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Modeling of dendritic solidification systems: reassessment of the continuum momentum equation

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Abstract—In recent years there has been renewed interest in modeling transport phenomena associated with the dendritic solidification of binary mixtures. Solidification occurs in a two-phase (*mushy*) region characterized by complex, solid–liquid interfacial geometries, and development of a model which is amenable to solution dictates the use of continuum (mixture theory) assumptions and/or volume-averaging procedures. A review of the recent literature would suggest that solidification models developed from mixture theory assumptions are less valid and less general than similar models based on volume-averaging, particularly with regard to the respective momentum equations which describe interdendritic fluid flow. In this paper, these different approaches are shown to yield identical macroscopic conservation equations, and the continuum momentum equation is reconsidered in an effort to reconcile matters which have lead to confusion about the validity of the continuum model. Consistency between recently presented momentum equations is demonstrated.

1. INTRODUCTION

THE SOLIDIFICATION of industrial alloys is a complex process which occurs over a temperature range and exhibits a two-phase region called the mushy zone. The mushy zone is comprised of solid dendrites and interdendritic liquid, and it separates the fully solidified and melted regions. Dendrites grow naturally with a very large specific surface area and with dendrite arm spacings of the order of 10 μm. In the macroscopic sense, such growth makes the liquid–solid interface highly irregular and virtually irresolvable. The nucleation and growth of crystals, microsegregation, the formation of inclusions such as pores, and internal cracking are important microscopic phenomena associated with solidification within the mushy zone, and these events are known to be strongly influenced by *macroscopic* momentum, heat, and mass transfer. Moreover, convection in the mushy zone is known to be responsible for macrosegregation [1, 2], which refers to the redistribution of alloy components on a macroscopic scale.

The inherent geometrical complexity of the solid–liquid interface in the mushy zone precludes a precise, microscopic description of the interdendritic fluid flow with macroscopic parameters. Nevertheless, numerous models which treat the effects of macroscopic transport phenomena during the solidification of alloys have been developed by incorporating empirical relationships between superficial fluid velocity (a macroscopic parameter) and permeability. The first such models [3–8] treated conditions only within the mushy zone and ignored the coupling which exists between flows in the bulk melt and mushy regions. Szekely and Jassal [9] and Ridder *et al.* [10] subsequently treated dendritic solidification with models which included coupling between the mushy and all-liquid zones. Separate conservation equations were written for the melt and mushy zones, and since the solutions to these equations could only be achieved numerically, each region was discretized with a separate grid. The solution procedure to these *multidomain* models therefore involved complicated schemes for remeshing each domain and matching boundary conditions at the moving liquidus interface. While providing significant improvement over previous models, the multidomain models required explicit tracking of the liquidus interface which, by practical considerations, restricted their use to problems with regular interface shapes.

In 1987, a set of equations for momentum, energy, and species transport in binary, solid–liquid, phase change systems was presented [11], which concurrently applied in all regions (solid, mush, and liquid) and required only a single, fixed numerical grid and a single set of boundary conditions to effect a solution. Hence, the solid, mushy, and liquid regions were implicitly coupled, and limitations of the multi-

NOMENCLATURE

B	body force
f	mass fraction
g	volume fraction
$\dot{G}$	momentum source due to phase interactions
$\mathbf{i}$	x-direction unit vector
$\mathbf{J}$	general diffusion flux
K	permeability
$\mathbf{n}$	unit normal vector
P	pressure-like parameter in momentum equation
S	general source term
t	time
u	x-direction velocity component
$\mathbf{V}$	velocity vector
x	x-direction.

Greek symbols

μ	viscosity
ρ	density
$\bar{\rho}$	partial density
σ	vector component of material stress tensor
$\bar{\sigma}$	average normal stress (mechanical pressure)
ϕ	general scalar quantity
Ω	angular velocity.

Subscripts

k	arbitrary phase k
l	liquid phase
s	solid phase
x	x-component.

Superscript

α	arbitrary constituent α.

domain models were avoided. In their formulation, the mushy zone was viewed as a solid–liquid mixture with macroscopic properties, and individual phase conservation equations were summed to form a set of mixture conservation equations. Limiting assumptions were invoked (a non-deforming solid phase, $T_s = T_l$, and no macroscopic species diffusion through the solid phase) to reduce the number of dependent variables, and the solidus and liquidus interfaces, as well as individual phase variables, were implicitly determined by solving the mixture equations. Applications of the so-called *continuum* model have confirmed important features of binary solidification that had previously been observed or surmised to exist but had eluded prediction [12–14]. Such features include an irregular liquidus interface shape, double-diffusive convection in the melt, the channeling of interdendritic flows, and characteristic macrosegregation patterns.

