

THEORY OF MULTIPHASE MIXTURES

A THERMOMECHANICAL FORMULATION

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Abstract—The paper presents a theory of mixtures with the nonzero interfacial area between the constituents of the mixture. The conservation laws are physically motivated by utilizing a volume averaging procedure and by the definition of a mapping transformation. It is shown that the theory constructed in this manner is consistent with the theory of mixtures with a vanishingly small interfacial area and that a second law of thermodynamics can be assigned for each phase of the mixture. The conservation laws are examined for invariance properties with the principle of the material frame indifference, and a particular constitutive assumption is discussed. Also presented in the paper are the conservation laws in the integral form and the jump conditions for the singular surfaces in the multiphase mixture.

1. INTRODUCTION

A general theory which describes the mixture of materials with *finite* interfacial areas between the reacting constituents of the mixture is incomplete at the present time. In principle, it is possible to describe such a mixture by the conservation laws for each continuum separately and by the jump conditions which serve as boundary conditions at the interfaces. In practice, however, this approach is usually prohibitive, and alternate methods of analysis are sought. So as to set forth properly the definition of such a mixture, I will from now on refer to it as the *multiphase mixture*. In this definition, the term *phase* will denote a portion of matter with a smoothly varying chemical composition, and phases are distinguished from one another by the well-defined boundary surfaces which are mathematically modeled as the surfaces of discontinuity.

When the interfacial area becomes negligibly small the multiphase mixture is modeled by the *theory of mixtures*. This theory has achieved maturity principally through the works of Truesdell (1969), Eringen & Ingram (1967), Muller (1968) and Bowen (1976).

With the final interfacial area a number of models have appeared in the literature which claim to give accurate representation of the conservation and balance equations of multiphase mixtures for specific as well as for general situations. Bedford & Drumheller (1983) reviewed recently a great number of works pertaining to immiscible (i.e. multiphase) mixtures of both the postulated and averaged variety. In the most physically appealing class of theories, the conservation and balance equations of multiphase mixtures are derived or motivated by integrating the local macroscopic conservation and balance equations of each phase over the space, time, and probability segments. Drew (1971) carried out time averaging of the global or integral formulation, while Ishii (1975) performed time averaging of the local phasic conservation and balance equations. Delhayé & Achard (1977) derived 2-phase flow 1-dimensional models by integrating the local phasic field equations over the volume, area, and time segment. Time, area, and line segment averagings produce singularities in some terms in the resulting averaged conservation and balance equations and various researchers have found it necessary to carry out double and triple integration procedures in order to smooth out these singularities. Trapp (1976) has presented the volume- and time-averaged field equations of mass and linear momentum, and discussed some constitutive properties of the averaged equations in the equilibrium state. Dobran (1981) brought some order to the averaging operators by deriving sufficient conditions for

the equivalence of time averaging and ensemble averaging operators in the area-averaged form of the conservation and balance equations. Nigmatulin (1979) also used volume averaging to derive two-phase flow equations for bubbly liquids and neglected surface tension and surface thermal effects at the interfaces between the phases. He also neglected any discussion of the entropy equation for each phase or for the mixture as a whole, and performed the decomposition of dependent variables (similarly to Ishii 1975 in his time averaging approach) into averaged and fluctuating quantities obtaining thus, in the averaged equations, the terms proportional to the fluctuating variables. The averaged form of continuity, momentum, and energy equations are, therefore, identical (except for the interpretation of averaged variables) in the formulations of Ishii and Nigmatulin. Drew's (1971) multiple averaging approach (two spatial and two time averagings) was motivated by the desire to smooth out any discontinuities in the averaged equations; however, it is not clear why indeed it is necessary to utilize so many averagings. His equations are also similar to the equations in the time- and space-averaged formulations.

All averaging approaches yield similar conservation and balance equations of multiphase mixtures; the difference between them is, however, in the interpretation of the averaged variables. When it is proposed that the averaged conservation and balance equations contain the dependent variables which are averages (or weighted averages) of the dependent variables over a material continuum, then the resulting equations contain various velocity, energy and entropy turbulent correlations (Ishii 1975; Nigmatulin 1979), distribution coefficients (Banerjee & Chen 1980), or covariance coefficients (Dobran 1981), and it is argued that constitutive equations are required for them. Furthermore, if any averaging procedure is to form a proper framework for a theory of multiphase mixtures then: (1) that averaging procedure should not be inconsistent with special physical situations; and (2) the averaging procedure should not be inconsistent with the application of the change of frame transformation to the field equations to study the invariance properties of these equations. The case in point is the time averaging procedure which yields the resulting equations singular whenever an interface becomes stationary in the flow field, and the application of a change of frame transformation principle to study the invariance properties of the theory (such as the principle of the material frame indifference) leads to an inconsistency (because this change of frame transformation involves a time-dependent rigid body rotation invariance).

The second basic approach used in the formulation of conservation and balance equations for multiphase mixtures involves *postulating* the field equations with a proper guidance, of course, from some specific physical situations or from the theory of mixtures (i.e. from the theory of single-phase multicomponent mixtures). A theory of this nature was proposed by Goodman & Cowin (1972) and subsequently refined leading to the most recent version as described by Passman *et al.* (1983). In this theory, the conservation equation of mass and balance equations of linear momentum, angular momentum and energy are postulated for each phase, whereas the entropy equation is only postulated for the mixture as a whole and not for each phase separately as it appears logically from the time- and space-averaged theories described above. Furthermore, the finite interfacial area associated with multiphase mixtures is modeled as *microstructures* and separate balance or transport equations for these microstructures (balance of the equilibrated force) are assumed. In addition, the postulated energy equation of each phase contains the effect of the constituent microstructure. Drumheller & Bedford (1980) derived their immiscible or multiphase field equations by utilizing the "Hamilton's extended variational principle." As in the postulated theory of multiphase mixtures of Goodman & Cowin and Passman *et al.*, the entropy equation for the mixture as a whole is only used. The finite interfacial area associated with the multiphase mixtures is modeled in the theory of Drumheller & Bedford through the virtual mass and expansion-contraction effects (the microstructure of the

mixture is modeled by its kinetic energy and generalized forces). The resulting variational analysis yields phasic equations of motion and equations which describe the evolution of microstructural properties of the mixture (the volumetric fractions, for example).

A basic difficulty with the postulated continuum theories of multiphase mixtures is that they all contain postulates in one form or another. Drummheller & Bedford's theory described above has from the outset a built-in constitutive assumption of the virtual mass and expansion-contraction effects, and the theory is constructed on the premise of a variational principle whose utility in the context of the complicated interrelation between the field equations and constitutive equations is altogether not clear. Similarly, the postulated balance equations of Goodman & Cowin also discussed above involve a postulatory basis. While a postulatory approach should not be refuted on the basis of an inability for a *a priori* justification, it is important, however, to keep a clear perspective of the method at all times even if the theory gives results that are consistent with the experiments. As discussed above, the balance of entropy equation for the mixture as a whole in the postulated theories is in variance with the averaging approaches which require an entropy equation for *each phase* in the multiphase mixture. Even Passman *et al.* (1983) admit that "We find this [the entropy balance equation for the mixture as a whole] to be one of the least pleasing results in the continuum theory of mixtures and evidence in itself that more research on fundamental questions is needed." It is worth noting that the principle from the single-phase multicomponent mixtures (Truesdell 1969) which states "The motion of the mixture is governed by the same equations as in a single body," is also used in the postulated multiphase theories. Again, this principle does not appear to valid in any theory of multiphase mixtures constructed from an averaging procedure and it also produces difficulties in the entropy balance equation for the mixture as a whole unless two different temperatures are defined—one for radiation and the other for conduction. The source terms in the field equations for the mixture as a whole can be thought as reflecting its structural properties that are different from single-phase multicomponent mixtures where the omission of these terms appears to be justifiable.

From the above discussion it is evident that there are two fundamental problems which need to be solved in order to complete the theory of multiphase mixtures. The first problem requires an agreement as to what constitutes a *complete* set of conservation and balance equations, while the second problem requires the descriptions of particular mixtures by means of constitutive equations.

In my view, the multiphase mixture theory should: (1) be *consistent* with the theory of mixtures when the interfacial area becomes negligibly small; and (2) be *consistent* with an averaging procedure that does not lead to any difficulties with simple physical situations (such as yielding singular field equations when an interface becomes stationary in the flow field) or lead to inconsistencies upon the application of the principle of the material frame indifference. The second consistency condition above is the existence property, since it simply requires that the conservation and balance equations of a multiphase mixture theory must yield the field equations identical to those which are obtained by performing the space averaging of the local macroscopic field equations of each phase. The simplest space averaging procedure which satisfies the requirements above is, clearly, the volume averaging. The volume averaging approach has not, however, been fully investigated in previous works nor have kinematic concepts, frame invariance or closure of the averaged field equations by the constitutive equations been discussed to any significant degree.

In this paper, the general equation of balance of each phase utilizing the volume averaging approach is presented in section 2 which satisfies the two consistency conditions discussed above. The conservation and balance equations for the multiphase mixture are presented in section 3 where the theory is also given a sufficient mathematical structure. It is shown there that a balance of entropy equation for each phase appears naturally in

the theory and how the microstructural properties of the mixture associated with the finite interfacial area can enter into the formulation. The restrictions imposed on the multiphase field equations by the principle of the material frame indifference are discussed in section 4, and a general discussion on the closure of the conservation and balance equations by the constitutive equations is presented in section 5. Section 6 deals with the integral form of the field equations where the jump conditions for the multiphase mixture are presented.

Notation

The paper uses a direct notation, and the underlying space is the 3-dimensional Euclidean space E^3 with the Cartesian coordinate system. Vectors and vector fields are denoted by the Latin bold-faced miniscules: \mathbf{a} , \mathbf{b} , \mathbf{x} , ... Second order tensors are viewed as linear transformations in E^3 , and are denoted by Latin bold-faced majuscules: \mathbf{A} , \mathbf{B} , \mathbf{T} , ... (except \mathbf{X} which is a vector of the reference position of the material body point). The product of two linear transformations is a linear transformation, $\mathbf{AB} = \mathbf{C}$, and the product of a linear transformation and a vector is a vector, $\mathbf{x} = \mathbf{T}\mathbf{u}$. \mathbf{T}^T is the transpose of \mathbf{T} , \mathbf{T}^{-1} is the inverse of \mathbf{T} , $\det \mathbf{T}$ is the determinant of \mathbf{T} , and the contraction of \mathbf{T} is its trace $\text{tr } \mathbf{T}$. The divergence operator is denoted by $\nabla \cdot$, ∇a is the gradient of a , and the gradient of a vector field \mathbf{b} is the linear transformation $\nabla \mathbf{b}$. \mathbf{I} is the unit linear transformation. The tensor product of two vectors \mathbf{a} and \mathbf{b} is denoted by $\mathbf{a} \otimes \mathbf{b}$, and it is identified as a linear transformation.

The basis in E^3 is denoted by the Cartesian triad of unit vectors $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$. The tensorial indices are denoted by the italic light-faced miniscules: i, j, \dots , and the summation convention always applies to them. The Greek light-faced symbols α and β always occur as subscripts and denote the phases of the multiphase mixture: $\alpha, \beta = 1, \dots, \gamma$. Summation over the phases is always denoted explicitly by the summation symbol Σ_α . Other symbols are defined in the text when they first appear and in the nomenclature.

2. FORMULATION OF THE THEORY

The objective of this section of the paper is to proceed through a series of physical arguments which will lead to the differential form of the conservation laws for the multiphase mixture. Section 6 of the paper turns this procedure around by postulating the integral forms of the conservation laws for each phase and, therefore, allows for the inclusion of the discontinuities into the theory of multiphase mixtures.

As noted in section 1, the volume averaging has clear physical advantages over all other averaging procedures. For this purpose, consider the flow field in figure 1 in the Euclidean space E_0^3 which consists of the phases $\alpha = 1, \dots, \gamma$, where each phase consists of a single chemical component. (It is easy to extend the theory to the case where each phase consists of a mixture of different chemical constituents with negligibly small interfacial areas.) Embedded in the space E_0^3 is an arbitrary fixed volume \mathcal{V} over which it is desirable to carry out the volume averaging operation. The volume \mathcal{V} consists of volumes $\mathcal{V}_\alpha = \Sigma_\delta \mathcal{V}_{\alpha\delta}$ such that $\mathcal{V} = \Sigma_\alpha \mathcal{V}_\alpha$.

For each phase α and volume $\mathcal{V}_{\alpha\delta}$, we have the macroscopic conservation laws of the continuum physics for the non-polar media (Eringen 1975):

$$\frac{\partial}{\partial t} (\rho_{\alpha\delta} \Psi_{\alpha\delta}) + \nabla^0 \cdot (\rho_{\alpha\delta} \Psi_{\alpha\delta} \mathbf{v}_{\alpha\delta}) + \nabla^0 \cdot \mathbf{J}_{\alpha\delta} - \rho_{\alpha\delta} \Phi_{\alpha\delta} = \rho_{\alpha\delta} B_{\alpha\delta}, \quad [2.1]$$

where $\Psi_{\alpha\delta}$, $\mathbf{J}_{\alpha\delta}$, $\Phi_{\alpha\delta}$ and $B_{\alpha\delta}$ are given in Table 1, and the operator ∇^0 operates in the space E_0^3 .

At the interface between the phases α and β we have the jump conditions (Eringen

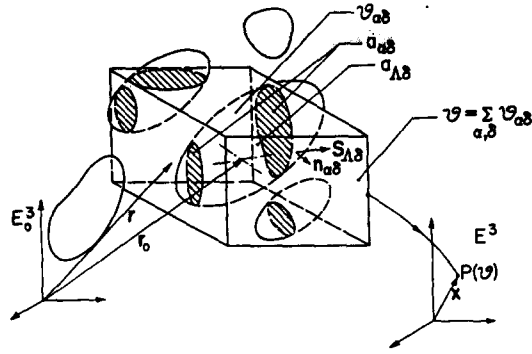


Figure 1. Representation of the multiphase mixture in different spaces.

1975):

$$(\dot{m}_{\alpha\beta}\Psi_{\alpha\beta} + J_{\alpha\beta}\mathbf{n}_{\alpha\beta}) + (\dot{m}_{\beta\eta}\Psi_{\beta\eta} + J_{\beta\eta}\mathbf{n}_{\beta\eta}) = \Delta_{\alpha\beta}, \quad [2.2]$$

where

$$\dot{m}_{\alpha\beta} = \rho_{\alpha\beta}(\mathbf{v}_{\alpha\beta} - \mathbf{S}_{\alpha\beta}) \cdot \mathbf{n}_{\alpha\beta} \quad [2.3]$$

is the interphase mass transfer rate which arises due to the phase change or chemical reactions, $\mathbf{S}_{\alpha\beta}$ is the velocity of the interface, $\mathbf{n}_{\alpha\beta}$ is the unit normal vector which points outward from $\mathcal{V}_{\alpha\beta}$, and $\Delta_{\alpha\beta}$ is the surface tension term (or possibly some other interfacial source). $\Delta_{\alpha\beta}$ is defined in Table 1. H , ∇_s^0 and ν in table 1 are the mean curvature of the interface, surface gradient vector, and the surface tension coefficient respectively. $\dot{m}_{\beta\eta}$ is defined similarly for the phase β . Clearly $\alpha \neq \beta$, $\mathbf{n}_{\alpha\beta} = -\mathbf{n}_{\beta\eta}$, and $\mathbf{S}_{\alpha\beta} = \mathbf{S}_{\beta\eta}$.

