Int. J. Engng Sci. Vol. 30, No. 10, pp. 1497–1505, 1992
Printed in Great Britain. All rights reserved

0020-7225/92 $5.00 + 0.00
Copyright © 1992 Pergamon Press Ltd

MODELING OF STRUCTURED MULTIPHASE MIXTURES

FLAVIO DOBRAN
Applied Science Department, New York University, New York, NY 10003, U.S.A.

Abstract—The usual modeling of multiphase mixtures involves a basic set of balance equations of mass, momentum, energy and entropy which are constructed by an averaging procedure or postulated. In modeling the structured multiphase mixtures, the intrinsic motion of particles can be described by an additional set of balance equations. Fundamental to the construction of the structured models of mixtures are the problems pertaining to the existence and number of these additional balance equations. By using the volume averaging procedure it is possible not only to derive the basic set of field equations, but also a very general set of additional balance equations which account for such properties as particle dilatation and rotation, demonstrating that the existing structured models of multiphase mixtures are very special cases of the material deformation.

1. INTRODUCTION

A multiphase mixture is characterized by the well-defined interfacial areas between the constituents of the mixture, with each phase having a smoothly varying chemical composition and steep gradients of properties close to the interface. In the mathematical modeling of such mixtures it should be, therefore, reasonable to employ the continuum field equations in each phase and provide the boundary conditions between the phases by another set of continuum field equations derived on the assumption that the interface can be modeled as a surface of discontinuity. The complexity of the continuum field equations and large number of interfaces which are commonly present in real multiphase flows prohibit, however, this modeling approach in favor of a more practical one.

The postulatory theories of mixtures and the theories of mixtures based on the averaging procedures are the superimposed continua models which ignore the three-dimensional interfacial structure in modeling multiphase flows. The former theories are based on various postulates and their motivation comes from the single phase multicomponent mixture theories, generalized variational approaches, and special models of the material deformation (Goodman and Cowin [1], Passman [2], Bedford and Drumheller [3], and Ahmadi [4], among others). These postulatory theories employ both the basic set of field equations (mass, momentum, energy and entropy) and an *additional* set of balance equations to model the structural properties of mixtures without accounting for the detailed motions of interfaces. The averaging theories of multiphase mixtures employ time or spatial averaging of local macroscopic field equations of each phase and account for the structural properties of mixtures through the constitutive equations (Drew [5], Ishii [6], Nigmatulin [7], Hassanizadeh and Gray [8], Celmins and Schmitt [9], Dobran [10]). As discussed by Dobran [11], the time averaging procedure has a drawback of not clearly separating turbulence from other structural effects of the mixture and it precludes a consistent utilization of the principle of material frame indifference on the averaged field equations which is a very powerful tool to study constitutive equations. Except for the volume averaging procedure, other spatial averaging approaches introduce nonremovable singularities into the models and consequently are not as suitable as the volume averaging approach to construct a consistent theory of mixtures.

In this paper a structured theory of multiphase mixtures (Dobran [11]) based on the volume averaging approach will be outlined. The utilization of the volume averaging procedure to construct a theory of multiphase mixtures strongly motivates the construction of a *physical theory* of mixtures, since it employs the well-established macroscopic field equations of each phase of the mixture. By adjoining to this procedure a basic deformation principle relating an

assumption of the motion of material particles relative to the center of mass it can then be shown that the resulting theory not only provides the basic set of field equations of multiphase mixtures, but also additional transport equations for modeling the structural characteristics of the mixture. The theory constructed in this manner reduces to the previous models of postulatory and averaged theories of mixtures only after considerably relaxing the material deformation assumption. The discussion of many details of the theory and results on constitutive equations is beyond the space limitations of this paper and the reader is urged to consult Dobran [11] for details.

2. BASIC FIELD EQUATIONS OF MULTIPHASE MIXTURES

2.1 Basic definitions and volume averaging procedure

The volume averaging procedure consists of averaging the macroscopic field equations of each phase (mass, momentum, energy and entropy) over an arbitrary fixed volume in space. Figure 1 illustrates a flow field in an Euclidean space $\mathscr{E}_0^3$ which consists of homogeneous continua or phases $\alpha = 1, \ldots, \gamma$. With each phase α is identified a subvolume $U^{(\alpha\delta)}$ which moves through space and changes with time as a result of mass, momentum, and energy transfer processes taking place within the mixture. At some initial time t_0 this volume is identified as $V^{(\alpha\delta)}$. The surface of the volume $U^{(\alpha\delta)}$ is denoted by $A^{(\alpha\delta)}$ which has a unit normal vector $\mathbf{n}^{(\alpha\delta)}$ and velocity $\mathbf{S}^{(\Lambda\delta)}$. A material point P of phase α is located within $\mathrm{d}U^{(\alpha\delta)}$ in the *spatial configuration* and within $\mathrm{d}V^{(\alpha\delta)}$ in the *reference configuration* or in an undeformed and unstressed state of the multiphase mixture where the point P is located by its spatial position vector $\mathbf{X}^{(\alpha\delta)}$. As the material undergoes mechanical and thermal deformations, the material point P moves to a position $\mathbf{x}^{(\alpha\delta)}$. The position vectors $\mathbf{X}^{(\alpha)}$ and $\mathbf{x}^{(\alpha)}$ denote the *center of mass positions of phase* α in the reference and spatial configurations, respectively, and the position vectors $\mathbf{\Sigma}^{(\alpha\delta)}$ and $\boldsymbol{\xi}^{(\alpha\delta)}$ represent the positions of the point P *relative to the center of mass* as shown in Fig. 1.