Other single-domain models of binary solidification have been presented in recent years. Voller and Prakash [15] presented a method of modeling dendritic solidification with a fixed grid, but their analysis ignored species transport. An enthalpy based energy equation and a momentum equation based on the superficial liquid velocity ($g_l\mathbf{V}_l$) were formulated to apply in all zones. Appropriate source terms were incorporated to account for latent heat evolution and solid–liquid interaction forces within the mushy zone. Variations and extensions of the continuum model [11] have been made by Voller *et al.* [16], who included non-equilibrium freezing effects and a deforming solid phase, and by Kececioglu and Rubinsky [17], who were concerned with the propagation of a discrete phase change interface through a porous material. Although a similar approach was adopted by Beckermann and Viskanta [18, 19], these authors chose to cite volume-averaging literature [20–22], rather than mixture theory literature [23–28], as justification for the conservation equations associated with individual phases. For predictions based on a stationary solid phase, results obtained from the volume-averaged model [18, 19] are consistent with those obtained from the continuum model [12, 14]. Very recently, Ni and Beckermann [29] proposed a model for which the volume-averaged, individual phase equations would have to be solved separately with the aid of interphase transport models. The model would permit relaxation of the assumptions pertaining to a non-deforming solid phase, thermal equilibrium ($T_s = T_l$), and negligible species diffusion through the solid phase, at the expense of solving twice as many partial differential equations. However, attempts to solve such a full set of equations have yet to be made.

Recent literature suggests some misunderstanding concerning the formulation and application of single-domain solidification models, especially with regard to the momentum equations. In a paper by Ganesan and Poirier [30], it was stated that, although several different momentum equations for treating interdendritic flow can be found in the literature, little fundamental justification had been provided for the models. Development of the continuum momentum equation [11] was said to rely too heavily on intuitive arguments related to phase interaction forces, while the volume-averaged momentum equation of Beckermann and Viskanta [18, 19] was noted for omitting development details. Moreover, recent reviews of dendritic solidification models [31–33] have suggested the existence of significant differences between models based on continuum theory [11] and local volume-averaging [18, 19].

The objective of this paper is to identify and clarify misunderstandings surrounding the development and application of continuum and volume-averaging models of dendritic solidification and to demonstrate that the two models yield essentially equivalent results. As the original derivation of the continuum momentum equation [11] has apparently contributed to the current state of confusion, a revised formulation of this equation is presented. While following the same basic approach of the original development [11], the revised formulation identifies and reconciles potentially confusing elements of the development. In addition, key features of the continuum and volume-averaging approaches are contrasted in an effort to clarify the essential elements of single-domain (or fixed-grid) solidification models, and inherent similarities of momentum equations based on the two methods are discussed.

2. THE CONTINUUM MOMENTUM EQUATION

In developing the continuum momentum equation, special attention will be given to points of contention concerning the original formulation [11]. The development parallels that of the original study, and the end result will be shown to be virtually equivalent. For convenience, only the x-component of momentum (in a Cartesian coordinate system) will be considered.

The continuum theory of mixtures can be applied to obtain the following general conservation equation [11]:

$$\frac{\partial}{\partial t}(\bar{\rho}_k \phi_k) + \nabla \cdot (\bar{\rho}_k \mathbf{V}_k \phi_k) = -\nabla \cdot (g_k \mathbf{J}_k) + g_k S_k \quad (1)$$

where g_k is the local volume fraction of phase k, $\bar{\rho}_k$ the partial density of phase k (i.e. $g_k \rho_k$), $\mathbf{V}_k$ the mass-averaged velocity of phase k, $\mathbf{J}_k$ the diffusion flux (per unit area of phase k) through phase k, S_k the total source/sink of a conserved quantity associated with phase k, and ϕ_k is an arbitrary, dependent scalar variable. The diffusive flux, $\mathbf{J}_k$, represents that which is not accommodated by the macroscopic advection term, $\bar{\rho}_k \mathbf{V}_k \phi_k$. An individual phase momentum equation is found by substituting the expressions $\phi_k = u_k$, $\mathbf{J}_k = -\sigma_{kx}$, and $S_k = \rho_k B_{kx} + \dot{G}_{kx}$ into equation (1). It follows that