In table 1, $\mathbf{T}_{\alpha\beta}$ is the stress tensor, $\mathbf{b}_{\alpha\beta}$ is the external body force per unit mass, $\mathbf{v}_{\alpha\beta}$ is the velocity, $\rho_{\alpha\beta}$ is the mass density, $\epsilon_{\alpha\beta}$ is the internal energy per unit mass, $\mathbf{q}_{\alpha\beta}$ is the heat flux vector, $s_{\alpha\beta}$ is the entropy per unit mass, $\mathbf{h}_{\alpha\beta}$ is the entropy flux vector, $\theta_{\alpha\beta}$ is the absolute temperature, $r_{\alpha\beta}$ is the heat generation rate per unit volume, and $\xi_{\alpha\beta}$ and Δ_s are the entropy production rates in the continuum and at the interface, respectively.

Volume averaging of the conservation equation [2.1] is carried out for each constituent phase α over the portion of the volume \mathcal{V} which the phase α occupies at time t , i.e. the following operation is carried out:

$$\sum_{\delta} \int_{\mathcal{V}_{\alpha\delta}} [\text{equation (2.1)}] d\mathcal{V} = 0. \quad [2.4]$$

To interchange the integration and differentiation operators in [2.4], it is necessary to define a mapping transformation of the volume \mathcal{V} in E_0^3 into a point $P(\mathcal{V})$ of E^3 as

Table 1. Coefficients of the conservation equations [2.1] and [2.2]

| CONSERVATION OF | $\Psi_{\alpha\beta}$ | $J_{\alpha\beta}$ | $\Phi_{\alpha\beta}$ | $\mathbf{B}_{\alpha\beta}$ | $\Delta_{\alpha\beta}$ |
|------------------|---|--|---|----------------------------|---|
| MASS | 1 | 0 | 0 | 0 | 0 |
| LINEAR MOMENTUM | $\mathbf{v}_{\alpha\beta}$ | $-\mathbf{T}_{\alpha\beta}$ | $\mathbf{b}_{\alpha\beta}$ | 0 | $(\Delta_m)_{\alpha\beta} = (2H\nu\eta + \nu\nabla_s^0)_{\alpha\beta}$ |
| ANGULAR MOMENTUM | $\mathbf{r} \wedge \mathbf{v}_{\alpha\beta}$ | $-\mathbf{r} \wedge \mathbf{T}_{\alpha\beta}$ | $\mathbf{r} \wedge \mathbf{b}_{\alpha\beta}$ | 0 | $\mathbf{r} \wedge (\Delta_m)_{\alpha\beta}$ |
| ENERGY | $\epsilon_{\alpha\beta} + \frac{\mathbf{v}_{\alpha\beta}^2}{2}$ | $\mathbf{q}_{\alpha\beta} - \mathbf{T}_{\alpha\beta}^T \mathbf{v}_{\alpha\beta}$ | $\mathbf{b}_{\alpha\beta} \cdot \mathbf{v}_{\alpha\beta}$ | $r_{\alpha\beta}$ | $(\Delta_e)_{\alpha\beta} = (2H\nu\eta \cdot \mathbf{S} + \Psi \cdot \mathbf{S} + \nu \nabla_s^0 \cdot \mathbf{S})_{\alpha\beta}$ |
| ENTROPY | $s_{\alpha\beta}$ | $\frac{h_{\alpha\beta}}{\theta_{\alpha\beta}}$ | $\frac{j_{\alpha\beta}}{\theta_{\alpha\beta}}$ | $\xi_{\alpha\beta} > 0$ | $(\Delta_s)_{\alpha\beta} > 0$ |

illustrated in figure 1. In appendix A, this mapping transformation is defined by [A.1]–[A.4], and it is discussed there that such a mapping can be made bijective.

Applying the transformations [A.1] and [A.2] to [2.4] yields the *general equation of balance for the phase α* .

$$\begin{aligned} & \frac{\partial}{\partial t} \mathcal{V}_\alpha \langle \rho_\alpha \Psi_\alpha \rangle + \nabla \cdot \mathcal{V}_\alpha \langle \rho_\alpha \Psi_\alpha \mathbf{v}_\alpha \rangle + \nabla \cdot \mathcal{V}_\alpha \langle \mathbf{J}_\alpha \rangle \\ & - \mathcal{V}_\alpha \langle \rho_\alpha \Phi_\alpha \rangle - \mathcal{V}_\alpha \langle \rho_\alpha B_\alpha \rangle = - \sum_\delta \int_{a_{\delta\delta}} (\dot{m}_{\alpha\delta} \Psi_{\alpha\delta} + J_{\alpha\delta} \mathbf{n}_{\alpha\delta}) da, \end{aligned} \quad [2.5]$$

where the volume-averaged quantities are defined as follows:

$$\langle F_\alpha \rangle \equiv \frac{1}{\mathcal{V}_\alpha} \sum_\delta \int_{\mathcal{V}_{\alpha\delta}} F_{\alpha\delta} d\mathcal{V}. \quad [2.6]$$

Since [2.5] is the outcome of mapping of each \mathcal{V}_α in E_0^3 , $\alpha = 1, \dots, \gamma$, into a point in E^3 , and each volume \mathcal{V} is also mapped into the same point, it is evident that at each place \mathbf{x} of E^3 there exist γ phases. There is nothing strange about this construction and of course it forms the basis for the theory of mixtures and for the Maxwell's kinetic theory of gases. My purpose for constructing the form of [2.5] was to provide the consistency of the theory of multiphase mixtures with the theory of mixtures with a vanishingly small interfacial area.

To motivate the meaning of the “phase velocity” in E^3 , and as well as the meaning of other independent variables, it is instructive to specialize [2.5] for the conservation of mass in Table 1. In such a case this equation is reduced to

$$\frac{\partial}{\partial t} \mathcal{V}_\alpha \langle \rho_\alpha \rangle + \nabla \cdot \mathcal{V}_\alpha \langle \rho_\alpha \mathbf{v}_\alpha \rangle = - \sum_\delta \int_{a_{\delta\delta}} \dot{m}_{\alpha\delta} da. \quad [2.7]$$

Equation [2.7] suggests that we define the (partial) *density of phase α* by the equation

$$\bar{\rho}_\alpha \equiv \frac{\mathcal{V}_\alpha}{\mathcal{V}} \langle \rho_\alpha \rangle, \quad [2.8]$$

and the *velocity of phase α* by

$$\tilde{\mathbf{v}}_\alpha \equiv \frac{\frac{\mathcal{V}_\alpha}{\mathcal{V}} \langle \rho_\alpha \mathbf{v}_\alpha \rangle}{\bar{\rho}_\alpha}. \quad [2.9]$$

Summing up α in [2.7] we also have that

$$\frac{\partial}{\partial t} \sum_\alpha \mathcal{V}_\alpha \langle \rho_\alpha \rangle + \nabla \cdot \sum_\alpha \mathcal{V}_\alpha \langle \rho_\alpha \mathbf{v}_\alpha \rangle = - \sum_{\alpha,\delta} \int_{a_{\delta\delta}} \dot{m}_{\alpha\delta} da. \quad [2.10]$$

Using [2.2] the right side of [2.10] is equal to zero, and using [2.8] and [2.9] we can define in [2.10] the *mixture density ρ* and the center of mass or *mixture velocity \mathbf{v}* as follows:

$$\begin{aligned} \rho & \equiv \sum_\alpha \bar{\rho}_\alpha \\ \rho \mathbf{v} & \equiv \sum_\alpha \bar{\rho}_\alpha \tilde{\mathbf{v}}_\alpha. \end{aligned} \quad [2.11]$$

The definitions [2.8], [2.9] and [2.11] are fully consistent with the theory of mixtures (Truesdell 1969, Bowen 1976).

Equation [2.5] suggests the definition of two types of averaged quantities. The density-weighted average of a physical property F_α will be denoted by \bar{F}_α , whereas the partial quantity of a physical variable G_α will be denoted by \bar{G}_α . The velocity of phase α is also defined as a density-weighted average since this is quantity directly measurable by a finite size instrument. Thus,

$$\begin{aligned}\bar{F}_\alpha &\equiv \frac{\langle \rho_\alpha F_\alpha \rangle}{\langle \rho_\alpha \rangle} = \frac{1}{\bar{\rho}_\alpha} \frac{\gamma_\alpha}{\gamma} \langle \rho_\alpha F_\alpha \rangle \\ \bar{G}_\alpha &\equiv \frac{\gamma_\alpha}{\gamma} \langle G_\alpha \rangle \\ \bar{C}_\alpha &\equiv \langle G_\alpha \rangle.\end{aligned}\quad [2.12]$$

3. CONSERVATION AND BALANCE EQUATIONS FOR MULTIPHASE MIXTURES

In the previous section, I have given a physical motivation for the derivation of the general equation of balance for phase α [2.5]. In this section, I will present the conservation and balance equations for the multiphase mixtures and assign sufficient mathematical structure to the theory. The latter is indispensable for the study of constitutive equations.

3.1 Kinematics

As in the theory of mixtures (Bowen 1976), the multiphase mixture can be thought to consist of γ diffusing bodies (phases) \mathcal{B}_α , $\alpha = 1, \dots, \gamma$, and each \mathcal{B}_α to belong to a differentiable manifold which is isomorphic to the 3-dimensional Euclidean space E^3 . Each body \mathcal{B}_α consists of *body points* (particles) X_α , and the *configuration* χ_α of \mathcal{B}_α is a homeomorphism of \mathcal{B}_α into E^3 . Corresponding to the body points X_α and the time t a *motion* is assigned to \mathcal{B}_α , and the position \mathbf{x} in E^3 of the body points X_α at time t is represented by

$$\mathbf{x} = \chi_\alpha(X_\alpha, t). \quad [3.1]$$

To each \mathcal{B}_α is assigned a *reference configuration* κ_α at time $t_0 > t$, and the place of the particle X_α in κ_α is given as follows:

$$\mathbf{X}_\alpha = \kappa_\alpha(X_\alpha, t_0). \quad [3.2]$$

Combining [3.1] and [3.2] we have

$$\mathbf{x} = \chi_\alpha(\kappa_\alpha^{-1}(X_\alpha, t_0), t) \equiv \chi_{\alpha\kappa}(\mathbf{X}_\alpha, t), \quad [3.3]$$

where $\chi_{\alpha\kappa}$ is the *deformation function* of \mathcal{B}_α .

The expression [3.3] is assumed invertible, $\mathbf{X}_\alpha = \chi_{\alpha\kappa}^{-1}(\mathbf{x}, t)$, for each α at each time t , and $\chi_{\alpha\kappa}$ and $\chi_{\alpha\kappa}^{-1}$ are differentiable as many times as necessary. The spatial coordinates are expressed by the lower case italic indices, $\mathbf{x} = x_i \mathbf{e}_i$, and the material coordinates are expressed by the upper case italic indices, $\mathbf{X}_\alpha = X_{\alpha I} \mathbf{e}_I$, where $\mathbf{e}_i \cdot \mathbf{e}_k = \delta_{ik}$ and $\mathbf{e}_I \cdot \mathbf{e}_K = \delta_{IK}$ are the Kronecker deltas.

The velocity and the acceleration of the body point X_α at time t and place \mathbf{x} are respectively:

$$\tilde{v}_\alpha = \frac{\partial \chi_{\alpha\alpha}(\mathbf{X}_\alpha, t)}{\partial t} \quad \dot{\tilde{v}}_\alpha = \frac{\partial^2 \chi_{\alpha\alpha}(\mathbf{X}_\alpha, t)}{\partial t^2}. \quad [3.4]$$

The backward primes affixed to the subscripted symbols with α always indicate the material derivative “following” the α th phase.

The *deformation gradient* of phase α is a linear transformation defined by

$$\mathbf{F}_\alpha = \text{GRAD } \chi_{\alpha\alpha}(\mathbf{X}_\alpha, t), \quad F_{\alpha kJ} = \frac{\partial x_k}{\partial X_{\alpha J}}$$

$$\mathbf{F}_\alpha^{-1} = \nabla \chi_{\alpha\alpha}^{-1}(\mathbf{x}, t), \quad F_{\alpha Jk}^{-1} = \frac{\partial X_{\alpha J}}{\partial x_k}, \quad [3.5]$$

and the *velocity gradient* of phase α is given by the expression:

$$\mathbf{L}_\alpha = \nabla \tilde{v}_\alpha(\mathbf{x}, t), \quad L_{\alpha ij} = \frac{\partial \tilde{v}_{\alpha i}}{\partial x_j}. \quad [3.6]$$

It then follows that

$$\mathbf{L}_\alpha = \dot{\mathbf{F}}_\alpha \mathbf{F}_\alpha^{-1}. \quad [3.7]$$

The *mixture density* and *mixture velocity* are defined respectively as

$$\rho = \sum_\alpha \bar{\rho}_\alpha \quad [3.8]$$

$$\rho \mathbf{v} = \sum_\alpha \bar{\rho}_\alpha \tilde{v}_\alpha, \quad [3.9]$$

and the *diffusion velocity* is defined as the difference between the phase velocity and the mixture velocity, i.e.

$$\mathbf{u}_\alpha \equiv \tilde{v}_\alpha - \mathbf{v}. \quad [3.10]$$

As pointed out by Bowen (1976), there are two mathematical identities which are useful for discussing the conservation laws (Truesdell & Toupin 1960, section 158). If Γ is a differentiable function of \mathbf{x} and t , then the time derivative “following” the α th phase and the time derivative “following” the mixture are respectively

$$\hat{\Gamma} = \frac{\partial \Gamma}{\partial t} + (\nabla \Gamma) \tilde{v}_\alpha, \quad \dot{\Gamma} = \frac{\partial \Gamma}{\partial t} + (\nabla \Gamma) \mathbf{v}, \quad [3.11]$$

and thus

$$\hat{\Gamma} - \dot{\Gamma} = (\nabla \Gamma) \mathbf{u}_\alpha. \quad [3.12]$$

If $\rho \Gamma \equiv \sum_\alpha \bar{\rho}_\alpha \tilde{\Gamma}_\alpha$, then it follows that

$$\rho \dot{\Gamma} = \sum_\alpha \left[\bar{\rho}_\alpha \hat{\tilde{\Gamma}}_\alpha - \nabla \cdot \bar{\rho}_\alpha \tilde{\Gamma}_\alpha \mathbf{u}_\alpha + \left(\frac{\partial \bar{\rho}_\alpha}{\partial t} + \nabla \cdot \bar{\rho}_\alpha \tilde{v}_\alpha \right) \tilde{\Gamma}_\alpha - \left(\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{v} \right) \tilde{\Gamma}_\alpha \right]. \quad [3.13]$$

3.2 Conservation of mass

Substituting the coefficients for the conservation of mass in table 1 into the general balance equation [2.5], and using the definitions [2.8], [2.9] and the identity [3.11]₁, we have an equation for the *conservation of mass of phase α* :

$$\dot{\bar{\rho}}_\alpha + \bar{\rho}_\alpha \nabla \cdot \tilde{\mathbf{v}}_\alpha = \hat{c}_\alpha, \quad [3.14]$$

where

$$\hat{c}_\alpha \equiv -\frac{1}{\mathcal{V}} \sum_\delta \int_{a_{\alpha\delta}} \dot{m}_{\alpha\delta} da \quad [3.15]$$

is the *mass supply* of phase α and arises due to the phase change or chemical reactions.