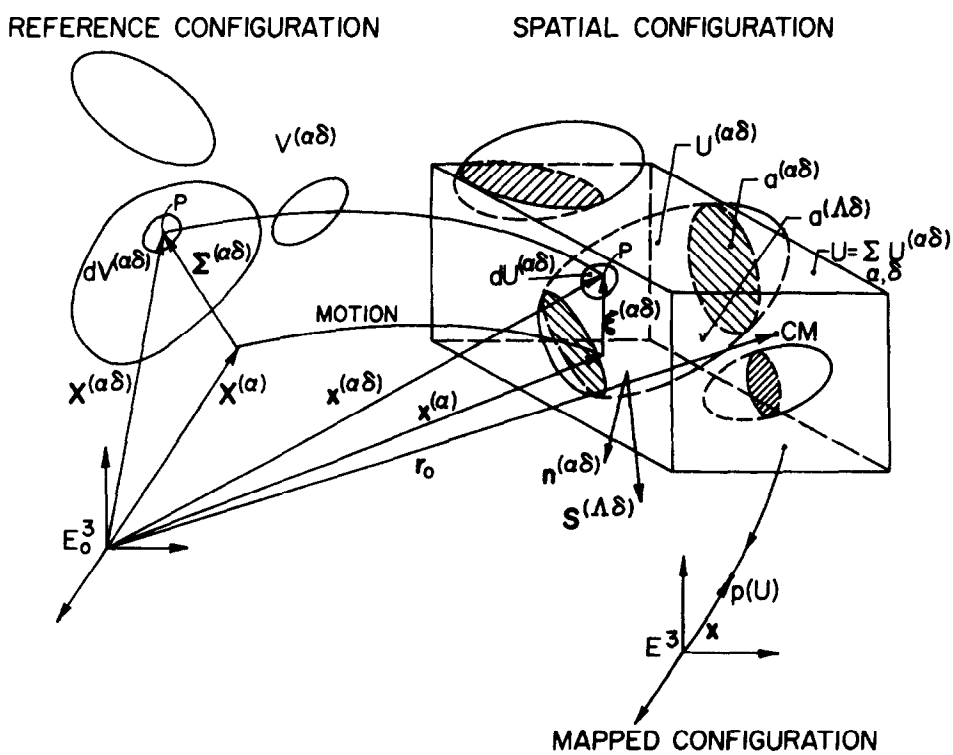

Fig. 1. Representation of a multiphase mixture in reference, spatial, and mapped configurations.

For each phase α and volume $U^{(\alpha\delta)}$, use may be made of the local macroscopic conservation and balance equations of mass, momentum, energy and entropy for the non-polar media (see, for example, Eringen [12]) which may be expressed in the following compact form:

$$\frac{\partial}{\partial t}(\rho^{(\alpha\delta)}\boldsymbol{\Psi}^{(\alpha\delta)}) + \nabla^0 \cdot (\rho^{(\alpha\delta)}\boldsymbol{\Psi}^{(\alpha\delta)}\mathbf{v}^{(\alpha\delta)}) + \nabla^0 \cdot \mathbf{J}^{(\alpha\delta)} - \rho^{(\alpha\delta)}\boldsymbol{\Phi}^{(\alpha\delta)} = \rho^{(\alpha\delta)}\mathbf{B}^{(\alpha\delta)} \tag{1}$$

where $\boldsymbol{\Psi}^{(\alpha\delta)}$, $\mathbf{J}^{(\alpha\delta)}$, $\boldsymbol{\Phi}^{(\alpha\delta)}$ and $\mathbf{B}^{(\alpha\delta)}$ are variables which depend on the particular conservation and balance law and are given in Table 1. ∇^0 is the gradient operator which operates in the space $\mathscr{E}_0^3$, $\rho^{(\alpha\delta)}$ is the mass density, $\mathbf{v}^{(\alpha\delta)}$ is the velocity, $\epsilon^{(\alpha\delta)}$ is the internal energy, $s^{(\alpha\delta)}$ is the entropy, $\mathbf{T}^{(\alpha\delta)}$ is the stress tensor, $\mathbf{q}^{(\alpha\delta)}$ is the heat flux vector, $r^{(\alpha\delta)}$ is the heat generation rate, $\mathbf{b}^{(\alpha\delta)}$ is the body force per unit mass, and $\theta^{(\alpha\delta)}$ is the temperature of a material point of phase α contained in $U^{(\alpha\delta)}$. Assuming that the interface can be modeled as a surface of discontinuity, use can also be made of the following *jump or boundary conditions* (Eringen [12]) when equation (1) is integrated over an averaging volume.