$$\frac{\partial}{\partial t}(\bar{\rho}_k u_k) + \nabla \cdot (\bar{\rho}_k \mathbf{V}_k u_k) = \nabla \cdot (g_k \sigma_{kx}) + \bar{\rho}_k B_{kx} + g_k \dot{G}_{kx} \quad (2)$$

where σ_{kx} is the vector component of the mean phase stress tensor which contributes to the x-direction momentum, B_{kx} is the mean body force acting on phase k in the x-direction, and $\dot{G}_{kx}$ represents all forces and rates of momentum exchange between phase k and all other phases per unit volume of phase k. In this formulation σ_{kx} represents the macroscopic state of stress within phase k. Stresses occurring at the microscopic interfaces between phases give rise to phase interaction forces and are macroscopically considered in $\dot{G}_{kx}$, along with direct momentum exchange through phase change.

Summing the individual phase momentum equations and imposing Newton's third law ($\Sigma\, g_k \dot{G}_{kx} = 0$), a mixture momentum equation may be expressed as

$$\frac{\partial}{\partial t}\left(\sum_k \bar{\rho}_k u_k\right) + \nabla \cdot \left(\sum_k \bar{\rho}_k \mathbf{V}_k u_k\right) = \nabla \cdot \left(\sum_k g_k \sigma_{kx}\right) + \left(\sum_k \bar{\rho}_k B_{kx}\right). \quad (3)$$

In the original derivation of the mixture momentum equation [11], the restriction associated with Newton's third law was not introduced, and instead a net phase interaction force was postulated to exist. This intuitive argument is removed from the current formulation, and the role of phase interaction forces is described below. Equation (3) simply states that the storage and advection of the momentum of a mixture of phases within a differential control volume must equal the net force acting on the volume. This force includes *unbalanced* internal stresses (e.g. viscous stresses and pressure) and externally imposed body forces (e.g. gravity). The momentum equation can be further refined by introducing definitions for mixture density, velocity, and body force

$$\rho = \sum_k \bar{\rho}_k \quad (4)$$

$$\rho \mathbf{V} = \sum_k \bar{\rho}_k \mathbf{V}_k \quad \text{and} \quad \rho u = \sum_k \bar{\rho}_k u_k \quad (5)$$

$$\rho B_x = \sum_k \bar{\rho}_k B_{kx} \quad (6)$$

and by substituting these definitions into equation (3). After rearranging the advection term, it follows that

$$\frac{\partial}{\partial t}(\rho u) + \nabla \cdot (\rho \mathbf{V} u) = \sum_k \nabla \cdot (g_k \sigma_{kx}) - \nabla \cdot \left[\sum_k \bar{\rho}_k (\mathbf{V}_k - \mathbf{V})(u_k - u)\right] + \rho B_x. \quad (7)$$

Equation (7) applies, in general, to multiphase systems which could, for example, include a large number of dispersed solid particles in a continuous liquid or a three-phase mixture of liquid, solid, and voids. However, if the equation is applied to a two-phase mixture of continuous solid and liquid, the identities $g_s + g_l = 1$, $\bar{\rho}_k = f_k \rho$ and $\mathbf{V}_l = (\mathbf{V} - \mathbf{V}_s)/f_l + \mathbf{V}_s$ allow the second term on the right-hand side of equation (7) to be rewritten as

$$\nabla \cdot \left[\sum_{k=s,l} \bar{\rho}_k (\mathbf{V}_k - \mathbf{V})(u_k - u)\right] = \nabla \cdot \left[\rho \frac{f_s}{f_l} (\mathbf{V} - \mathbf{V}_s)(u - u_s)\right]. \quad (8)$$

This term is non-zero *only* within the mushy zone, and it is a measure of the difference between the total net advection of momentum (from both phases individually) and the advection represented by mixture parameters on the left-hand side of equation (7). This term will subsequently be shown to be negligible.