Summing up all phases α in [3.14] and utilizing the definitions [3.8], [3.9], [3.11]₂ and [2.2] with $\Delta_{\alpha\delta} = 0$ in table 1, we have an equation for the *conservation of mass for the mixture*

$$\dot{\rho} + \rho \nabla \cdot \mathbf{v} = 0, \quad [3.16]$$

and the *compatibility condition on the mass supplies*

$$\sum_\alpha \hat{c}_\alpha = 0. \quad [3.17]$$

Equations [3.14] and [3.16] reduce the identity [3.13] to the following:

$$\rho \dot{\Gamma} = \sum_\alpha [\bar{\rho}_\alpha \dot{\Gamma}_\alpha - \nabla \cdot \bar{\rho}_\alpha \tilde{\mathbf{r}}_\alpha \mathbf{u}_\alpha + \hat{c}_\alpha \tilde{\mathbf{r}}_\alpha] \quad [3.18]$$

3.3 Balance of the linear momentum

The *linear momentum equation for the phase α* is obtained by substituting the coefficients for the balance of linear momentum from table 1 into [2.5] and using the definitions [2.12],

$$\bar{\rho}_\alpha \dot{\tilde{\mathbf{v}}}_\alpha = \nabla \cdot \tilde{\mathbf{T}}_\alpha + \bar{\rho}_\alpha \tilde{\mathbf{b}}_\alpha + \hat{\mathbf{p}}_\alpha, \quad [3.19]$$

where the *linear momentum supply or source* is defined by

$$\hat{\mathbf{p}}_\alpha \equiv -\hat{c}_\alpha \tilde{\mathbf{v}}_\alpha - \frac{1}{\mathcal{V}} \sum_\delta \int_{a_{\alpha\delta}} (\dot{m}_{\alpha\delta} \mathbf{v}_{\alpha\delta} - \mathbf{T}_{\alpha\delta} \mathbf{n}_{\alpha\delta}) da - \nabla \cdot \mathbf{C}_{1\alpha}. \quad [3.20]$$

$\mathbf{C}_{1\alpha}$ is the velocity covariance coefficient (a linear transformation) and is defined in appendix B.

The linear momentum supply or source $\hat{\mathbf{p}}_\alpha$ in multiphase mixtures arises due to the three effects: (1) from the action of the surface traction force $\mathbf{T}_{\alpha\delta} \mathbf{n}_{\alpha\delta}$ which is imposed by other phases upon the phase α ; (2) from the phase change or chemical reactions; and (3) from the divergence of the covariance $\mathbf{C}_{1\alpha}$ which arises due to the finite interfacial area between the phases. These effects can be considered as giving rise to the microstructural characteristics of the mixture and must be modeled by the constitutive equations. One such constitutive decomposition which is popular in two-phase flow modeling is presented in Appendix C, since in the past the modeling of $\hat{\mathbf{p}}_\alpha$ has been of considerable controversy.

The *linear momentum equation for the mixture* is obtained by summing up α in [3.19]

and using [3.18] with $\tilde{\Gamma}_\alpha = \tilde{\mathbf{v}}_\alpha$. The result is:

$$\rho \dot{\mathbf{v}} = \nabla \cdot \mathbf{T} + \rho \mathbf{b} + \hat{\mathbf{p}}_m. \quad [3.21]$$

In the above equation, the stress tensor for the mixture \mathbf{T} , the mixture body force \mathbf{b} , and the mixture momentum supply $\hat{\mathbf{p}}_m$ are defined respectively by the expressions:

$$\begin{aligned} \mathbf{T} &\equiv \sum_\alpha (\tilde{\mathbf{T}}_\alpha - \bar{\rho}_\alpha \mathbf{u}_\alpha \otimes \mathbf{u}_\alpha) \\ \rho \mathbf{b} &\equiv \sum_\alpha \bar{\rho}_\alpha \tilde{\mathbf{b}}_\alpha \\ \hat{\mathbf{p}}_m &\equiv -\frac{1}{\mathcal{V}} \sum_{\alpha, \delta} \int_{a_{\alpha\delta}} (\Delta_m)_{\alpha\delta} da - \nabla \cdot \left(\sum_\alpha \mathbf{C}_{1\alpha} \right). \end{aligned} \quad [3.22]$$

The surface tension term $(\Delta_m)_{\alpha\delta}$ in [3.22]₃ is defined in table 1.

Combining [3.20] and [3.22]₃, we have the *compatibility condition for the momentum supply* for the mixture, i.e.

$$\hat{\mathbf{p}}_m = \sum_\alpha (\hat{c}_\alpha \tilde{\mathbf{v}}_\alpha + \hat{\mathbf{p}}_\alpha) = \sum_\alpha (\hat{c}_\alpha \mathbf{u}_\alpha + \hat{\mathbf{p}}_\alpha). \quad [3.23]$$

Notice that in [3.22]₁, the stress tensor for the mixture is symmetric if and only if $\sum_\alpha \tilde{\mathbf{T}}_\alpha$ is symmetric since $\mathbf{u}_\alpha \otimes \mathbf{u}_\alpha$ is always symmetric. Thus, it is possible that \mathbf{T} is symmetric even if $\tilde{\mathbf{T}}_\alpha$ are not symmetric individually.

Whereas in the theory of single-phase multicomponent mixtures the momentum supply for the mixture as a whole is assumed to be equal to zero, this does not appear to be true in the theory of multiphase mixtures for two reasons: (1) the surface tension effect can be important; and (2) the divergence of the velocity covariance $\mathbf{C}_{1\alpha}$ is likely to be of importance whenever the interfacial area is finite. The mixture supply vector $\hat{\mathbf{p}}_m$ renders [3.21] different from the momentum equation for a single body. Since it is common in the theory of mixtures (Truesdell 1969) to accept the principle: "The motion of the mixture is governed by the same equations as is a single body," the acceptance of this principle in the theory of the multiphase mixtures does not appear to be justifiable. Passman *et al.* (1983) also adopted the above principle in their theory of immiscible or multiphase mixtures and noted that it does lead to difficulties in the interpretation of the entropy balance equation for the mixture as a whole. To bypass this difficulty and still retain the principle, the above authors found it necessary to define two different temperatures—one for conduction and the other for radiation.

3.4 Balance of the angular momentum

From table 1 and [2.5], the *angular momentum equation for the phase α* becomes

$$\bar{\rho}_\alpha \frac{\mathbf{x} \wedge \mathbf{v}_\alpha}{\mathbf{x} \wedge \mathbf{v}_\alpha} = \nabla \cdot (\mathbf{x} \wedge \tilde{\mathbf{T}}_\alpha) + \mathbf{x} \wedge (\bar{\rho}_\alpha \tilde{\mathbf{b}}_\alpha + \hat{\mathbf{p}}_\alpha) + \hat{\mathbf{m}}_\alpha, \quad [3.24]$$

where the *angular momentum supply or source* is defined by the expression:

$$\begin{aligned} \hat{\mathbf{m}}_\alpha &\equiv -\mathbf{x} \wedge (\hat{\mathbf{p}}_\alpha + \hat{c}_\alpha \mathbf{v}_\alpha) - \frac{1}{\mathcal{V}} \sum_\delta \int_{a_{\alpha\delta}} \mathbf{r} \wedge (\dot{m}_{\alpha\delta} \mathbf{v}_{\alpha\delta} - \mathbf{T}_{\alpha\delta} \mathbf{n}_{\alpha\delta}) da \\ &\quad - \bar{\rho}_\alpha \overbrace{(\mathbf{r} - \mathbf{x}) \wedge \mathbf{v}_\alpha} - \hat{c}_\alpha \overbrace{(\mathbf{r} - \mathbf{x}) \wedge \mathbf{v}_\alpha} + \nabla \cdot \overbrace{(\mathbf{r} - \mathbf{x}) \wedge \tilde{\mathbf{T}}_\alpha} \end{aligned}$$

$$+ \overline{\bar{\rho}_\alpha(\mathbf{r} - \mathbf{x}) \wedge \mathbf{g}_\alpha} - \nabla \cdot \overline{\bar{\rho}_\alpha(\mathbf{r} \wedge \mathbf{v}_\alpha)(\mathbf{v}_\alpha - \bar{\mathbf{v}}_\alpha)}. \quad [3.25]$$

Expanding [3.24] and using the linear momentum equation [3.19] for the phase α we have

$$\hat{\mathbf{m}}_\alpha + \mathbf{e}_i \epsilon_{ijk} \bar{T}_{akj} = 0, \quad [3.26]$$

where ϵ_{ijk} is the alternating symbol. Denoting by $\hat{\mathbf{M}}_\alpha$ the skew-symmetric linear transformation (Bowen 1976), [3.26] is written as follows:

$$\hat{\mathbf{M}}_\alpha = \hat{\mathbf{T}}_\alpha - \hat{\mathbf{T}}_\alpha^T, \quad [3.27]$$

where the components of $\hat{\mathbf{M}}_\alpha$ are:

$$\hat{M}_{\alpha 11} = \hat{M}_{\alpha 22} = \hat{M}_{\alpha 33} = 0$$

$$\hat{M}_{\alpha 23} = -\hat{M}_{\alpha 32} = \hat{m}_{\alpha 1}$$

$$\hat{M}_{\alpha 31} = -\hat{M}_{\alpha 13} = \hat{m}_{\alpha 2}$$

$$\hat{M}_{\alpha 12} = -\hat{M}_{\alpha 21} = \hat{m}_{\alpha 3}.$$

The angular momentum equation for the mixture is obtained by summing up α in [3.24] i.e.

$$\overline{\rho \mathbf{x} \wedge \mathbf{v}} = \nabla \cdot (\mathbf{x} \wedge \mathbf{T}) + \mathbf{x} \wedge \rho \mathbf{b} + \hat{\mathbf{m}}_m + \mathbf{x} \wedge \hat{\mathbf{p}}_m, \quad [3.28]$$

and

$$\hat{\mathbf{m}}_m = \sum_\alpha \hat{\mathbf{m}}_\alpha$$

is the angular momentum supply for the mixture. Expanding [3.28], and using the linear momentum equation for the mixture [3.21] and the definition [3.27], it follows that

$$\hat{\mathbf{m}}_m + \mathbf{e}_i \epsilon_{ijk} T_{kj} = 0 \quad [3.29]$$

$$\hat{\mathbf{M}} = \sum_\alpha \hat{\mathbf{M}}_\alpha = \mathbf{T} - \mathbf{T}^T.$$

The angular momentum supply vector for the mixture is also obtained by summing up α in [3.25], and using [3.23] and [3.22].

$$\begin{aligned} \hat{\mathbf{m}}_m = & -\frac{1}{\mathcal{V}} \sum_{\alpha, \beta} \int_{a_{\alpha\beta}} (\mathbf{r} - \mathbf{x}) \wedge (\Delta_m)_{\alpha\beta} + \mathbf{x} \wedge \nabla \cdot \sum_\alpha \mathbf{C}_{1\alpha} \\ & - \sum_\alpha \overline{\bar{\rho}_\alpha(\mathbf{r} - \mathbf{x}) \wedge \mathbf{v}_\alpha} - \sum_\alpha \overline{\hat{c}_\alpha(\mathbf{r} - \mathbf{x}) \wedge \mathbf{v}_\alpha} \\ & + \nabla \cdot \sum_\alpha \overline{(\mathbf{r} - \mathbf{x}) \wedge \mathbf{T}_\alpha} + \sum_\alpha \overline{\bar{\rho}_\alpha(\mathbf{r} - \mathbf{x}) \wedge \mathbf{g}_\alpha} \\ & - \nabla \cdot \sum_\alpha \overline{\bar{\rho}_\alpha(\mathbf{r} \wedge \mathbf{v}_\alpha)(\mathbf{v}_\alpha - \bar{\mathbf{v}}_\alpha)}. \end{aligned} \quad [3.30]$$

In the theory of mixtures without body couples and couple stresses $\hat{\mathbf{m}}_m = \mathbf{0}$. From [3.30], however, this does not appear to be true necessarily in the theory of multiphase mixtures even in the absence of body couples and couple stresses because of the presence of interfacial forces and nonlocal effects (the covariance effect). From [3.29] and [3.30] we can see that the vanishing of the interfacial forces and nonlocal effects is only sufficient condition for $\hat{\mathbf{m}}_m = \mathbf{0}$ or for the mixture stress tensor to be symmetric. However, the vanishing of the angular momentum supply for the mixture is both sufficient and necessary for the stress tensor of the mixture to be symmetric. These observations are consistent with a physical observation that it is possible to have a situation with $\hat{\mathbf{T}}_\alpha = \hat{\mathbf{T}}_\alpha^T$ and $(\Delta_m)_{\alpha\delta} \neq \mathbf{0}$.