$$(m^{(\alpha\delta)}\boldsymbol{\Psi}^{(\alpha\delta)} + \mathbf{J}^{(\alpha\delta)}\mathbf{n}^{(\alpha\delta)}) + (m^{(\beta\eta)}\boldsymbol{\Psi}^{(\beta\eta)} + \mathbf{J}^{(\beta\eta)}\mathbf{n}^{(\beta\eta)}) = \boldsymbol{\Delta}^{(\alpha\delta)} \tag{2}$$

where

$$m^{(\alpha\delta)} = \rho^{(\alpha\delta)}(\mathbf{v}^{(\alpha\delta)} - \mathbf{S}^{(\Lambda\delta)}) \cdot \mathbf{n}^{(\alpha\delta)} \tag{3}$$

is the interphase mass transfer rate and $\boldsymbol{\Delta}^{(\alpha\delta)}$ is the interfacial source term. This source term is given in Table 1 for the case of surface tension force, with ∇_s^0 representing the surface gradient operator and ν representing the surface tension coefficient. Notice in equations (2) and (3) that $\alpha \neq \beta$, $\mathbf{n}^{(\alpha\delta)} = -\mathbf{n}^{(\beta\eta)}$ and $\mathbf{S}^{(\Lambda\delta)} = \mathbf{S}^{(\beta\eta)}$ for a subvolume δ of phase α in contact with a subvolume η of phase β. The condition $\zeta^{(\alpha\delta)} \geq 0$ represents the *local axiom of dissipation* normally adopted in single phase models of continua (Truesdell and Noll [13]) and used in the present theory.

The volume averaging procedure involves selecting an *arbitrary fixed volume in space U* as illustrated in Fig. 1 and averaging equation (1) over all subvolumes $U^{(\alpha\delta)}$ of phase α in the volume $U_\alpha = \sum_\delta U^{(\alpha\delta)}$ of phase α which is contained within U. The surface of $U^{(\alpha\delta)}$ which is fully contained within U is denoted by $a^{(\Lambda\delta)}$, whereas the surface of intersection of $U^{(\alpha\delta)}$ with U is denoted by $a^{(\alpha\delta)}$. The volume averaging procedure is then expressed by

$$\sum_\delta \int_{U^{(\alpha\delta)}} (\text{equation (1)})\, \mathrm{d}U = 0 \tag{4}$$

and has the property of mapping the entire contents of the flow field at time t in the averaging volume located in the spatial configuration into a point $p(U)$ located at $\mathbf{x}$, such that the mapped configuration space $\mathscr{E}^3$ (to which $\mathbf{x}$ belongs) is the *subspace* of $\mathscr{E}_0^3$ as schematically illustrated in Fig. 1.

2.2 *The general phasic equation of balance and basic field equations of multiphase mixtures*

Carrying out the procedure as expressed by equation (4) and using the Leibnitz's and Divergence Theorems to interchange the integration and differentiation operators yields the

Table 1. Coefficients of the conservation and balance equations

Conservation or balance of	$\boldsymbol{\Psi}^{(\alpha\delta)}$	$\mathbf{J}^{(\alpha\delta)}$	$\boldsymbol{\Phi}^{(\alpha\delta)}$	$\mathbf{B}^{(\alpha\delta)}$	$\boldsymbol{\Delta}^{(\alpha\delta)}$
Mass	1	O	O	O	O
Linear momentum	$\mathbf{v}^{(\alpha\delta)}$	$-\mathbf{T}^{(\alpha\delta)}$	$\mathbf{b}^{(\alpha\delta)}$	O	$(\boldsymbol{\Delta}_m)^{(\alpha\delta)} = (2H\nu\mathbf{n} + \nabla_s\nu)^{(\alpha\delta)}$
Angular momentum	$\mathbf{r} \wedge \mathbf{v}^{(\alpha\delta)}$	$-\mathbf{r} \wedge \mathbf{T}^{(\alpha\delta)}$	$\mathbf{r} \wedge \mathbf{b}^{(\alpha\delta)}$	O	$\mathbf{r} \wedge (\boldsymbol{\Delta}_m)^{(\alpha\delta)}$
Energy	$\epsilon^{(\alpha\delta)} + \frac{1}{2}\mathbf{v}^{(\alpha\delta)} \cdot \mathbf{v}^{(\alpha\delta)}$	$\mathbf{q}^{(\alpha\delta)} - \mathbf{T}^{(\alpha\delta)T}\mathbf{v}^{(\alpha\delta)}$	$\mathbf{b}^{(\alpha\delta)} \cdot \mathbf{v}^{(\alpha\delta)}$	$r^{(\alpha\delta)}$	$(\Delta_\epsilon)^{(\alpha\delta)} = (2H\nu\mathbf{n} \cdot \mathbf{S} + \nabla_s\nu\mathbf{S} + \nu\,\nabla_s \cdot \mathbf{S})^{(\alpha\delta)}$
Entropy	$s^{(\alpha\delta)}$	$\frac{\mathbf{h}^{(\alpha\delta)}}{\theta^{(\alpha\delta)}}$	$\frac{r^{(\alpha\delta)}}{\theta^{(\alpha\delta)}}$	$\zeta^{(\alpha\delta)} \geq 0$	$(\Delta_s)^{(\alpha\delta)} \geq 0$

general equation of balance of phase α

$$\frac{\partial}{\partial t} U_\alpha \langle \rho_\alpha \mathbf{\Psi}_\alpha \rangle + \nabla \cdot U_\alpha \langle \rho_\alpha \mathbf{\Psi}_\alpha \mathbf{v}_\alpha \rangle + \nabla \cdot U_\alpha \langle \mathbf{J}_\alpha \rangle - U_\alpha \langle \rho_\alpha \mathbf{\Phi}_\alpha \rangle - U_\alpha \langle \rho_\alpha \mathbf{B}_\alpha \rangle$$

$$= -\sum_\delta \int_{a^{(\Lambda\delta)}} (m^{(\alpha\delta)} \mathbf{\Psi}^{(\alpha\delta)} + \mathbf{J}^{(\alpha\delta)} \mathbf{n}^{(\alpha\delta)})\, \mathrm{d}a \tag{5}$$

where the volume-averaged quantities are defined as follows:

$$\langle F_\alpha \rangle = \frac{1}{U_\alpha} \sum_\delta \int_{U^{(\alpha\delta)}} F^{(\alpha\delta)}\, \mathrm{d}U \tag{6}$$