If, in addition, fluid behavior is assumed to be Newtonian, the following constitutive relation for the intrinsic mean phase stress vector [11, 30] holds:

$$\sigma_{kx} = \frac{1}{g_k}\mu_k\nabla(g_k u_k) - \frac{2}{3g_k}\mu_k\nabla\cdot(g_k\mathbf{V}_k)\mathbf{i} + \frac{1}{g_k}\mu_k\frac{\partial}{\partial x}(g_k\mathbf{V}_k) - \bar{\sigma}_k\mathbf{i} \quad (9)$$

where $\bar{\sigma}_k$ is the mean mechanical pressure of phase k. Substituting this relation into the liquid stress term, it follows after some manipulation, that

$$\nabla\cdot(g_1\sigma_{1x}) = \nabla\cdot\left(\mu_1\frac{\rho}{\rho_1}\nabla u\right) - \mu_1\frac{\rho}{\rho_1}u_s\nabla^2 f_s - 2\mu_1\frac{\rho}{\rho_1}\nabla u_s\cdot\nabla f_s - \frac{\partial}{\partial x}(g_1 P) \quad (10a)$$

where

$$P = \bar{\sigma}_1 - \frac{\mu_1}{3}\frac{\nabla\cdot(g_1\mathbf{V}_1)}{g_1}. \quad (10b)$$

In developing equation (10), it is assumed that viscous stresses arising from local density variations are negligible and that viscosity is locally invariant ($\nabla\mu_1 \approx 0$). Also, the solid phase is considered to be rigid, such that $\nabla^2 u_s = 0$. Collectively, the first three terms on the right-hand side of equation (10a) represent viscous straining of the liquid. The straining rate has deliberately been expressed in terms of mixture kinematics and the kinematic motion of the solid phase. The second term on the right-hand side of equation (10a) is written in terms of solid translation, and the third term is written in terms of solid rotation, where $\nabla u_s = -\mathbf{\Omega}_s \times \mathbf{i}$. Since the solid fraction gradient is zero in single-phase regions, the second and third terms on the right-hand side of equation (10a) vanish outside the mushy zone. In the all-liquid region, the first and last terms on the right-hand side of equation (10a) simply represent conventional viscous and pressure force variations. In the all-solid region, all terms on the right-hand side of equation (10a) vanish, since the liquid stress is not defined in this region.

Consideration must now be given to the stress in the solid phase, since this phase may transmit forces. However, since the solid phase is assumed to be nondeformable, equation (9) is of little use. An acceptable expression for the solid stress term may instead be obtained by rearranging equation (2), yielding

$$\nabla\cdot(g_s\sigma_{sx}) = \frac{\partial}{\partial t}(\bar{\rho}_s u_s) + \nabla\cdot(\bar{\rho}_s\mathbf{V}_s u_s) - \bar{\rho}_s B_{sx} - g_s\dot{G}_{sx}. \quad (11)$$

The last term on the right-hand side of equation (11) represents normal (pressure) and shear (viscous) forces imparted on the solid by the liquid, as well as direct momentum exchange through phase change. Phase change effects are assumed to be negligible, and the phase interactions on the solid are equal and opposite to those on the liquid. Therefore

$$\nabla\cdot(g_s\sigma_{sx}) = \frac{\partial}{\partial t}(\bar{\rho}_s u_s) + \nabla\cdot(\bar{\rho}_s\mathbf{V}_s u_s) - \bar{\rho}_s B_{sx} + g_1\dot{G}_{1x} = \frac{\partial}{\partial t}(\bar{\rho}_s u_s) + \nabla\cdot(\bar{\rho}_s\mathbf{V}_s u_s) - \bar{\rho}_s B_{sx} + P\frac{\partial g_1}{\partial x} + g_1\dot{G}_{1x,D} \quad (12)$$

where $P(\partial g_1/\partial x)$ represents the net normal force interaction and $g_1\dot{G}_{1x,D}$ represents drag force on the liquid due to relative phase motion. The drag term ($g_1\dot{G}_{1x,D}$) accounts for shear forces acting on the liquid phase at the solid–liquid interface.