3.5 Balance of energy

The energy equation for phase α is obtained from [2.5] by utilizing the coefficients from table 1, and [3.14] and [3.19],

$$\bar{\rho}_\alpha \dot{\hat{\epsilon}}_\alpha = \text{tr}(\hat{\mathbf{T}}_\alpha^T \nabla \hat{\mathbf{v}}_\alpha) - \nabla \cdot \hat{\mathbf{q}}_\alpha + \bar{\rho}_\alpha \hat{r}_\alpha + \hat{\epsilon}_\alpha, \quad [3.31]$$

where the energy supply or source is defined by

$$\begin{aligned} \hat{\epsilon}_\alpha \equiv & -\hat{\mathbf{p}}_\alpha \cdot \hat{\mathbf{v}}_\alpha - \hat{c}_\alpha \left(\hat{\tilde{\epsilon}}_\alpha + \frac{1}{2} \hat{\mathbf{v}}_\alpha \cdot \hat{\mathbf{v}}_\alpha \right) - \frac{1}{\mathcal{V}} \sum_\delta \int_{a_{\alpha\delta}} [\dot{m}_{\alpha\delta} \left(\epsilon_{\alpha\delta} + \frac{1}{2} \mathbf{v}_{\alpha\delta} \cdot \mathbf{v}_{\alpha\delta} \right) \\ & + (\mathbf{q}_{\alpha\delta} - \mathbf{T}_{\alpha\delta}^T \mathbf{v}_{\alpha\delta}) \cdot \mathbf{n}_{\alpha\delta}] da + c_{4\alpha} + \nabla \cdot (\mathbf{c}_{3\alpha} - \mathbf{c}_{2\alpha}) \\ & + \frac{\bar{\rho}_\alpha}{2} (\widehat{\mathbf{v}}_\alpha \cdot \widehat{\mathbf{v}}_\alpha - \widehat{\mathbf{v}}_\alpha \cdot \widehat{\mathbf{v}}_\alpha) + \frac{\hat{c}_\alpha}{2} (\widehat{\mathbf{v}}_\alpha \cdot \widehat{\mathbf{v}}_\alpha - \widehat{\mathbf{v}}_\alpha \cdot \widehat{\mathbf{v}}_\alpha), \end{aligned} \quad [3.32]$$

and where the covariance coefficients $c_{4\alpha}$, $c_{3\alpha}$ and $c_{2\alpha}$ are defined in appendix B. The covariance coefficients represent the effect of the finite interfacial area and do not appear in the theory of single-phase multi component mixtures.

Equations [3.25] and [3.32] hint that momentum and energy supplies are complex functions of multiphase variables and that their constitutive form should include the nonlocal effects. The region of nonlocality is clearly equal to the size of the averaging volume \mathcal{V} and this volume should be incorporated into the constitutive assumption. It is through such a description that the averaging volume \mathcal{V} can reenter into the framework of the present theory and the resulting multiphase field equations become then the integro-differential equations. By the principle of equipresence, the nonlocal effects must enter into the entire set of constitutive variables. The surface tension and nonlocal effects associated with the mixture can be thought of as describing its microstructural characteristics and as such they are not easy to model in full generality.

The energy equation for the mixture can take two convenient forms. An equation in terms of the mixture kinetic energy follows most simply from [2.5] when α is summed up. The result is:

$$\rho \left(\epsilon + \frac{1}{2} \mathbf{v} \cdot \mathbf{v} \right) = \nabla \cdot (\mathbf{t}^T \mathbf{v} - \mathbf{q}) + \rho r + \rho \mathbf{v} \cdot \mathbf{b} + \hat{e}_m, \quad [3.33]$$

where the mixture properties are defined by the following relations:

$$\begin{aligned} \rho \epsilon & \equiv \sum_\alpha \left[\bar{\rho}_\alpha \hat{\epsilon}_\alpha + \frac{\bar{\rho}_\alpha}{2} \mathbf{u}_\alpha \cdot \mathbf{u}_\alpha \right] \\ \rho r & \equiv \sum_\alpha [\bar{\rho}_\alpha \hat{r}_\alpha + \bar{\rho}_\alpha \mathbf{b}_\alpha \cdot \mathbf{u}_\alpha] \end{aligned}$$

$$\mathbf{q} \equiv \sum_{\alpha} \left[\bar{\mathbf{q}}_{\alpha} - \bar{\mathbf{T}}_{\alpha}^T \mathbf{u}_{\alpha} + \bar{\rho}_{\alpha} \tilde{\epsilon}_{\alpha} \mathbf{u}_{\alpha} + \frac{1}{2} \bar{\rho}_{\alpha} (\mathbf{u}_{\alpha} \cdot \mathbf{u}_{\alpha}) \mathbf{u}_{\alpha} \right] \quad [3.34]$$

$$\begin{aligned} \hat{e}_m \equiv \sum_{\alpha} \left[c_{4\alpha} + \nabla \cdot (\mathbf{c}_{3\alpha} - \mathbf{c}_{2\alpha}) + \frac{\bar{\rho}_{\alpha}}{2} (\tilde{\mathbf{v}}_{\alpha} \cdot \tilde{\mathbf{v}}_{\alpha} - \widehat{\mathbf{v}}_{\alpha} \cdot \widehat{\mathbf{v}}_{\alpha}) \right. \\ \left. + \frac{\hat{c}_{\alpha}}{2} (\tilde{\mathbf{v}}_{\alpha} \cdot \tilde{\mathbf{v}}_{\alpha} - \widehat{\mathbf{v}}_{\alpha} \cdot \widehat{\mathbf{v}}_{\alpha}) \right] - \frac{1}{\mathcal{V}} \sum_{\alpha, \delta} \int_{a, \delta} (\Delta_{\epsilon})_{\alpha\delta} da. \end{aligned}$$

$(\Delta_{\epsilon})_{\alpha\delta}$ in [3.34]₄ is the rate of work by the surface tension forces and it is given in table 1.

The kinetic energy of the mixture can be eliminated from [3.33] using the linear momentum equation for the mixture [3.21], i.e.

$$\rho \dot{\epsilon} = \text{tr}(\mathbf{T}^T \nabla \mathbf{v}) - \nabla \cdot \mathbf{q} + \rho r + (\hat{e}_m - \mathbf{v} \cdot \hat{\mathbf{p}}_m). \quad [3.35]$$

Combining [3.23], [3.32] and [3.34]₄ results in the *compatibility condition for the energy supply* for the mixture.

$$\hat{e}_m - \mathbf{v} \cdot \hat{\mathbf{p}}_m = \sum_{\alpha} \left[\hat{\epsilon}_{\alpha} + \mathbf{u}_{\alpha} \cdot \hat{\mathbf{p}}_{\alpha} + \hat{c}_{\alpha} \left(\tilde{\epsilon}_{\alpha} + \frac{1}{2} \mathbf{u}_{\alpha} \cdot \mathbf{u}_{\alpha} \right) \right]. \quad [3.36]$$

In the theory of mixtures the energy supply for the mixture as a whole is assumed to be equal to zero. For multiphase mixtures, this does not appear to be justifiable unless the interfacial sources and nonlocal effects are absent. In most practical applications, however, the work of the interfacial forces will not be significant when compared to other work terms in [3.33] and [3.35].

3.6 The second law of thermodynamics

For the single phase material continuum, it is a common practice to assume that the entropy flux \mathbf{h} is equal to the heating flux \mathbf{q} since the kinetic theory of gases confirms approximately this assumption. In his theory of mixtures, Muller (1968) has proposed for each constituent that $\mathbf{h} \neq \mathbf{q}$ and considered constitutive equations for them. If it is assumed that for the single-phase material $\mathbf{h} = \mathbf{q}$ then within the scope of the present theory, it should be justifiable to set $\bar{\mathbf{h}}_{\alpha} = \bar{\mathbf{q}}_{\alpha}$ and I will do so here. In section 6 of the paper, the proposed integral relations do not invoke this conjecture.

The *second law of thermodynamics for the phase α* is obtained from [2.5] by utilizing the coefficients for entropy in table 1, i.e.

$$\bar{\rho}_{\alpha} \tilde{s}_{\alpha} + \nabla \cdot \left(\frac{\bar{\mathbf{q}}_{\alpha}}{\theta_{\alpha}} \right) - \frac{\bar{\rho}_{\alpha} \tilde{r}_{\alpha}}{\theta_{\alpha}} + \hat{c}_{\alpha} \tilde{s}_{\alpha} + \hat{s}_{\alpha} = \bar{\rho}_{\alpha} \tilde{\xi}_{\alpha} \geq 0. \quad [3.37]$$

The *entropy supply or source* for phase α is defined by

$$\hat{s}_{\alpha} \equiv \nabla \cdot (\mathbf{c}_{5\alpha} + \mathbf{c}_{6\alpha}) - c_{7\alpha} + \frac{1}{\mathcal{V}} \sum_{\delta} \int_{a, \delta} \left[\dot{m}_{\alpha\delta} s_{\alpha\delta} + \frac{\mathbf{q}_{\alpha\delta}}{\theta_{\alpha\delta}} \cdot \mathbf{n}_{\alpha\delta} \right] da, \quad [3.38]$$

and it is not necessarily positive. $\mathbf{c}_{5\alpha}$, $\mathbf{c}_{6\alpha}$ and $c_{7\alpha}$ are the covariance coefficients which represent the effect of the finite interfacial area and are defined in appendix B. The definition of the absolute temperature $\bar{\theta}_{\alpha}$ in [3.37] differs from the definition by Drew (1971). According to this author the average temperature for phase α should be $\bar{\theta}_{\alpha}$, i.e. the density-weighted average. To me this definition is not physical. A different temperature

for each phase is necessary in the theory to allow for the thermal nonequilibrium between the phases.

The *second law of thermodynamics for the mixture* is obtained by summing up α in [3.38] and using the identity [3.18] with $\tilde{f}_\alpha = \tilde{s}_\alpha$. The result is

$$\rho \dot{s} + \nabla \cdot \sum_\alpha \left(\frac{\tilde{q}_\alpha}{\tilde{\theta}_\alpha} + \tilde{\rho}_\alpha \tilde{s}_\alpha \mathbf{u}_\alpha \right) - \sum_\alpha \frac{\tilde{\rho}_\alpha \tilde{r}_\alpha}{\tilde{\theta}_\alpha} + \hat{s}_m = \rho \xi \geq 0, \quad [3.39]$$

where the mixture entropy, the mixture entropy production rate, and the mixture entropy supply are defined respectively as follows:

$$\begin{aligned} \rho s &\equiv \sum_\alpha \tilde{\rho}_\alpha \tilde{s}_\alpha \\ \rho \xi &\equiv \sum_\alpha \tilde{\rho}_\alpha \tilde{\xi}_\alpha \geq 0 \\ \hat{s}_m &\equiv \sum_\alpha \hat{s}_\alpha = \sum_\alpha [\nabla \cdot (\mathbf{c}_{5\alpha} + \mathbf{c}_{6\alpha}) - c_{7\alpha}] + \frac{1}{\mathcal{V}} \sum_{\alpha, \delta} \int_{a_{\alpha\delta}} (\Delta_s)_{\alpha\delta} da \end{aligned} \quad [3.40]$$

$(\Delta_s)_{\alpha\delta}$ is the entropy production rate at the interface and it is positive semidefinite (see table 1).

In the theory of the single-phase multicomponent mixtures the entropy supply for the mixture as a whole is assumed to be equal to zero, whereas in the theory of multiphase mixtures it is not reasonable to hypothesize that either \hat{s}_α or \hat{s}_m are equal to zero. Comparing [3.39] with a similar equation in the theory of mixtures (Bowen 1976, [1.6.11]) it is seen that both equations are very similar although the variables have different interpretations in the two theories.

There is another important difference between the theory of mixtures and theory of multiphase mixtures and this is in the interpretation of the *axiom of dissipation* (Truesdell 1969). In the mixture theories of Truesdell & Bowen, the axiom of dissipation refers to the statement that the *mixture* entropy production is positive semidefinite, whereas Eringen & Ingram (1967) postulate that the axiom of dissipation should also hold for each constituent of the mixture. Truesdell's argument in favor for the axiom is provided by the Maxwell's kinetic theory of gases in which there is no basis whatever for an entropy inequality for each constituent. Eringen and Ingram do not offer an explanation for postulating their local axiom of dissipation. It should be noted that in the theory of mixtures there is a disagreement whether only the global or the local axioms of dissipation should be utilized to study the constitutive equations. Indeed, Green & Naghdi (1971), and Bedford & Ingram (1971) have considered an entropy inequality for each constituent of the mixture. The serious drawback of the entropy inequality for each constituent of the single-phase mixture is that it yields the equilibrium chemical potential which depends only on the properties of that constituent. Except for the ideal mixtures, this result is in variance with the single-phase equilibrium thermodynamics. When an entropy inequality for the mixture is only used, this inconsistency does not arise (Bowen 1976).

The theory of multiphase mixtures appears to yield naturally the axiom of dissipation *for each phase* as is illustrated by the development which gives [3.37]. As long as the interfacial area remains finite, it is not inconsistent with the equilibrium thermodynamics to have a second law of thermodynamics for each phase. This deduction follows from the study of constitutive equations for the multiphase mixtures that is presented by Dobran (1984).

The multiphase mixture theory presented above agrees with the theory of Drmheller

& Bedford (1980) when in their momentum and energy equations the source terms, the virtual mass effect, and the expansion-contraction effect are identified with the source terms in this paper. In this respect, the conservation laws presented in this paper are more fundamental since they are not constructed from any *a priori* constitutive assumption. The conservation laws of Drew (1971) for multiphase mixtures have also a built-in constitutive assumption of "suitable" length and time scales. In addition, I do not agree in this formulation with the definition of the average phase temperature and the study of constitutive equations becomes less direct utilizing these conservation laws since the time averaging also affects the principle of the material frame indifference. The time-averaged 2-phase conservation laws of Ishii (1975) are similar to the conservation laws based on the volume averaging approach except that Ishii's equations contain turbulent fluxes instead of the covariance coefficients. His theory assumes that the stress tensor for each phase is symmetric and that the entropy inequality exists for each phase. The drawbacks of the time-averaged model are, however, that its conservation laws are singular whenever an interface becomes stationary and the study of constitutive equations becomes less direct for the reason indicated above. Nigmatulin's (1979) volume averaging theory is incomplete as already discussed in section 1. It does not contain the interfacial source terms, arbitrary number of phases, the entropy balance equation, and the theory is not given a rigorous mathematical structure such as kinematics. It should be stressed (see also a discussion by Dobran 1983a) that the purpose of utilizing an averaging procedure in the "derivation" of multiphase field equations is to give the theory an existence property and that this together with a rigorous definition of kinematic concepts can form a framework for the construction of constitutive equations for special mixtures.

The postulated multiphase mixture theories of Goodman & Cowin, Passman *et al.*, and Drumheller & Bedford discussed in section 1 have mixture source terms absent in the linear momentum, angular momentum and entropy balance equations. As already noted in a number of occasions, the mixture source terms in the presented theory of multiphase mixtures do not appear to vanish unless the mixture is endowed with the absence of interfacial sources and nonlocal effects. In this respect the axiom from the single-phase multicomponent mixture theory that the motion of the mixture is governed by the same equations as is a single body does not appear to be justifiable for multiphase mixtures. This is to say that an argument can be raised that some source terms for the mixture can indeed be incorporated into the field properties whose constitutive equations could then account for this inclusion. An example is the momentum supply $\hat{\mathbf{p}}_m$ which could be incorporated into the stress tensor term in [3.22]₁, but in general for other source terms this does not appear to be possible without invoking postulates of the form of the final field equations.