In the discussion to follow use will also be made of the *density-weighted average variables*, $\tilde{F}_\alpha$, *partial variables*, $\bar{F}_\alpha$, and *phase average variables*, $\bar{\bar{F}}_\alpha$, i.e.

$$\tilde{F}_\alpha = \frac{\langle \rho_\alpha F_\alpha \rangle}{\langle \rho_\alpha \rangle} = \frac{1}{\bar{\rho}_\alpha} \frac{U_\alpha}{U} \langle \rho_\alpha F_\alpha \rangle \tag{7}$$

$$\bar{F}_\alpha = \frac{U_\alpha}{U} \langle F_\alpha \rangle \tag{8}$$

$$\bar{\bar{F}}_\alpha = \langle F_\alpha \rangle \tag{9}$$

The *partial density of phase* α is defined as

$$\bar{\rho}_\alpha = \frac{U_\alpha}{U} \langle \rho_\alpha \rangle \tag{10}$$

whereas the *mixture density* is obtained by summing up the partial densities of phases, i.e.

$$\rho = \sum_\alpha \bar{\rho}_\alpha \tag{11}$$

The *velocity of phase* α, $\tilde{\mathbf{v}}_\alpha$, and the *mixture velocity*, $\mathbf{v}$, are defined as

$$\tilde{\mathbf{v}}_\alpha = \frac{1}{\bar{\rho}_\alpha} \frac{U_\alpha}{U} \langle \rho_\alpha \mathbf{v}_\alpha \rangle \tag{12}$$

$$\rho \mathbf{v} = \sum_\alpha \bar{\rho}_\alpha \tilde{\mathbf{v}}_\alpha \tag{13}$$

The above definition of phase velocity as the density-weighted velocity can be motivated by specializing equation (5) for the case of conservation of mass from Table 1, i.e.

$$\frac{\partial \bar{\rho}_\alpha}{\partial t} + \nabla \cdot \bar{\rho}_\alpha \tilde{\mathbf{v}}_\alpha = \grave{\bar{\rho}}_\alpha + \bar{\rho}_\alpha \nabla \cdot \tilde{\mathbf{v}}_\alpha = \hat{c}_\alpha \tag{14}$$

where the backward prime affixed to $\bar{\rho}_\alpha$ indicates the *material derivative* following the motion of the αth phase. The mass source term $\hat{c}_\alpha$ represents the effect of phase change or chemical reactions and is expressed as

$$\hat{c}_\alpha = -\frac{1}{U} \sum_\delta \int_{a^{(\Lambda\delta)}} m^{(\alpha\delta)}\, \mathrm{d}a \tag{15}$$

The conservation of mass equation for the mixture as a whole is obtained by summing over α equation (14) and requiring that the mass sources satisfy $\sum_\alpha \hat{c}_\alpha = 0$. Thus

$$\dot{\rho} + \rho \nabla \cdot \mathbf{v} = 0 \tag{16}$$

where the dot over ρ denotes the material derivative of ρ following the motion of the mixture with velocity $\mathbf{v}$.

The linear momentum balance of phase α is obtained from equation (5) and Table 1, i.e.

$$\bar{\rho}_\alpha \dot{\bar{\mathbf{v}}}_\alpha = \nabla \cdot \bar{\mathbf{T}}_\alpha + \bar{\rho}_\alpha \bar{\mathbf{b}}_\alpha + \hat{\mathbf{p}}_\alpha \tag{17}$$

where $\hat{\mathbf{p}}_\alpha$ is the *linear momentum supply or source* representing the momentum interaction between the phases as a result of mass transfer, interfacial forces, and structural characteristics of the mixture (see Dobran [11]).

The angular momentum balance of phase α represents the nonsymmetry of the phasic stress tensor $\bar{\mathbf{T}}_\alpha$ and can be written as

$$\hat{\mathbf{M}}_\alpha = \bar{\mathbf{T}}_\alpha - \bar{\mathbf{T}}_\alpha^T \tag{18}$$

where the superscript T over $\bar{\mathbf{T}}_\alpha$ represents the transpose operation. The nonsymmetry of the stress tensor can be produced by particle spins, couple stresses, and body moments.

The internal energy balance of phase α is obtained from Table 1 and equation (5), i.e.

$$\bar{\rho}_\alpha \dot{\bar{\epsilon}}_\alpha = \mathrm{tr}(\bar{\mathbf{T}}_\alpha^T \nabla \bar{\mathbf{v}}_\alpha) - \nabla \cdot \bar{\mathbf{q}}_\alpha + \bar{\rho}_\alpha \bar{r}_\alpha + \hat{\epsilon}_\alpha \tag{19}$$

where the *energy source* $\hat{\epsilon}_\alpha$ results from interphase interactions and structural properties of the mixture (see Dobran [11] for a detailed expression).