By substituting equations (8), (10) and (12) into equation (7), the momentum equation becomes

$$\frac{\partial}{\partial t}(\rho u) + \nabla\cdot(\rho\mathbf{V}u) = \nabla\cdot\left(\mu_1\frac{\rho}{\rho_1}\nabla u\right) - \mu_1\frac{\rho}{\rho_1}u_s\nabla^2 f_s - 2\mu_1\frac{\rho}{\rho_1}\nabla u_s\cdot\nabla f_s - \nabla\cdot\left[\rho\frac{f_s}{f_1}(\mathbf{V}-\mathbf{V}_s)(u-u_s)\right] + g_1\rho_1 B_{1x} - g_1\frac{\partial P}{\partial x} + g_1\dot{G}_{1x,D} + \frac{\partial}{\partial t}(\bar{\rho}_s u_s) + \nabla\cdot(\bar{\rho}_s\mathbf{V}_s u_s). \quad (13)$$

In equation (13) only the liquid body force term ($g_1\rho_1 B_{1x}$) has survived, and the pressure interaction term has cancelled part of the liquid pressure gradient to yield $g_1(\partial P/\partial x)$. Both conditions result from the manner in which the solid stress term was expressed in equation (12). The drag interaction term in equation (13) must be replaced with an expression amenable to computation. Ganesan and Poirier [30] provide a good discussion of appropriate models for the drag interaction term, including Darcy's law. Darcy's law is deemed appropriate only under the restrictive conditions of slow, steady fluid motion through a porous medium of uniform liquid volume fraction in which the macroscopic advection and viscous terms (liquid–liquid interactions) are negligible. Darcy's law can be expressed as

$$\frac{\partial P}{\partial x} - \rho_1 B_{1x} = -\frac{\mu}{K_x}g_1(u_1 - u_s) \quad (14)$$

where the permeability, K_x, may be isotropic or orthotropic. A version of Darcy's law with a more general anisotropic permeability can also be written, but it is not essential to the current discussion. While not being strictly appropriate [30], Darcy's law can be applied to determine the drag interaction term in equation (13)

$$\dot{G}_{lx,D} = -\frac{\mu}{K_x}\, g_l(u_l-u_s) \tag{15}$$

where it has been assumed that the only significant terms in equation (13) are those associated with drag interaction, pressure gradient, and liquid body force. Since permeabilities of dendritic structures are typically of the order of 10^{-11} m^2 (or smaller) [34], the drag interaction term does indeed dominate over the advection and viscous terms within the mushy zone. While more detailed procedures have been proposed for modeling the solid–liquid drag interaction term [30], there is insufficient data to support the use of such schemes. Therefore, Darcy's law is used in the current formulation with the understanding that higher-order models can be substituted as justification arises.

As mentioned earlier, the second, third and fourth terms on the right-hand side of equation (13) are non-zero only in the two-phase region, where they are negligible in comparison to the drag interaction term. Hence, these terms are ignored, and the continuum momentum equation reduces to

$$\frac{\partial}{\partial t}(\rho u)+\nabla\cdot(\rho \mathbf{V} u) = \nabla\cdot\left(\mu_l\frac{\rho}{\rho_l}\nabla u\right) - g_l\frac{\mu_l}{K_x}\frac{\rho}{\rho_l}(u-u_s)+g_l\rho_l B_{lx}-g_l\frac{\partial P}{\partial x}+\frac{\mathrm{D}}{\mathrm{D}t}(\bar{\rho}_s u_s) \tag{16}$$

where $g_l(u_l-u_s) = \rho/\rho_l(u-u_s)$ and the solid acceleration is expressed as a substantial derivative.

Another objective of the continuum formulation was to develop equations which are amenable to solution with existing numerical algorithms. The SIMPLER algorithm [35], for example, couples momentum component and continuity equations implicitly through the pressure gradient term, which is scaled by g_l in equation (16). To avoid changing existing algorithms to account for the scaling of the pressure gradient by g_l, equation (14), which is essentially valid whenever g_s is non-zero, can be multiplied by g_s, rearranged to yield an identity with zero, and added to the right-hand side of equation (16) to yield†

$$\frac{\partial}{\partial t}(\rho u)+\nabla\cdot(\rho \mathbf{V} u) = \nabla\cdot\left(\mu_l\frac{\rho}{\rho_l}\nabla u\right) - \frac{\mu_l}{K_x}\frac{\rho}{\rho_l}(u-u_s)+\rho_l B_{lx}-\frac{\partial P}{\partial x}+\frac{\mathrm{D}}{\mathrm{D}t}(\bar{\rho}_s u_s). \tag{17}$$

Equations (16) and (17) are considered to be equivalent, but equation (17) is easier to implement into existing solution algorithms.