Furthermore, upon reflecting a moment on the supply terms for the mixture or for each phase (\hat{c}_α , $\hat{\mathbf{p}}_\alpha$, $\hat{\mathbf{p}}_m$, $\hat{\mathbf{M}}_\alpha$, $\hat{\mathbf{M}}_m$, \hat{e}_α , \hat{e}_m , \hat{s}_α , \hat{s}_m) it can be seen that these terms contain the microstructural characteristics of the mixture. As such they are more general than the terms proposed by Drumheller & Bedford (1980) and Passman *et al.* (1983), among others. This being the case, then, it is clear that care must be exercised in assuming the form of microstructural characteristics in the multiphase field equations.

4. RESTRICTIONS IMPOSED ON THE CONSERVATION LAWS BY THE PRINCIPLE OF THE MATERIAL FRAME INDIFFERENCE

In classical physics, it is only required that the conservation laws remain the same in all frames moving with the constant velocities. This change of frame from \mathcal{f} to \mathcal{f}^* is represented by the Galilei group of transformations, i.e.

$$\mathbf{x}^* = \mathbf{Q}(t)\mathbf{x} + \mathbf{c}(t), \quad [4.1]$$

where $d\mathbf{Q}/dt = \mathbf{0}$ and $\mathbf{c} = \mathbf{w}t$. \mathbf{Q} represents an orthogonal linear transformation (a fixed rotation of the frame \mathcal{F}^* with respect to the frame \mathcal{F}), and \mathbf{w} is the fixed velocity of the frame \mathcal{F}^* with respect to the frame \mathcal{F} .

For the phase α , the *principle of the material frame indifference* is stated as follows: Given a deformation function $\chi_{\alpha\alpha}$, the change of frame \mathcal{F} from E^3 to E^3 induces also a change in the motion of the body point X_α , namely:

$$\chi_{\alpha\alpha}^*(X_\alpha, t) = \mathbf{c}(t) + \mathbf{Q}(t)\chi_{\alpha\alpha}(X_\alpha, t), \dagger \quad [4.2]$$

where $\mathbf{c}(t)$ is an arbitrary time-dependent translation vector, and $\mathbf{Q}(t)$ is a time-dependent orthogonal linear transformation which represents a rigid body rotation, i.e.

$$\begin{aligned} \mathbf{Q}(t)\mathbf{Q}(t)^T &= \mathbf{I} \\ \det \mathbf{Q} &\equiv +1, \quad \dot{\mathbf{Q}}\mathbf{Q}^T = -(\dot{\mathbf{Q}}\mathbf{Q}^T)^T. \end{aligned} \quad [4.3]$$

Under the change of frame [4.2], the defining properties of objective scalars, vectors and second order tensors are as follows:

$$\begin{aligned} f^*(\mathbf{x}^*, t) &= f(\mathbf{x}, t) \\ \mathbf{y}^*(\mathbf{x}^*, t) &= \mathbf{Q}(t)\mathbf{y}(\mathbf{x}, t) \\ \mathbf{M}^*(\mathbf{x}^*, t) &= \mathbf{Q}(t)\mathbf{M}(\mathbf{x}, t)\mathbf{Q}(t)^T. \end{aligned} \quad [4.4]$$

The change of frame [4.2] requires that $\bar{\rho}_\alpha^* = \bar{\rho}_\alpha$, $\dot{\bar{\rho}}_\alpha^* = \dot{\bar{\rho}}_\alpha$, $\nabla^* \cdot \bar{\mathbf{v}}_\alpha^* = \nabla \cdot \bar{\mathbf{v}}_\alpha$, and from the conservation of mass equation [3.14], the mass supply must transform according to

$$\hat{c}_\alpha^* = \hat{c}_\alpha. \quad [4.5]$$

The forces are primitive entities in mechanics, and, as such, they are required to transform as vectors according to [4.4]. In the linear momentum equation [3.19], therefore, $\nabla^* \cdot \bar{\mathbf{T}}_\alpha^* = \nabla \cdot \bar{\mathbf{T}}_\alpha$, $\hat{\mathbf{b}}_\alpha^* = \mathbf{Q}\hat{\mathbf{b}}_\alpha$, and

$$\hat{\mathbf{p}}_\alpha^* = \mathbf{Q}(t)\hat{\mathbf{p}}_\alpha. \quad [4.6]$$

From [4.2] the velocity and acceleration transform as

$$\begin{aligned} \bar{\mathbf{v}}_\alpha^* &= \dot{\mathbf{Q}}(t)\mathbf{x} + \mathbf{Q}(t)\bar{\mathbf{v}}_\alpha + \dot{\mathbf{c}}(t) \\ \bar{\mathbf{v}}_\alpha^* &= \ddot{\mathbf{Q}}(t)\mathbf{x} + \mathbf{Q}(t)\bar{\mathbf{v}}_\alpha + 2\dot{\mathbf{Q}}(t)\bar{\mathbf{v}}_\alpha + \ddot{\mathbf{c}}(t), \end{aligned} \quad [4.7]$$

and are, clearly, *not* frame indifferent.

From the mixture linear momentum equation [3.21] or from [3.23] we must also have that

$$\hat{\mathbf{p}}_m^* = \mathbf{Q}(t)\hat{\mathbf{p}}_m. \quad [4.8]$$

†The origin of time in the two frames is here taken to be the same without the loss of generality.

Since $\hat{\mathbf{T}}_\alpha^* = \mathbf{Q}\hat{\mathbf{T}}_\alpha\mathbf{Q}^T$, the angular momentum skew-symmetric linear transformation [3.27] and [3.29] are required to transform according to the following rules:

$$\begin{aligned}\hat{\mathbf{M}}_\alpha^* &= \mathbf{Q}\hat{\mathbf{M}}_\alpha\mathbf{Q}^T \\ \hat{\mathbf{M}}^* &= \mathbf{Q}\hat{\mathbf{M}}\mathbf{Q}^T.\end{aligned}\quad [4.9]$$

In the energy equation [3.31] for phase α we have $\tilde{c}_\alpha^* = \tilde{c}_\alpha$, $\tilde{e}_\alpha^* = \tilde{e}_\alpha$, $\tilde{r}_\alpha^* = \tilde{r}_\alpha$, and $\mathbf{v}^* \cdot \hat{\mathbf{q}}_\alpha^* = \mathbf{v} \cdot \hat{\mathbf{q}}_\alpha$. The velocity gradient \mathbf{L}_α can be decomposed into a symmetric part \mathbf{D}_α and into a skew-symmetric part \mathbf{W}_α , i.e.

$$\mathbf{L}_\alpha = \nabla \tilde{\mathbf{v}}_\alpha = \frac{1}{2}(\mathbf{L}_\alpha + \mathbf{L}_\alpha^T) + \frac{1}{2}(\mathbf{L}_\alpha - \mathbf{L}_\alpha^T) = \mathbf{D}_\alpha + \mathbf{W}_\alpha, \quad [4.10]$$

and thus

$$\text{tr}(\hat{\mathbf{T}}_\alpha^T \nabla \tilde{\mathbf{v}}_\alpha) = \text{tr}(\hat{\mathbf{T}}_\alpha^T \mathbf{D}_\alpha) - \frac{1}{2} \text{tr}(\hat{\mathbf{M}}_\alpha \mathbf{W}_\alpha).$$

Since

$$\text{tr}(\hat{\mathbf{T}}_\alpha^T \mathbf{D}_\alpha^*) = \text{tr}(\hat{\mathbf{T}}_\alpha^T \mathbf{D}_\alpha)$$

and

$$\text{tr}(\hat{\mathbf{M}}_\alpha^* \mathbf{W}_\alpha^*) = \text{tr}(\hat{\mathbf{M}}_\alpha \mathbf{W}_\alpha) + \text{tr}(\hat{\mathbf{M}}_\alpha \mathbf{Q}^T \dot{\mathbf{Q}}),$$

then

$$\text{tr}(\hat{\mathbf{T}}_\alpha^T \mathbf{v}^* \tilde{\mathbf{v}}_\alpha^*) = \text{tr}(\hat{\mathbf{T}}_\alpha^T \nabla \tilde{\mathbf{v}}_\alpha) - \frac{1}{2} \text{tr}(\hat{\mathbf{M}}_\alpha \mathbf{Q}^T \dot{\mathbf{Q}}), \quad [4.11]$$

and [3.31] requires that

$$\hat{e}_\alpha^* = \hat{e}_\alpha + \frac{1}{2} \text{tr}(\hat{\mathbf{M}}_\alpha \mathbf{Q}^T \dot{\mathbf{Q}}). \quad [4.12]$$

The energy supply \hat{e}_α is, therefore, not frame indifferent unless the angular momentum supply $\hat{\mathbf{M}}_\alpha$ is equal to zero. Note, however, that in the Galilei frame of reference $\dot{\mathbf{Q}} = 0$ and \hat{e}_α is frame indifferent.

From the mixture energy equation [3.35] or from the compatibility condition [3.36] and from [3.29] it follows that the mixture energy supply for the multiphase mixture

$$\hat{e}_m^* - \mathbf{v}^* \cdot \hat{\mathbf{p}}_m^* = \hat{e}_m - \mathbf{v} \cdot \hat{\mathbf{p}}_m + \frac{1}{2} \text{tr}(\hat{\mathbf{M}}\mathbf{Q}^T\dot{\mathbf{Q}}) \quad [4.13]$$

is not frame indifferent unless $\hat{\mathbf{M}} = 0$.

Under the change of frame [4.2], the entropy supply in [3.37] must remain frame indifferent

$$\hat{s}_\alpha^* = \hat{s}_\alpha, \quad [4.14]$$

since $\bar{s}_\alpha^* = \bar{s}_\alpha$, $\dot{\bar{s}}_\alpha^* = \dot{\bar{s}}_\alpha$, $\nabla^* \cdot (\bar{\mathbf{q}}_\alpha^*/\bar{\theta}_\alpha^*) = \nabla \cdot (\bar{\mathbf{q}}_\alpha/\bar{\theta}_\alpha)$, $\hat{c}_\alpha^* = \hat{c}_\alpha$, $\bar{\theta}_\alpha^* = \bar{\theta}_\alpha$, $\bar{r}_\alpha^* = \bar{r}_\alpha$ and $\xi_\alpha^* = \xi_\alpha$. Using [4.14] in [3.40] implies that

$$\hat{s}_m^* = \hat{s}_m, \quad [4.15]$$

and is also demanded by the mixture entropy equation [3.39].

The energy supply can be made frame indifferent by including into the energy equation [3.31] the rate of work due to the couple $\hat{\mathbf{M}}_\alpha$. The form of this work term will arise naturally when we examine a particular constitutive assumption in the next section.

5. GENERAL DISCUSSION ON THE CLOSURE OF THE CONSERVATION AND BALANCE EQUATIONS BY THE CONSTITUTIVE EQUATIONS

The conservation laws for the phase α are expressed by [3.14], [3.19], [3.27] and [3.31], and the compatibility conditions between the phasic and mixture conservation laws are expressed by [3.17], [3.23], [3.29] and [3.36]. The second law of thermodynamics [3.37] only requires that the assumed material response or the *constitutive assumption* is consistent with it.

According to Coleman & Noll (1963), the *thermodynamic process* is defined by $\mathbf{x} = \chi_{\alpha\alpha}(\mathbf{X}_\alpha, t)$ and by the following fields which depend on \mathbf{x} and t :

$$\bar{\rho}_\alpha, \hat{c}_\alpha, \bar{\mathbf{T}}_\alpha, \bar{\mathbf{b}}_\alpha, \hat{\mathbf{p}}_\alpha, \hat{\mathbf{M}}_\alpha (\text{or } \bar{\mathbf{T}}_\alpha^T), \bar{\epsilon}_\alpha, \bar{\mathbf{q}}_\alpha, \quad [5.1]$$

$$\bar{r}_\alpha, \hat{c}_\alpha, \bar{s}_\alpha, \bar{\theta}_\alpha \text{ and } \hat{s}_\alpha \text{ for } \alpha = 1, \dots, \gamma.$$

Furthermore, to define the thermodynamic process [5.1] it is *sufficient* to assign the constitutive equations for \hat{c}_α , $\bar{\mathbf{T}}_\alpha$, $\hat{\mathbf{p}}_\alpha$, $\hat{\mathbf{M}}_\alpha$, $\bar{\epsilon}_\alpha$, $\bar{\mathbf{q}}_\alpha$, \hat{c}_α , \bar{s}_α and \hat{s}_α at \mathbf{X}_α by the *history* of the fields $\mathbf{x} = \chi_{\alpha\alpha}(\mathbf{X}_\alpha, t)$ and $\bar{\theta}_\beta(\mathbf{x}, t)$. The remaining fields $\bar{\rho}_\alpha$, $\bar{\mathbf{b}}_\alpha$ and \bar{r}_α in the list [5.1] are determined from the conservation laws, and local, nonlocal, and memory effects of the material response are included in the history.

A fairly general constitutive assumption is the following:

$$\begin{aligned} & (\hat{c}_\alpha, \bar{\mathbf{T}}_\alpha, \hat{\mathbf{p}}_\alpha, \hat{\mathbf{M}}_\alpha, \bar{\epsilon}_\alpha, \bar{\mathbf{q}}_\alpha, \hat{c}_\alpha, \bar{s}_\alpha, \hat{s}_\alpha) \\ & = f(\bar{\theta}_\beta, \dot{\bar{\theta}}_\beta, \nabla \bar{\theta}_\beta, \mathbf{F}_\beta, \dot{\mathbf{F}}_\beta, \text{GRAD } \mathbf{F}_\beta, \bar{\mathbf{v}}_\beta, \dot{\bar{\mathbf{v}}}_\beta), \end{aligned} \quad [5.2]$$

and no confusion should arise in the notation where each constitutive variable of the phase α ($\alpha = 1, \dots, \gamma$) depends on all other variables in the functional expression f , and $\bar{\theta}_\beta, \dots, \dot{\bar{\mathbf{v}}}_\beta$ is interpreted to mean $\bar{\theta}_1, \dots, \bar{\theta}_\gamma, \dots, \dot{\bar{\mathbf{v}}}_1, \dots, \dot{\bar{\mathbf{v}}}_\gamma$.

The above constitutive assumption allows for the propagation of thermal waves, $\dot{\bar{\theta}}_\beta$ (this, of course, does not imply that by including $\dot{\bar{\theta}}_\beta$ an independent constitutive variable proves the existence of such waves); for heat conduction, $\nabla \bar{\theta}_\beta$; for viscous effects, $\dot{\mathbf{F}}_\beta$; for density gradients, $\text{GRAD } \mathbf{F}_\beta$; for viscous drag, $\bar{\mathbf{v}}_\beta$; and for the virtual mass effects, $\dot{\bar{\mathbf{v}}}_\beta$. It does not include the nonlocal effects discussed in section 3.6 and, therefore, its applicability is limited to mixtures with sufficiently small interfacial areas. By including into the theory the above independent variables it is assumed that the resulting theory would be able to predict at least some simple physical phenomena for both fluid and solid mixtures. For a fluid, for example, $\text{GRAD } \mathbf{F}_\beta$ would be replaced by $\nabla \bar{\rho}_\beta$, whereas for isotropic solids by the gradient of left Cauchy–Green tensor (see, e.g. Bowen 1976). The virtual mass effect is assumed to account for the acceleration of the continuous phase when the dispersed phase is moving relative to it.