The role of entropy in continuum mechanics is debatable and especially in mixture theories. Single phase multicomponent mixture theory (Bowen [14]) requires only the satisfaction of the *global axiom of dissipation* or entropy inequality for the mixture as a whole, with the same rule being adopted in the construction of the postulatory theory of multiphase mixtures (Passman [2]). In the theory of multiphase mixtures which is *consistent* with volume averaging of local macroscopic field equations where the local axiom of dissipation has proven very useful in modeling, it should thus be legitimate to state that each sub-body δ of phase α produces $\zeta^{(\alpha\delta)} \geq 0$ as stated in Table 1. From this table and equation (5), the entropy inequality for each phase can thus be established as

$$\bar{\rho}_\alpha \dot{\bar{s}}_\alpha + \nabla \cdot \left(\frac{\bar{\mathbf{q}}_\alpha}{\bar{\bar{\theta}}_\alpha} \right) - \frac{\bar{\rho}_\alpha \bar{r}_\alpha}{\bar{\bar{\theta}}_\alpha} + \hat{c}_\alpha \bar{s}_\alpha + \hat{s}_\alpha \geq 0 \tag{20}$$

where $\hat{s}_\alpha$ is the *entropy source of phase* α arising from interphase entropy transfer and structural characteristics of the mixture. This entropy source is not necessarily positive semidefinite.

When the momentum, energy and entropy equations (17), (19) and (20) are summed over α to obtain the balance of linear momentum, energy and entropy for the mixture as a whole, the momentum, energy and entropy source terms ($\hat{\mathbf{p}}_\alpha$, $\hat{\epsilon}_\alpha$ and $\hat{s}_\alpha$) do not necessarily add to zero as required in the single phase flow multicomponent theory of mixtures (Bowen [14]). The reason for this is that the mixture source terms in the present theory include the *nonlocal* effect as brought about by the volume averaging process and can be considered as the structural effect of multiphase mixture. This structural characteristics of the mixture can be seen more clearly by introducing an assumption of material deformation relative to the center of mass of each phase as discussed in the following section.

3. THE MATERIAL DEFORMATION ASSUMPTION AND ADDITIONAL BALANCE EQUATIONS OF MULTIPHASE MIXTURES

The single phase micromorphic theory of Eringen [15] and Twiss and Eringen [16] rests on a basic material deformation postulate. The construction of a structured theory of multiphase mixtures may also be based on a similar material deformation assumption where the material particles of each phase relative to the center of mass undergo a homogeneous deformation

expressed by the following equations:

$$\xi_k^{(\alpha\delta)} = \Pi_{kK}^{(\alpha)}\Sigma_K^{(\alpha\delta)} \tag{21}$$

$$\Sigma_K^{(\alpha\delta)} = \Xi_{Kk}^{(\alpha)}\xi_k^{(\alpha\delta)} \tag{22}$$

This material deformation assumption implies that the motion of material of phase α is comprised of an arbitrary deformation of the center of mass, a rotation of the mass points about the center of mass, and an affine deformation of material particles relative to the center of mass carrying ellipsoids into ellipsoids.

Differentiating equation (21) it can then be shown that

$$\dot{\xi}_k^{(\alpha\delta)} = \dot{\Pi}_{kK}^{(\alpha)}\Sigma_K^{(\alpha\delta)} = \dot{\Pi}_{kK}^{(\alpha)}\Xi_{Kl}^{(\alpha)}\xi_l^{(\alpha\delta)} = \nu_{kl}^{(\alpha)}\xi_l^{(\alpha\delta)} \tag{23}$$

where $\nu_{kl}^{(\alpha)}$ is the *gyration tensor*. If $\nu_{kl}^{(\alpha)}$ is a skew-symmetric tensor, equation (23) then represents a *rotation* of material particles relative to the center of mass, whereas if $\nu_{kl}^{(\alpha)} = \delta_{ij}f(\mathbf{x}, t)$ then this tensor represents pure dilatation or stretching. Using equation (23),

$$\mathbf{v}^{(\alpha\delta)} = \left(\frac{\partial \mathbf{x}^{(\alpha\delta)}}{\partial t}\right)_{\mathbf{x}^{(\alpha\delta)}}, \qquad \mathbf{v}^{(\alpha)} = \left(\frac{\partial \mathbf{x}^{(\alpha)}}{\partial t}\right)_{\mathbf{x}^{(\alpha)}} \tag{24}$$

and

$$\mathbf{x}^{(\alpha\delta)} = \mathbf{x}^{(\alpha)} + \boldsymbol{\xi}^{(\alpha\delta)} \tag{25}$$

(see Fig. 1) gives a relation between the velocity of a particle of phase α, $\mathbf{v}^{(\alpha\delta)}$, and the center of mass velocity of the same phase, $\mathbf{v}^{(\alpha)}$, i.e.

$$v_k^{(\alpha\delta)} = v_k^{(\alpha)} + \nu_{kl}^{(\alpha\delta)}\xi_l^{(\alpha\delta)} \tag{26}$$