Equation [5.2] satisfies a number of principles of the constitutive equations. These are causality, determinism, equipresence, homogeneous material invariance and local action. A constitutive equation will be also required to satisfy the principle of the material frame indifference, and by a simple inspection, [5.2] does not satisfy this principle.

In the frame \mathcal{f}^* we can write [5.2] as follows:

$$\begin{aligned} & (\hat{c}_\alpha^*, \hat{\mathbf{T}}_\alpha^*, \hat{\mathbf{p}}_\alpha^*, \hat{\mathbf{M}}_\alpha^*, \tilde{c}_\alpha^*, \tilde{\mathbf{q}}_\alpha^*, \hat{e}_\alpha^*, \tilde{s}_\alpha^*, \hat{s}_\alpha^*) \\ & - f(\bar{\theta}_\beta^*, \dot{\bar{\theta}}_\beta^*, \nabla^* \bar{\theta}_\beta^*, \mathbf{F}_\beta^*, \dot{\mathbf{F}}_\beta^*, \text{GRAD } \mathbf{F}_\beta^*, \tilde{\mathbf{v}}_\beta^*, \dot{\tilde{\mathbf{v}}}_\beta^*), \end{aligned} \quad [5.3]$$

Using now the results of section 4 for the transformation of scalar, vector and second order tensor fields from the frame \mathcal{f} to the frame \mathcal{f}^* , [5.3] becomes:

$$\begin{aligned} & (\hat{c}_\alpha, \mathbf{Q}\hat{\mathbf{T}}_\alpha\mathbf{Q}^T, \mathbf{Q}\hat{\mathbf{p}}_\alpha, \mathbf{Q}\hat{\mathbf{M}}_\alpha\mathbf{Q}^T, \tilde{c}_\alpha, \mathbf{Q}\tilde{\mathbf{q}}_\alpha, \hat{e}_\alpha + \frac{1}{2} \text{tr}(\hat{\mathbf{M}}_\alpha\mathbf{Q}^T\dot{\mathbf{Q}}), \tilde{s}_\alpha, \hat{s}_\alpha) \\ & - f(\bar{\theta}_\beta, \dot{\bar{\theta}}_\beta, \nabla\bar{\theta}_\beta, \mathbf{Q}\mathbf{F}_\beta, \dot{\mathbf{Q}}\mathbf{F}_\beta + \mathbf{Q}\dot{\mathbf{F}}_\beta, \text{GRAD } \mathbf{Q}\mathbf{F}_\beta, \\ & \dot{\mathbf{Q}}\mathbf{x} + \mathbf{Q}\dot{\tilde{\mathbf{v}}}_\beta + \dot{c}, \dot{\mathbf{Q}}\mathbf{x} + 2\dot{\mathbf{Q}}\tilde{\mathbf{v}}_\beta + \mathbf{Q}\dot{\tilde{\mathbf{v}}} + \dot{c}). \end{aligned} \quad [5.4]$$

Two sets of necessary conditions are next considered. Select first $\mathbf{Q} = \mathbf{I}$, $\dot{\mathbf{Q}} = \mathbf{0}$, $\dot{c} = -\dot{\tilde{\mathbf{v}}}_\gamma$, $\ddot{\mathbf{Q}} = \mathbf{0}$, $\ddot{c} = -\dot{\tilde{\mathbf{v}}}_\gamma$ and substitute into [5.4]. The equation which results is next required to hold in the frame \mathcal{f}^* in a similar manner as [5.3]. Using the transformation properties for the tensor fields from section 4 again, the resulting equation is reduced to the form which is similar to [5.4]. The second set of necessary conditions are now selected as $\mathbf{Q} = \mathbf{I}$ and $\dot{\mathbf{Q}} = -\mathbf{W}_\gamma$, and the result is reduced to the frame indifferent form

$$\begin{aligned} & (\hat{c}_\alpha, \hat{\mathbf{T}}_\alpha, \hat{\mathbf{p}}_\alpha, \hat{\mathbf{M}}_\alpha, \tilde{c}_\alpha, \tilde{\mathbf{q}}_\alpha, \hat{e}_\alpha - \frac{1}{2} \text{tr}(\hat{\mathbf{M}}_\alpha\mathbf{W}_\gamma), \tilde{s}_\alpha, \hat{s}_\alpha) \\ & - f(\bar{\theta}_\beta, \dot{\bar{\theta}}_\beta, \mathbf{F}_\beta, \nabla\bar{\theta}_\beta, \mathbf{D}_\beta, \mathbf{W}_\beta - \mathbf{W}_\gamma, \text{GRAD } \mathbf{F}_\beta, \\ & \tilde{\mathbf{v}}_\beta - \tilde{\mathbf{v}}_\gamma, \dot{\tilde{\mathbf{v}}}_\beta - \dot{\tilde{\mathbf{v}}}_\gamma - 2\mathbf{W}_\gamma(\tilde{\mathbf{v}}_\beta - \tilde{\mathbf{v}}_\gamma)). \end{aligned} \quad [5.5]$$

The two sets of necessary conditions considered above are also sufficient for [5.5] to hold true for all $\mathbf{Q}\mathbf{Q}^T = \mathbf{I}$ and $\dot{\mathbf{Q}}\mathbf{Q}^T = -(\dot{\mathbf{Q}}\mathbf{Q}^T)^T$.

It is noted from [5.5] that

$$\hat{e}_\alpha - \frac{1}{2} \text{tr}(\hat{\mathbf{M}}_\alpha\mathbf{W}_\gamma)$$

is frame indifferent although \hat{e}_α is not (Cit. [4.12]). This being the case, we can redefine the energy supply in [3.32] as follows:

$$\hat{e}_\alpha = \hat{e}_{\alpha R} + \frac{1}{2} \text{tr}(\hat{\mathbf{M}}_\alpha\mathbf{W}_\gamma), \quad [5.6]$$

where the last term in the equation represents the rate of work due to the couple $\hat{\mathbf{M}}_\alpha$. The redefined energy supply $\hat{e}_{\alpha R}$ is now frame indifferent as it is easy to show.

Equation [5.5] also shows that the constitutive variables can depend on the difference of accelerations, $\ddot{\mathbf{v}}_\beta - \ddot{\mathbf{v}}_\gamma$, only in the linear approximation, and that for the single phase continuum there is no dependence on the spin rate \mathbf{W} . This last conclusion is well-known. A simpler version of [5.5] was also obtained by Bowen (1976).

The constitutive assumption [5.2] assumes that no volumetric fractions enter as independent variables, since the conservation and balance equations for a multiphase mixture presented in section 3 do not explicitly contain these variables. This is in contrast to the formulations of Drumheller & Bedford (1980) and Passman *et al.* (1983) who include such fractions for modeling the microstructural characteristics of the mixture and, consequently, require additional balance equations to close the governing field equations. Equation [5.2] was also required to satisfy the principle of equipresence by which there should be *non a priori* reason for discriminating any kinematical variable which enters in the different response functionals f in [5.2]. While in the theory of single-phase multicomponent mixtures this is generally an established procedure, in the theories of multiphase mixtures this is certainly not the case due to an argument that the phases are physically separated and should, therefore, obey different rules. Drew (1976) and as well as most recently Passman *et al.* (1983) advocate the principle of phase separation whereby the material-specific dependent variables of the α th phase only depend on the independent variables of this phase, whereas the supply or source variables depend on all of the independent variables. By not advocating the principle of phase separation, Dobran (1984) showed that it is possible theoretically for the stress tensor of phase α to be affected by other phases and by their rotational motion. This result appears reasonable in view of a similar result in the theory of single-phase multicomponent mixtures (Bowen 1976) and it thus provides a further consistency between the two theories.

6. INTEGRAL FORM OF THE CONSERVATION LAWS AND JUMP CONDITIONS FOR THE MULTIPHASE MIXTURE

The conservation and balance equations for a multiphase mixture were derived in section 3 through physical as well as through the metaphysical arguments. The entire metaphysics, however, rests in the definition of the mapping transformations in Appendix A. These mapping transformations have allowed us to place into one-to-one correspondence the theory of multiphase mixtures and the theory of mixtures. In fact, the presented "derivation" of the theory of multiphase mixtures provides a very good motivation for the "derivation" of the theory of mixtures.

The theory of multiphase mixtures is more complex than the theory of single-phase multicomponent mixtures for two reasons. First, this complexity is reflected in the apparent nonvanishing of the linear momentum, angular momentum, energy and entropy source terms for the mixture, and second, the constitutive equations of greater complexity should be constructed in order to account for the nonlocal effects.

In previous sections, it was assumed that in the space E^3 all the fields of the conservation laws possess sufficient smoothness. Then, what about the possibility of relaxing this smoothness assumption of the fields in order to account for the discontinuities in the multiphase mixtures? It is apparent that to study such entities, we need the *integral form* of the field equations for each phase α , and to construct such forms, it is necessary to demand that, in the regions of E^3 with sufficient smoothness, the integral form of the conservation and balance equations must reduce to the differential form of section 3.

With the above as a guide, let \mathcal{V} be a volume region in E^3 which contains the phases of the multiphase mixture, and let \int denote the integration over the volume \mathcal{V} . The boundary of \mathcal{V} is $\partial\mathcal{V}$ and the integration over the boundary will be denoted by \oint . The backward prime, as before, denotes the time derivative "following" the phase α , and the

dot ($\dot{\cdot}$) denotes the time derivative "following" the mixture. The conservation laws in the integral form for the phase α and for the multiphase mixture are the *postulates*:

6.1 Conservation of mass

$$\begin{aligned} \overline{\int_{\mathcal{V}} \bar{\rho}_\alpha d\mathcal{V}} &= \int_{\mathcal{V}} \hat{c}_\alpha d\mathcal{V} \\ \overline{\int_{\mathcal{V}} \rho d\mathcal{V}} &= 0. \end{aligned} \quad [6.1]$$

6.2 Balance of the linear momentum

$$\begin{aligned} \overline{\int_{\mathcal{V}} \bar{\rho}_\alpha \tilde{\mathbf{v}}_\alpha d\mathcal{V}} &= \oint_{\partial\mathcal{V}} \mathbf{T}_\alpha \mathbf{n} da + \int_{\mathcal{V}} \bar{\rho}_\alpha \tilde{\mathbf{b}}_\alpha d\mathcal{V} + \int_{\mathcal{V}} (\hat{\mathbf{p}}_\alpha + \hat{c}_\alpha \tilde{\mathbf{v}}_\alpha) d\mathcal{V} \\ \overline{\int_{\mathcal{V}} \rho \mathbf{v} d\mathcal{V}} &= \oint_{\partial\mathcal{V}} \mathbf{T} \mathbf{n} da + \int_{\mathcal{V}} \rho \mathbf{b} d\mathcal{V} + \int_{\mathcal{V}} \hat{\mathbf{p}}_m d\mathcal{V} \end{aligned} \quad [6.2]$$

6.3 Balance of the angular momentum

$$\begin{aligned} \overline{\int_{\mathcal{V}} \mathbf{x} \wedge \bar{\rho}_\alpha \tilde{\mathbf{v}}_\alpha d\mathcal{V}} &= \oint_{\partial\mathcal{V}} \mathbf{x} \wedge \mathbf{T}_\alpha \mathbf{n} da + \int_{\mathcal{V}} \mathbf{x} \wedge (\bar{\rho}_\alpha \tilde{\mathbf{b}}_\alpha + \hat{\mathbf{p}}_\alpha + \hat{c}_\alpha \tilde{\mathbf{v}}_\alpha) d\mathcal{V} + \int_{\mathcal{V}} \hat{\mathbf{m}}_\alpha d\mathcal{V} \\ \overline{\int_{\mathcal{V}} \mathbf{x} \wedge \rho \mathbf{v} d\mathcal{V}} &= \oint_{\partial\mathcal{V}} \mathbf{x} \wedge \mathbf{T} \mathbf{n} da + \int_{\mathcal{V}} \mathbf{x} \wedge \rho \mathbf{b} d\mathcal{V} + \int_{\mathcal{V}} \mathbf{x} \wedge \hat{\mathbf{p}}_m d\mathcal{V} \\ &\quad + \int_{\mathcal{V}} \hat{\mathbf{m}}_m d\mathcal{V}. \end{aligned} \quad [6.3]$$

6.4 Balance of energy

$$\begin{aligned} \overline{\int_{\mathcal{V}} \bar{\rho}_\alpha \left(\tilde{\epsilon}_\alpha + \frac{1}{2} \tilde{\mathbf{v}}_\alpha \cdot \tilde{\mathbf{v}}_\alpha \right) d\mathcal{V}} &= \oint_{\partial\mathcal{V}} \tilde{\mathbf{v}}_\alpha \cdot \mathbf{T}_\alpha \mathbf{n} da - \oint_{\partial\mathcal{V}} \bar{\mathbf{q}}_\alpha \cdot \mathbf{n} da + \int_{\mathcal{V}} \bar{\rho}_\alpha \tilde{r}_\alpha d\mathcal{V} \\ &\quad + \int_{\mathcal{V}} \tilde{\mathbf{v}}_\alpha \cdot \bar{\rho}_\alpha \tilde{\mathbf{b}}_\alpha d\mathcal{V} + \int_{\mathcal{V}} \left[\hat{c}_\alpha \left(\tilde{\epsilon}_\alpha + \frac{1}{2} \tilde{\mathbf{v}}_\alpha \cdot \tilde{\mathbf{v}}_\alpha \right) + \tilde{\mathbf{v}}_\alpha \cdot \hat{\mathbf{p}}_\alpha + \hat{\epsilon}_\alpha \right] d\mathcal{V} \\ \overline{\int_{\mathcal{V}} \rho \left(\epsilon + \frac{1}{2} \mathbf{v} \cdot \mathbf{v} \right) d\mathcal{V}} &= \oint_{\partial\mathcal{V}} \mathbf{v} \cdot \mathbf{T} \mathbf{n} da - \oint_{\partial\mathcal{V}} \mathbf{q} \cdot \mathbf{n} da + \int_{\mathcal{V}} \rho r d\mathcal{V} \\ &\quad + \int_{\mathcal{V}} \rho \mathbf{v} \cdot \mathbf{b} d\mathcal{V} + \int_{\mathcal{V}} (\hat{\epsilon}_m + \mathbf{v} \cdot \hat{\mathbf{p}}_m) d\mathcal{V}. \end{aligned} \quad [6.4]$$

6.5 The second law of thermodynamics

$$\begin{aligned}
 \overline{\int_{\mathcal{V}} \bar{\rho}_\alpha \bar{s}_\alpha d\mathcal{V}} + \oint_{\partial\mathcal{V}} \frac{\bar{\mathbf{h}}_\alpha \cdot \mathbf{n}}{\bar{\theta}_\alpha} da - \int_{\mathcal{V}} \frac{\bar{\rho}_\alpha \bar{r}_\alpha}{\bar{\theta}_\alpha} d\mathcal{V} + \int_{\mathcal{V}} \hat{s}_\alpha d\mathcal{V} &= \int_{\mathcal{V}} \bar{\rho}_\alpha \bar{\xi}_\alpha d\mathcal{V} \geq 0 \\
 \overline{\int_{\mathcal{V}} \rho s d\mathcal{V}} + \oint_{\partial\mathcal{V}} \sum_\alpha \left(\frac{\bar{\mathbf{h}}_\alpha}{\bar{\theta}_\alpha} + \bar{\rho}_\alpha \bar{s}_\alpha \mathbf{u}_\alpha \right) \cdot \mathbf{n} da - \int_{\mathcal{V}} \sum_\alpha \frac{\bar{\rho}_\alpha \bar{r}_\alpha}{\bar{\theta}_\alpha} d\mathcal{V} & \quad [6.5] \\
 + \int_{\mathcal{V}} \hat{s}_m d\mathcal{V} &= \int_{\mathcal{V}} \rho \xi d\mathcal{V} \geq 0.
 \end{aligned}$$

The mixture properties ρ , v , \mathbf{T} , \mathbf{b} , $\hat{\mathbf{p}}_m$, $\hat{\mathbf{m}}_m$, ϵ , r , \mathbf{q} , \hat{e}_m , s , ξ and \hat{s}_m in the above equations are expressed by [3.8], [3.9], [3.22], [3.30], [3.34] and [3.40] respectively. In the balance of the angular momentum equation [6.3] the external couples and couple stresses have been excluded, and [6.5] do not assume that the entropy flux vector $\bar{\mathbf{h}}_\alpha$ is equal to the heat flux vector $\bar{\mathbf{q}}_\alpha$. Equations [6.1]–[6.5] are also identical to the equations in the theory of mixtures (Bowen 1976) when it is assumed that $\hat{\mathbf{p}}_m = \mathbf{0}$, $\hat{\mathbf{m}}_m = \mathbf{0}$, $\hat{e}_m = 0$ and $\hat{s}_m = 0$.

To derive the jump conditions for multiphase mixtures, let \mathcal{V} be a volume region which contains a fixed amount of matter of the phase α , and let a singular surface \mathcal{S} separate \mathcal{V} into \mathcal{V}^+ and \mathcal{V}^- in which the field $\bar{\rho}_\alpha \bar{\Psi}_\alpha$ is differentiable. It is then easy to establish the following *transport theorem* (similar to Eringen 1975, section 2.3):

$$\begin{aligned}
 \overline{\int_{\mathcal{V}^+ + \mathcal{V}^-} \bar{\rho}_\alpha \bar{\Psi}_\alpha d\mathcal{V}} &= \int_{\mathcal{V}^+ + \mathcal{V}^-} \left(\frac{\partial}{\partial t} \bar{\rho}_\alpha \bar{\Psi}_\alpha + \nabla \cdot \bar{\rho}_\alpha \Psi_\alpha \tilde{\mathbf{v}}_\alpha \right) d\mathcal{V} \\
 &+ \int_{\mathcal{S}} [\bar{\rho}_\alpha \Psi_\alpha (\tilde{\mathbf{v}}_\alpha - \mathbf{w}_\mathcal{S})] \cdot \mathbf{n}_\mathcal{S} da, \quad [6.6]
 \end{aligned}$$

where the *jump* of Ω is defined by the expression:

$$[\Omega] \equiv \Omega^+ - \Omega^-.$$

In [6.6] $\mathbf{w}_\mathcal{S}$ is the velocity of the singular surface \mathcal{S} , and $\mathbf{n}_\mathcal{S}$ is the unit normal vector to \mathcal{S} which points into \mathcal{V}^+ .

Application of the transport theorem [6.6] to the integral conservation laws [6.1]–[6.5] yields the differential form of the conservation laws of section 3 in \mathcal{V}^+ and \mathcal{V}^- , and the following jump conditions across the singular surface \mathcal{S} :

Conservation of mass

$$\begin{aligned}
 [\bar{\rho}_\alpha (\tilde{\mathbf{v}}_\alpha - \mathbf{w}_\mathcal{S})] \cdot \mathbf{n}_\mathcal{S} &= 0 \\
 [\rho (\mathbf{v} - \mathbf{w}_\mathcal{S})] \cdot \mathbf{n}_\mathcal{S} &= 0. \quad [6.7]
 \end{aligned}$$

Balance of the linear momentum

$$\begin{aligned}
 [\bar{\rho}_\alpha \tilde{\mathbf{v}}_\alpha \otimes (\tilde{\mathbf{v}}_\alpha - \mathbf{w}_\mathcal{S}) - \hat{\mathbf{T}}_\alpha] \mathbf{n}_\mathcal{S} &= \mathbf{0} \\
 [\rho \mathbf{v} \otimes (\mathbf{v} - \mathbf{w}_\mathcal{S}) - \mathbf{T}] \mathbf{n}_\mathcal{S} &= \mathbf{0}. \quad [6.8]
 \end{aligned}$$

Balance of energy

$$\left[\bar{\rho}_\alpha \left(\tilde{\epsilon}_\alpha + \frac{1}{2} \tilde{v}_\alpha \cdot \tilde{v}_\alpha \right) (\tilde{v}_\alpha - \mathbf{w}_\mathcal{I}) + \bar{q}_\alpha - \mathbf{T}_\alpha^T \tilde{v}_\alpha \right] \cdot \mathbf{n}_\mathcal{I} = 0$$

$$\left[\rho \left(\epsilon + \frac{1}{2} \mathbf{v} \cdot \mathbf{v} \right) (\mathbf{v} - \mathbf{w}_\mathcal{I}) + \mathbf{q} - \mathbf{T}^T \mathbf{v} \right] \cdot \mathbf{n}_\mathcal{I} = 0.$$
[6.9]

Second law of thermodynamics

$$\left[\bar{\rho}_\alpha \tilde{s}_\alpha (\tilde{v}_\alpha - \mathbf{w}_\mathcal{I}) + \frac{\bar{h}_\alpha}{\bar{\theta}_\alpha} \right] \cdot \mathbf{n}_\mathcal{I} \geq 0$$

$$\left[\rho s (\mathbf{v} - \mathbf{w}_\mathcal{I}) + \sum_\alpha \left(\frac{\bar{h}_\alpha}{\bar{\theta}_\alpha} + \bar{\rho}_\alpha \tilde{s}_\alpha \mathbf{u}_\alpha \right) \right] \cdot \mathbf{n}_\mathcal{I} \geq 0.$$
[6.10]

The similarity of the jump conditions [6.7]–[6.10] to [2.2] is evident in the form but not in the principles. The above jump conditions for the *mixture* are identical to the results of Eringen & Ingram (1967) in their theory of mixtures. For the application of the above results on the jump conditions the reader is referred to Dobran (1983b).

7. SUMMARY AND CONCLUSIONS

The theory of multiphase mixtures presented in this paper is shown to be consistent with the theory of mixtures of Truesdell (1969) or Bowen (1976) when the interfacial area is reduced to zero. This theory is also consistent with the physical models which are rigorously constructed by the volume averaging process.

The conservation and balance equations in the theory of multiphase mixtures are similar to the field equations in the theory of mixtures, except that in the former theory, these equations contain the effect of the finite interfacial area. This effect in the theory manifests itself through the interfacial sources (surface tension) and through the covariance coefficients which can be assumed to represent the nonlocal material response or the microstructural characteristics of the mixture. Another significant difference between the two theories is in the equations for the second law of thermodynamics. In the theory of multiphase mixtures presented in this paper, the second law of thermodynamics of each phase contains the entropy source term which represents the effect of the microstructural characteristics of the mixture, and the axiom of dissipation can be assigned for each phase.

The multiphase field equations were examined by the principle of material frame indifference and the constitutive variables were identified and discussed for a particular constitutive assumption. The jump conditions for the multiphase mixture were also derived for each phase and for the mixture by postulating the integral form of the conservation and balance equations.

NOMENCLATURE

- $\tilde{\mathbf{b}}_\alpha$ body force of phase α
- \mathbf{b} body force of the mixture defined by [3.22]₂
- \mathbf{c} arbitrary time-dependent translation vector in [4.2]
- $\mathbf{c}_{\beta\alpha}, \mathbf{C}_{\beta\alpha}$ covariance coefficients defined in Appendix B
- $\hat{\epsilon}_\alpha$ mass supply or phase change rate of phase α defined by [3.15]
- \mathbf{D}_α symmetric part of velocity gradient of phase α

| | |
|--------------------------|---|
| \hat{e}_m | energy supply or source of the mixture defined by [3.36] |
| F_α | deformation gradient of phase α defined by [3.5] ₁ |
| G_α | GRAD F_α |
| GRAD | gradient with respect to the material coordinates defined by [3.5] _{1,2} |
| \hat{h}_α | entropy flux of phase α in [6.5] |
| I | unit tensor |
| L_α | velocity gradient of phase α defined by [3.6] |
| \hat{M}_α | angular momentum supply or source of phase α defined by [3.27] |
| \hat{M} | angular momentum supply or source of the mixture defined by [3.29] ₂ |
| \hat{p}_α | linear momentum supply or source of phase α |
| \hat{p}_m | linear momentum supply or source for the mixture defined by [3.23] |
| \hat{q}_α | heat flux vector of phase α |
| q | heat flux vector of the mixture defined by [3.34] ₃ |
| Q | time-dependent orthogonal linear transformation in [4.2] |
| \tilde{r}_α | heat generation rate of phase α |
| r | heat generation rate of the mixture defined by [3.34] ₂ |
| \tilde{s}_α | entropy of phase α |
| s | entropy of the mixture defined by [3.40] ₁ |
| \hat{s}_α | entropy supply or source of phase α |
| \hat{s}_m | entropy supply or source of the mixture defined by [3.40] ₃ |
| t | time |
| \hat{T}_α | stress tensor of phase α |
| T | stress tensor of the mixture defined by [3.22] ₁ |
| u_α | diffusion velocity defined by [3.10] |
| \tilde{v}_α | velocity of phase α defined by [3.4] ₁ |
| $\tilde{\dot{v}}_\alpha$ | acceleration of phase α defined by [3.4] ₂ |
| v | center of mass velocity of the mixture defined by [3.9] |
| \dot{v} | acceleration of the mixture |
| \mathcal{V} | averaging volume |
| W_α | antisymmetric part of velocity gradient of phase α |
| x | position vector |
| X_α | reference position vector of a particle of phase α |
| X_α | particle of phase α |

Greek symbols

| | |
|-----------------------|---|
| \tilde{e}_α | internal energy of phase α |
| \hat{e}_α | energy supply or source of phase α |
| ϵ | energy of the mixture defined by [3.34] ₁ |
| $\bar{\theta}_\alpha$ | temperature of phase α |
| κ_α | reference configuration of phase α |
| $\bar{\rho}_\alpha$ | partial density of phase α |
| ρ | density of mixture defined by [3.8] |
| $\chi_{\alpha\kappa}$ | deformation function of phase α defined by [3.3] |

Subscripts

| | |
|-------------------------|-------------------------------|
| m | pertains to the mixture |
| α, β, δ | phase of a multiphase mixture |
| γ | total number of phases |

Superscripts

| | |
|------|-----------|
| T | transpose |
| -1 | inverse |

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APPENDIX A

Definition of the mapping transformation

Figure 1 illustrates the flow field in an Euclidean space E_0^3 which consists of continua $\alpha = 1, \dots, \gamma$. Embedded in this space is a fixed volume \mathcal{V} , and at time t a volume $\mathcal{V}_\alpha = \sum_\delta \mathcal{V}_{\alpha\delta}$ of the phase α is contained within \mathcal{V} . The surfaces of $\mathcal{V}_{\alpha\delta}$ are $a_{\alpha\delta}$ and $a_{\delta\alpha}$, where $a_{\alpha\delta}$ is the surface of intersection between \mathcal{V} and $\mathcal{V}_{\alpha\delta}$, and $a_{\delta\alpha}$ is the surface of $\mathcal{V}_{\alpha\delta}$ which is fully contained within \mathcal{V} .

Consider a mapping of the averaging volume \mathcal{V} in E_0^3 into a point $P(\mathcal{V})$ in E^3 . That is, (1) associate with the space E_0^3 the averaging volumes \mathcal{V} with the domain of definition contained in E_0^3 , (2) assign to each \mathcal{V} a mapping function such that its image point in E^3 is the point $P(\mathcal{V})$ with the location \mathbf{x} , and (3) identify the center $\dagger r_0$ of \mathcal{V} to be identical to the place \mathbf{x} of $P(\mathcal{V})$ such that to each distinct \mathcal{V} corresponds a distinct center r_0 . (The particular selection of $r_0 = \mathbf{x}$ reenters into the theory through the constitutive assumption as it is clearly evidenced by equation (3.25) for the angular momentum supply for phase α .) The mapping defined above is *onto*. It is also *one-to-one*, since to each point $P(\mathcal{V})$ at the place \mathbf{x} corresponds a unique \mathcal{V} at $r_0 = \mathbf{x}$.

In this appendix, the transformations which are needed in [2.4] to accomplish the above bijective mapping are considered. These transformations utilize Leibnitz's and Green-Gauss's Divergence Theorems. For this purpose, let $\mathbf{F}_{\alpha\delta}$ represent a differentiable field in $\mathcal{V}_{\alpha\delta}$, and on $a_{\alpha\delta}$ and $a_{\delta\alpha}$. Then with the nomenclature in figure 1 we have:

Leibnitz's theorem

$$\sum_\delta \int_{\mathcal{V}_{\alpha\delta}} \frac{\partial \mathbf{F}_{\alpha\delta}}{\partial t} d\mathcal{V} = \frac{\partial}{\partial t} \sum_\delta \int_{\mathcal{V}_{\alpha\delta}} \mathbf{F}_{\alpha\delta} d\mathcal{V} - \sum_\delta \int_{a_{\delta\alpha}} \mathbf{F}_{\alpha\delta} \mathbf{S}_{\delta\alpha} \cdot \mathbf{n}_{\alpha\delta} da, \quad [\text{A.1}]$$

where $\mathbf{S}_{\delta\alpha}$ is the velocity of surface $a_{\delta\alpha}$.