Multiplying this equation by $\rho^{(\alpha\delta)}$ and integrating over the volume of phase α contained in the averaging volume U as shown in Fig. 1 gives

$$\mathbf{v}^{(\alpha)} = \bar{\mathbf{v}}_\alpha \tag{27}$$

since the *center of mass of phase* α is defined by the following relation:

$$\sum_\delta \int_{U^{(\alpha\delta)}} \rho^{(\alpha\delta)}\xi_l^{(\alpha\delta)}\,\mathrm{d}U = 0 \tag{28}$$

Similarly, it can also be shown that

$$\mathbf{a}^{(\alpha)} = \dot{\bar{\mathbf{v}}}_\alpha \tag{29}$$

Thus the density-weighted velocities and accelerations of each phase are equal to the corresponding velocities and accelerations of the center of mass. These results are clearly a consequence of the material deformation assumption and do not follow directly from the volume averaging procedure. In this way the position $\mathbf{x}$ in the mapped configuration space in Fig. 1 may be associated with the center of mass of the mixture in the averaging volume U.

The material deformation assumption expressed by equation (21) allows for the derivation of additional balance equations of multiphase mixtures for modeling the structural properties of the mixture. The *balance equation for the equilibrated inertia* is obtained by taking a moment about the center of mass of the conservation of mass equation (1) and performing volume averaging of the resulting expression, i.e.

$$\sum_\delta \int_{U^{(\alpha\delta)}} \xi_k^{(\alpha\delta)}\xi_l^{(\alpha\delta)}\left(\frac{\partial}{\partial t}\rho^{(\alpha\delta)} + \frac{\partial}{\partial x_m^{(\alpha\delta)}}\rho^{(\alpha\delta)}v_m^{(\alpha\delta)}\right)\mathrm{d}U = 0 \tag{30}$$

or after some algebraic manipulations as described in Dobran [11], we obtain

$$\bar{\rho}_\alpha(\dot{\bar{i}}_{\alpha kl} - \nu_{km}^{(\alpha)}\bar{i}_{\alpha ml} - \nu_{lm}^{(\alpha)}\bar{i}_{\alpha km}) = -\hat{c}_\alpha(\bar{i}_{\alpha kl} - \hat{i}_{\alpha kl}) - (\bar{\rho}_\alpha\hat{I}_{\alpha mkl})_{,m} \tag{31}$$

where $\bar{i}_{\alpha kl}$ is the *equilibrated inertia* of phase α defined by

$$\bar{i}_{\alpha kl} = \frac{1}{\bar{\rho}_\alpha}\frac{1}{U}\sum_\delta \int_{U^{(\alpha\delta)}} \rho^{(\alpha\delta)}\xi_k^{(\alpha\delta)}\xi_l^{(\alpha\delta)}\,\mathrm{d}U \tag{32}$$

and $\hat{i}_{\alpha kl}$ and $\hat{I}_{\alpha mkl}$ are the *equilibrated source inertia* and *hyperinertia tensor,* respectively (see [11] for definitions) that must be determined by the constitutive equations.

A *balance equation for the equilibrated moments* is obtained by taking a moment of the momentum equation (1) and integrating over the volume of phase α in the averaging volume U, i.e.

$$\sum_{\delta} \int_{U^{(\alpha\delta)}} x_j^{(\alpha\delta)} \left[\frac{\partial}{\partial t} \rho^{(\alpha\delta)} v_k^{(\alpha\delta)} + \frac{\partial}{\partial x_m^{(\alpha\delta)}} \rho^{(\alpha\delta)} v_k^{(\alpha\delta)} v_m^{(\alpha\delta)} - T_{kl,l}^{(\alpha\delta)} - \rho^{(\alpha\delta)} b_k^{(\alpha\delta)} \right] \mathrm{d}U = 0 \tag{33}$$

producing:

$$\bar{\rho}_\alpha \bar{i}_{\alpha jn} (\dot{v}_{kn}^{(\alpha)} + v_{km}^{(\alpha)} v_{mn}^{(\alpha)}) = \bar{S}_{\alpha jk} + \bar{\rho}_\alpha \bar{l}_{\alpha jk} + \bar{\lambda}_{\alpha jkm,m} - \bar{\rho}_\alpha v_{kn,m}^{(\alpha)} \hat{I}_{\alpha mjn} - \bar{\rho}_\alpha v_{mq}^{(\alpha)} \bar{v}_{\alpha k,m} \bar{i}_{\alpha jq} \tag{34}$$

In this equation $\bar{l}_{\alpha jk}$ is the *body force moment*

$$\bar{l}_{\alpha jk} = \frac{1}{\bar{\rho}_\alpha} \frac{1}{U} \sum_{\delta} \int_{U^{(\alpha\delta)}} \rho^{(\alpha\delta)} \xi_j^{(\alpha\delta)} b_k^{(\alpha\delta)} \, \mathrm{d}U \tag{35}$$

$\bar{\lambda}_{\alpha jkm}$ is the *intrinsic stress moment*

$$\bar{\lambda}_{\alpha jkm} = \frac{1}{U} \sum_{\delta} \int_{U^{(\alpha\delta)}} \xi_j^{(\alpha\delta)} T_{km}^{(\alpha\delta)} \, \mathrm{d}U \tag{36}$$

and $\bar{S}_{\alpha jk}$ is the *surface traction moment* defined by

$$\bar{S}_{\alpha jk} = \frac{1}{U} \sum_{\delta} \int_{a^{(\Lambda\delta)}} \xi_j^{(\alpha\delta)} T_{km}^{(\alpha\delta)} n_m^{(\alpha\delta)} \, \mathrm{d}a \tag{37}$$

that must be specified by the constitutive equations.

The balance equations for the equilibrated inertia and moments reveal the structural properties of the mixture. They arise when the local force balance equation in each phase, representing the continuous distribution of forces, is replaced by an averaged equation. This result is thus consistent with the particle mechanics where the forces acting on a collection of particles may be replaced by a resultant force and a resultant couple. The extrinsic forces acting on the entire set of particles are thus replaced by a resultant body force $\bar{\mathbf{b}}_\alpha$ and a resultant couple $\bar{\mathbf{l}}_\alpha$, whereas the forces acting on the surface of U_α are replaced by a resultant surface traction force $\bar{\mathbf{T}}_\alpha \mathbf{n}_\alpha$ and a couple $\bar{\mathbf{S}}_\alpha$. In a continuum of each phase, the interparticle forces cancel out by Newton's third law of action and reaction and there is no net resultant force. When a particle of small volume is isolated from the body, however, the internal forces produce a stress and a couple stress when the effect of the body on particle is considered in terms of the resultant forces and couples. The result of this, in the averaged field equations, is the existence of the stress field $\bar{\mathbf{T}}_\alpha$ and of a hyperstress field $\bar{\boldsymbol{\lambda}}_\alpha$.

The basic deformation assumption expressed by equation (21) also allows the momentum, energy and entropy sources ($\hat{\mathbf{p}}_\alpha$, $\hat{\epsilon}_\alpha$ and $\hat{s}_\alpha$) to be expressed in terms of the structural properties of the mixture. Since these results are rather complicated, the reader is referred to Dobran [11] for details.

4. DISCUSSION

The theory of multiphase mixtures outlined above reproduces the basic and additional balance equations of the averaged and postulatory theories of mixtures when the material deformation assumption expressed by equation (21) is simplified. A simple example of an affine deformation consists of rotation and dilatation which may be expressed as follows:

$$v_{ij}^{(\alpha)} = \hat{v}_{ij}^{(\alpha)} + \dot{\phi}_\alpha \delta_{ij} \tag{38}$$

where $\grave{\phi}_\alpha$ denotes the material derivative of a function ϕ_α of phase α expressing the dilatational rate, whereas $\hat{v}_{ij}^{(\alpha)}$ is a skew-symmetric tensor expressing the rotational effect, i.e.

$$\hat{v}_{ij}^{(\alpha)} = -\hat{v}_{ji}^{(\alpha)}, \qquad \hat{v}_{ii}^{(\alpha)} = 0 \tag{39}$$

The function ϕ_α representing the dilatation or stretching effect may be assumed to be the *volumetric fraction* of phase α in the averaging volume U. Such an association is clearly a constitutive assumption and may not be a valid choice as discussed below.

Assuming the validity of the decomposition expressed by equation (38), setting ϕ_α to be equal to the volumetric fraction of phase α, ignoring the rotational effect, and assuming that the *inertia tensor is isotropic*, i.e.

$$\tilde{i}_{\alpha ij} = \tilde{i}_\alpha \delta_{ij} \tag{40}$$

produces the basic and additional balance equations which are consistent with the *postulatory* theories of multiphase mixtures. This consistency is particularly strong with the most developed theory of structured mixtures as proposed by Goodman and Cowin [1] and subsequently refined by Passman [2], and demonstrates that this theory has an existence within the volume averaging and very special assumption of the material deformation relative to the center of mass. This special theory has, however, a fundamental defect which is not apparent until a consideration is given to the *theory of constraints* of multiphase mixtures. This theory basically violates the incompressibility constraint

$$\check{W}_\alpha = p_\alpha\left(\grave{\phi}_\alpha + \phi_\alpha \nabla \cdot \tilde{\mathbf{v}}_\alpha - \frac{\hat{c}_\alpha}{\bar{\rho}_\alpha}\right) \tag{41}$$

of the work expended per unit volume in phase α due to this constraint which is required to vanish for all hydrostatic pressures p_α. The details of this proof are somewhat long and will not be presented here. To resolve this problem it is only *sufficient* to revise the (somewhat arbitrary) assumption of the material deformation expressed by equation (38) to the following:

$$v_{ij}^{(\alpha)} = \hat{v}_{ij}^{(\alpha)} + \frac{\grave{\phi}_\alpha}{\phi_\alpha}\delta_{ij} \tag{42}$$

where $\grave{\phi}_\alpha/\phi_\alpha$ now represents the effect of dilatation.

Based on the assumption expressed by equation (42) it is then possible to develop linear and nonlinear constitutive equations of compressible, incompressible, fluid and solids multiphase mixtures, with and without the dilatational and rotational effects of material particles relative to the center of mass of each phase. Such a study, which also involves a detailed discussion of the concepts and principles of the constitutive theory, is presented by Dobran [11] and will not be repeated here. In the following I will only discuss some of the fundamental results to illustrate the capability of the presented theory to reproduce some well-known results of multiphase flows and its ability to predict novel phenomena.