Divergence theorem. Using the Green-Gauss's divergence theorem and the fundamental theorem of calculus it is easy to show that

$$\sum_\delta \int_{\mathcal{V}_{\alpha\delta}} \nabla^0 \cdot \mathbf{F}_{\alpha\delta} d\mathcal{V} = \sum_\delta \nabla \cdot \int_{\mathcal{V}_{\alpha\delta}} \mathbf{F}_{\alpha\delta} d\mathcal{V} + \sum_\delta \int_{a_{\delta\alpha}} \mathbf{F}_{\alpha\delta} \cdot \mathbf{n}_{\alpha\delta} da, \quad [\text{A.2}]$$

\dagger The center r_0 should be selected as the center of mass of \mathcal{V} in order to correspond to the definition of the center of mass velocity in [3.9].

where ∇^0 is defined in E_0^3 and ∇ is defined in E^3 at P . The mappings [A.1] and [A.2] are also linear, and we thus have

$$\sum_{\alpha,\beta} \int_{\mathcal{V}_{\alpha\beta}} \frac{\partial \mathbf{F}_{\alpha\beta}}{\partial t} d\mathcal{V} = \frac{\partial}{\partial t} \sum_{\alpha,\beta} \int_{\mathcal{V}_{\alpha\beta}} \mathbf{F}_{\alpha\beta} d\mathcal{V} - \sum_{\alpha,\beta} \int_{a_{\alpha\beta}} \mathbf{F}_{\alpha\beta} \mathbf{S}_{\alpha\beta} \cdot \mathbf{n}_{\alpha\beta} da, \quad [\text{A.3}]$$

$$\sum_{\alpha,\beta} \int_{\mathcal{V}_{\alpha\beta}} \nabla^0 \cdot \mathbf{F}_{\alpha\beta} d\mathcal{V} = \nabla \cdot \sum_{\alpha,\beta} \int_{\mathcal{V}_{\alpha\beta}} \mathbf{F}_{\alpha\beta} d\mathcal{V} + \sum_{\alpha,\beta} \int_{a_{\alpha\beta}} \mathbf{F}_{\alpha\beta} \cdot \mathbf{n}_{\alpha\beta} da. \quad [\text{A.4}]$$

A simple example. The transformation equations [A.1] and [A.2] are general and they are applicable to a phase α in the averaging volume \mathcal{V} such as shown in figure 1. To clarify the averaging procedure summarized above consider a special case of two-phase flow through a duct as shown in figure 2 where the averaging volume \mathcal{V} coincides with the duct walls and by the planes at $z = z_1$ and $z = z_2$. The volume of phase α in \mathcal{V} is \mathcal{V}_α , $a_\alpha(z_1, t)$ and $a_\alpha(z_2, t)$ are the surfaces of intersection between \mathcal{V} and \mathcal{V}_α at z_1 and z_2 respectively, and a_A is the surface of \mathcal{V}_α which is fully contained in \mathcal{V} . In this case the Leibnitz's and Divergence Theorems can be written as follows:

$$\int_{\mathcal{V}_\alpha} \frac{\partial \mathbf{F}_\alpha}{\partial t} d\mathcal{V} = \frac{\partial}{\partial t} \int_{\mathcal{V}_\alpha} \mathbf{F}_\alpha d\mathcal{V} - \int_{a_A} \mathbf{F}_\alpha \mathbf{S}_A \cdot \mathbf{n}_\alpha da, \quad [\text{A.5}]$$

$$\int_{\mathcal{V}_\alpha} \nabla \cdot \mathbf{F}_\alpha d\mathcal{V} = \int_{a_A} \mathbf{F}_\alpha \cdot \mathbf{n}_\alpha da + \int_{a_\alpha(z_2, t)} \mathbf{F}_\alpha \cdot \mathbf{n}_z da - \int_{a_\alpha(z_1, t)} \mathbf{F}_\alpha \cdot \mathbf{n}_z da. \quad [\text{A.6}]$$

But, by the fundamental theorem of calculus,

$$\int_{a_\alpha(z_2, t)} \mathbf{F}_\alpha \cdot \mathbf{n}_z da - \int_{a_\alpha(z_1, t)} \mathbf{F}_\alpha \cdot \mathbf{n}_z da = \frac{\partial}{\partial z} \int_{\mathcal{V}_\alpha} \mathbf{F}_\alpha \cdot \mathbf{n}_z d\mathcal{V}, \quad [\text{A.7}]$$

and [A.6] reduces to

$$\int_{\mathcal{V}_\alpha} \nabla \cdot \mathbf{F}_\alpha d\mathcal{V} = \frac{\partial}{\partial z} \int_{\mathcal{V}_\alpha} \mathbf{F}_\alpha \cdot \mathbf{n}_z d\mathcal{V} + \int_{a_A} \mathbf{F}_\alpha \cdot \mathbf{n}_\alpha da. \quad [\text{A.8}]$$

Comparing [A.5] and [A.8] with [A.1] and [A.2] it can be seen that the former equations are a special case of the latter equations.

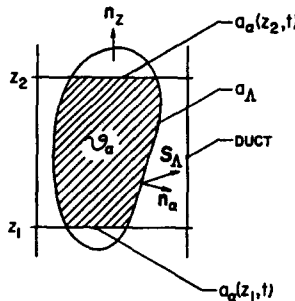


Figure 2. A simple case of two-phase flow through a duct.

APPENDIX B

The covariance coefficients

This appendix lists the covariance coefficients which appear in the paper.

$$c_{1\alpha} = \frac{\mathcal{V}_\alpha}{\mathcal{V}} \langle \rho_\alpha \mathbf{v}_\alpha \otimes \mathbf{v}_\alpha \rangle - \bar{\rho}_\alpha \tilde{\mathbf{v}}_\alpha \otimes \tilde{\mathbf{v}}_\alpha$$

$$c_{2\alpha} = \frac{\mathcal{V}_\alpha}{\mathcal{V}} \left\langle \rho_\alpha \left(\epsilon_\alpha + \frac{1}{2} \mathbf{v}_\alpha \cdot \mathbf{v}_\alpha \right) \mathbf{v}_\alpha \right\rangle - \bar{\rho}_\alpha \left(\tilde{\epsilon}_\alpha + \frac{1}{2} \tilde{\mathbf{v}}_\alpha \cdot \tilde{\mathbf{v}}_\alpha \right) \tilde{\mathbf{v}}_\alpha$$

$$c_{3\alpha} = \frac{\mathcal{V}_\alpha}{\mathcal{V}} \langle \mathbf{T}_\alpha^T \mathbf{v}_\alpha \rangle - \bar{\mathbf{T}}_\alpha^T \tilde{\mathbf{v}}_\alpha$$

$$c_{4\alpha} = \frac{\mathcal{V}_\alpha}{\mathcal{V}} \langle \rho_\alpha \mathbf{v}_\alpha \cdot \mathbf{b}_\alpha \rangle - \bar{\rho}_\alpha \tilde{\mathbf{v}}_\alpha \cdot \tilde{\mathbf{b}}_\alpha$$

$$c_{5\alpha} = \frac{\mathcal{V}_\alpha}{\mathcal{V}} \langle \rho_\alpha s_\alpha \mathbf{v}_\alpha \rangle - \bar{\rho}_\alpha \tilde{s}_\alpha \tilde{\mathbf{v}}_\alpha$$

$$c_{6\alpha} = \frac{\mathcal{V}_\alpha}{\mathcal{V}} \left\langle \frac{\mathbf{h}_\alpha}{\theta_\alpha} \right\rangle - \frac{\bar{\mathbf{h}}_\alpha}{\bar{\theta}_\alpha}$$

$$c_{7\alpha} = \frac{\mathcal{V}_\alpha}{\mathcal{V}} \left\langle \frac{\rho_\alpha r_\alpha}{\theta_\alpha} \right\rangle - \frac{\bar{\rho}_\alpha \tilde{r}_\alpha}{\bar{\theta}_\alpha}$$

In the above expressions, the density-weighted mean values and the mean values over the volume are defined respectively by

$$\tilde{f}_\alpha \equiv \frac{\langle \rho_\alpha f_\alpha \rangle}{\langle \rho_\alpha \rangle} = \frac{1}{\bar{\rho}_\alpha} \frac{\mathcal{V}_\alpha}{\mathcal{V}} \langle \rho_\alpha f_\alpha \rangle$$

$$\bar{f}_\alpha \equiv \frac{\mathcal{V}_\alpha}{\mathcal{V}} \langle f_\alpha \rangle$$

$$\bar{f}_\alpha \equiv \langle f_\alpha \rangle.$$

APPENDIX C

On the modeling of linear momentum supply or source $\hat{\mathbf{p}}_\alpha$ and its consequences

It is common in the two-phase flow modeling (see, for example, Ishii 1975) to perform a reduction of the linear momentum supply or source $\hat{\mathbf{p}}_\alpha$ expressed by [3.20] by decomposing the stress tensor $\mathbf{T}_{\alpha\delta}$ into the pressure $P_{\alpha\delta}$ and viscous stress $\tau_{\alpha\delta}$, i.e.

$$\mathbf{T}_{\alpha\delta} = -P_{\alpha\delta} \mathbf{I} + \tau_{\alpha\delta}. \quad [\text{C.1}]$$

Substituting for $\mathbf{F}_{\alpha\delta} = \mathbf{I}$ in [A.4] results in the following equation

$$\frac{1}{\mathcal{V}} \sum_\delta \int_{a,\delta} \mathbf{I}_{n_{\alpha\delta}} d\mathbf{a} = -\nabla \cdot \frac{1}{\mathcal{V}} \sum_\delta \int_{\mathcal{V}_{\alpha\delta}} \mathbf{I} d\mathcal{V} = -\nabla \left(\frac{\mathcal{V}_\alpha}{\mathcal{V}} \right). \quad [\text{C.2}]$$

Assuming that the pressure P_{ab} in [C.1] when integrated over the interfacial area is equal to an average interfacial pressure P_i and using above equations in [3.20] results in the following expression for $\hat{\mathbf{p}}_\alpha$:

$$\begin{aligned} \hat{\mathbf{p}}_\alpha &= -\hat{c}_\alpha \tilde{\mathbf{v}}_\alpha - \frac{1}{\mathcal{V}} \sum_\delta \int_{a_{\delta\delta}} (\dot{m}_{\alpha\delta} \mathbf{v}_{\alpha\delta} - \boldsymbol{\tau}_{\alpha\delta} \mathbf{n}_{\alpha\delta}) da \\ -\nabla \cdot \mathbf{C}_{1\alpha} + P_i \nabla \left(\frac{\mathcal{V}_\alpha}{\mathcal{V}} \right) &= \hat{\mathbf{p}}_\alpha^+ + P_i \nabla \left(\frac{\mathcal{V}_\alpha}{\mathcal{V}} \right). \end{aligned} \quad [\text{C.3}]$$

Equation [C.3] leads to important consequences when it is substituted into [3.19] and when the stress tensor $\hat{\mathbf{T}}_\alpha$ is assumed to be decomposed as follows:

$$\hat{\mathbf{T}}_\alpha \equiv -P_\alpha \left(\frac{\mathcal{V}_\alpha}{\mathcal{V}} \right) \mathbf{I} + \bar{\boldsymbol{\tau}}_\alpha \quad [\text{C.4}]$$

where P_α is the pressure and $\bar{\boldsymbol{\tau}}_\alpha$ is the viscous stress tensor for phase α . With these substitutions, [3.19] becomes

$$\bar{\rho}_\alpha \dot{\tilde{\mathbf{v}}}_\alpha = - \left(\frac{\mathcal{V}_\alpha}{\mathcal{V}} \right) \nabla P_\alpha + \nabla \cdot \bar{\boldsymbol{\tau}}_\alpha + \bar{\rho}_\alpha \hat{\mathbf{b}}_\alpha + \hat{\mathbf{p}}_\alpha^+ + (P_i - P_\alpha) \nabla \left(\frac{\mathcal{V}_\alpha}{\mathcal{V}} \right) \quad [\text{C.5}]$$

where $\hat{\mathbf{p}}_\alpha^+$ is defined by [C.3]. If, however, only the decomposition [C.4] is invoked in [3.19] then this equation is reduced to

$$\bar{\rho}_\alpha \dot{\tilde{\mathbf{v}}}_\alpha = - \nabla \left(P_\alpha \frac{\mathcal{V}_\alpha}{\mathcal{V}} \right) + \nabla \cdot \bar{\boldsymbol{\tau}}_\alpha + \bar{\rho}_\alpha \hat{\mathbf{b}}_\alpha + \hat{\mathbf{p}}_\alpha. \quad [\text{C.6}]$$

Equations [C.5] and [C.6] differ from each other in three important ways: (1) in [C.5] the volumetric fraction ($\mathcal{V}_\alpha/\mathcal{V}$) is outside of the gradient of pressure, whereas in [C.6] it is inside the gradient; (2) the two momentum supplies $\hat{\mathbf{p}}_\alpha$ and $\hat{\mathbf{p}}_\alpha^+$ are defined differently (cit. [C.3]) and, therefore, are expected to be represented by different constitutive equations; and (3) [C.5] contains the effect associated with the imbalance of pressures across the interfaces. In the two-phase flow modeling it is usually assumed that $P_i = P_\alpha$ and argued on physical grounds that [C.5] is a better equation to use than [C.6] (Harlow & Amsden 1975; Lyczkowski *et al.* 1978, among others). Equation [C.5] was also used by Homsy (1983) with $P_i = P_{\text{fluid}}$ in modeling the fluid-particle suspensions.

Lyczkowski *et al.* (1978) used [C.5] and [C.6] with $P_i = P_\alpha = P(\nabla \cdot \bar{\boldsymbol{\tau}}_\alpha$ was modelled through a wall shear stress term) to study the stability properties. They also assumed that the linear momentum supplies or sources $\hat{\mathbf{p}}_\alpha$ and $\hat{\mathbf{p}}_\alpha^+$ are equal to each other and that they can be modeled through a relative velocity effect (the viscous drag force) and a relative acceleration effect (the virtual mass force). The study showed that the solution space with real characteristics is larger for [C.6] than for [C.5] and that both equations yield in some solution domain the complex characteristics. The real characteristics are necessary (but not sufficient) for a well-posed initial value problem, while the complex characteristics produce an ill-posed initial value problem that is unsatisfactory because all finite difference schemes consistent with the differential equations are unstable (Richtmyer & Morton 1967).

The above controversy in modeling the momentum equation can be due to the premature assumptions invoked in modeling the momentum supply or source $\hat{\mathbf{p}}_\alpha$ and stress tensor $\hat{\mathbf{T}}_\alpha$ in equation [3.19]. A reasonable way to construct the constitutive equations for

these variables is to require that they depend on the kinematical variables appearing in the conservation and balance equations and demanding then that such a constitutive assumption should be consistent with a change of frame transformation. In section 5 of the paper this procedure is indeed followed, and in Dobran (1984) the constitutive equations for a multiphase mixture of fluids are studied in greater detail.