A linearized theory of constitutive equations for isotropic mixtures of fluids without the phase change can reproduce the Rayleigh-type bubble equation when the bubble volumetric fraction in a two-phase mixture is very small, i.e.

$$\bar{\pi}_1 - \bar{\pi}_2 = \beta_1 - \beta_2 + \bar{\rho}_2 R\ddot{R} + 2\bar{\rho}_2\dot{R}\dot{R} + \frac{4\mu_2^*}{R}\dot{R} + i^* - \grave{\bar{\rho}}_2 R\dot{R} \tag{43}$$

where $\bar{\pi}$ is the pressure, $\beta_1 - \beta_2$ is the difference in *configuration pressures* that can be related to the surface tension and radius of curvature of the bubble $(2\sigma/R)$, $\bar{\rho}_\alpha$ is the material density, R is the radius of the bubble, μ^* is an *effective viscosity coefficient* of the phases, i^* is an *effective inertia coefficient* for liquid and bubbles, and where the subscript 1 and 2 denote the dispersed (bubble) and continuous (liquid) phases, respectively. The difference between equation (43) and the classical bubble equation (cit. Van Wijngaarden [17]) is a factor of 2 multiplying the

inertia term $\dot{R}\dot{R}$ in the former equation instead of 3/2. This difference in factors multiplying the inertia terms may be associated with the averaging procedure describing an *average bubble* in the mixture, whereas the classical bubble equation is derived by considering only one bubble in an infinite fluid. The effects of viscosity and phase compressibilities on the bubble growth have been discussed previously [17], whereas the effect of phase inertias has not and constitutes a novel feature in the bubble equation.

Another result of the linearized theory of constitutive equations with structure is the prediction of a Mohr–Coulomb-type yield criterion of limited equilibrium in the limit when the multiphase flow is brought to rest. This prediction comes from the stress tensor result of the theory, showing that the phases can support nonzero shear stresses at rest in the presence of nonzero volumetric fraction gradients. This is an important and consistent result with the granular flow experiments (Savage [18]).

The rotational and dilatational effects considerably complicate a linearized theory of constitutive equations and a full nonlinear theory becomes very complex and not practical [11]. Since a linear theory is not fully adequate for modeling complex multiphase flows, the nonlinear effects should be introduced selectively; first in the phenomenological coefficients in the constitutive equations of a linear theory, and second in the full tensor representation of constitutive variables in terms of the invariants of independent variables in these equations.

5. SUMMARY AND CONCLUSIONS

Starting from the volume averaging approach and an assumption of the material deformation of each phase relative to the center of mass it is possible not only to establish the basic field equations of averaged and postulatory theories of multiphase mixtures, but also an additional (and much more general) set of balance equations to model the structural characteristics of the mixture. The basic field equations of conservation and balance of mass, momentum, energy and entropy describe the center of mass evolution of each phase, whereas the additional balance equations describe the evolution of phase properties, or structural characteristics, relative to the center of mass. These structural properties are the consequence of the nonlocal theory introduced by the volume averaging process and may be approximated to various degrees in future works. The theory also reproduces the well-known and classical results of multiphase flows and may be used for modeling of dense multiphase mixtures where the structural effects of the mixture may be very important.

REFERENCES

[1] M. A. GOODMAN and S. C. COWIN, *J. Fluid. Mech.* **45**, 321–339 (1971).
[2] S. L. PASSMAN, *Int. J. Engng Sci.* **15**, 117–129 (1977).
[3] A. BEDFORD and D. S. DRUMHELLER, *Arch. Rat. Mech. Anal.* **68**, 37–51 (1978).
[4] G. AHMADI, *Int. J. Engng. Sci.* **23**, 1–25 (1985).
[5] D. A. DREW, *Stud. Appl. Math.* **L**, 133–166 (1971).
[6] M. ISHII, *Thermo-Fluid Dynamic Theory of Two-Phase Flows.* Eyrolles, Paris (1975).
[7] R. I. NIGMATULIN, *Int. J. Multiphase Flow* **5**, 353–385 (1979).
[8] M. HASSANIZADEH and W. G. GRAY, *Adv. Water Resources* **2**, 131–144 (1979).
[9] A. K. R. CELMINS and J. A. SCHMITT, Three dimensional modeling of gas combusting solid two-phase flows. *Multi-phase Flow and Heat Transfer III*, Part B. Elsevier, Amsterdam (1984).
[10] F. DOBRAN, *Int. J. Multiphase Flow* **10**, 273–305 (1984).
[11] F. DOBRAN, *Theory of Structured Multiphase Mixtures. Lecture Notes in Physics* **372**. Springer, Berlin (1991).
[12] A. C. ERINGEN, *Continuum Physics II.* Academic Press, New York (1975).
[13] C. TRUESDELL and W. NOLL, The Nonlinear Field Theories of Mechanics. *Handbuch der Physik Band III/1.* Springer, Berlin (1965).
[14] R. BOWEN, Theory of mixtures. *Continuum Physics III.* Academic Press, New York (1976).
[15] A. C. ERINGEN, *Int. J. Engng Sci.* **2**, 205–217 (1964).
[16] R. J. TWISS and A. C. ERINGEN, *Int. J. Engng Sci.* **9**, 1019–1044 (1971).
[17] L. VAN WIJNGAARDEN, *Ann. Rev. Fluid Mech.* **4**, 369–376 (1972).
[18] S. B. SAVAGE, *J. Fluid. Mech.* **92**, 53–96 (1979).