Although solid velocity components appear in equation (17), the dependent variable is the mixture velocity, which is well defined in all regions. In an all-liquid region, the Darcy term vanishes with $K_x = \infty$, as does the solid acceleration term with $\bar{\rho}_s = 0$. Thus, in an all-liquid region, equation (17) reduces to the familiar, single-phase relation. The solid velocity must be determined for the mushy and all-solid regions, requiring another equation for the solid motion. However, the need to solve another equation is eliminated by considering conditions in which the solid motion can be prescribed [11], and since the solid is assumed to be continuous and rigid, its motion is described entirely by prescribing its translation and rotation at a single point. This assumption could be relaxed without changing the general methodology of the continuum model, but the complexity of the model would be greatly enhanced. The Darcy term in equation (17) ensures that $u = u_s$ in an all-solid region, provided that the permeability model yields $K_x = 0$ when $g_s = 1$. Hence, equation (17) can be appropriately applied in all regions of a solidification system. As previously discussed [10, 12, 30, 34, 36], the Darcy damping term depends strongly on the permeability model.

The current formulation of the continuum momentum equation differs from the original development [11] in two important ways. First, Newton's third law is explicitly asserted in equation (3). In the original development [11], the general mixture momentum equation included a non-zero, phase interaction term. Secondly, instead of assuming that the solid is free of internal stress [11], equation (11) is exploited, which introduces solid–liquid interactions into the mixture momentum equation. Equation (17) is slightly different than the original form of the continuum momentum equation [11]. First, the last term on the right-hand side of equation (17) is not found in the original mixture momentum equation. The solid acceleration term accounts for a portion of the solid stress variation. It is negligible or zero for most solidification conditions, but has been retained because it may be important in situations for which the solid is oscillating. Secondly, the body force term in equation (17) ($\rho_l B_{lx}$) depends only on the liquid phase, whereas the body force term of the original continuum momentum equation included contributions from both phases [11]. However, previous applications of the continuum momentum equation [12, 14] have been consistent with equation (17), with the Boussinesq approximation having been invoked to account for the effects of temperature and solute concentration on the density of the liquid phase. Finally, the definitions of the pressure-like parameter P differ between the current and original formulations. In equation (10b), P is defined in terms of liquid parameters only, whereas the original definition for P was a volume fraction-weighted average of parameters associated with both phases.

3. COMPARISON OF CONTINUUM AND VOLUME-AVERAGED MODELING APPROACHES

Two different approaches have been adopted to yield single-domain, solid–liquid phase change

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† Equation (14) and the last step which yielded equation (17) are valid only under the assumption of a non-deforming dendritic structure.

models. Both approaches begin by considering a macroscopic domain which contains an arbitrary number of phases. In the continuum approach [11, 17], general conservation principles are applied to a macroscopically small control volume, and an integral conservation equation is obtained for an arbitrary, individual phase, with the integrands written in terms of macroscopic parameters of the physical system. The integral equations can be transformed into differential equations when the macroscopic parameters are assumed to be continuously differentiable functions of space and time. Source terms are included in the individual phase conservation equations to account for interactions with other phases. The fact that microscopic interfaces exist between the different phases necessitates the inclusion of phase interaction terms.

In the volume-averaging approach [18, 30, 37] conventional continuum relationships are assumed to be valid within a given phase at the microscopic level. By integrating the microscopic relations over an appropriately sized control volume (i.e. one which is small in the macroscopic view but large in the microscopic view), the scale of the problem is changed [37], and macroscopic parameters are defined in terms of microscopic parameters. Conservation equations are written in terms of the new macroscopic quantities, and phase interactions are described with microscopic surface integrals, evaluated over the acknowledged interfacial surfaces.

The general conservation equation which provides a starting point for both the continuum and volume-average models [11, 18] is equation (1). However, because it deals more systematically with the relationship between microscopic and macroscopic parameters, the volume-average approach may be preferable. In this approach, phase interaction terms are a natural consequence of the development and are expressed as surface integrals over microscopic solid–liquid interfaces [29]. The approach may therefore be better suited to understanding how microscopic events influence macroscopic behavior and to the development of micro–macroscopic models [38–40]. However, it is important to recognize that, although a phase interaction term can be represented as an integral over the interfacial area contained within a small averaging volume, final evaluation in terms of the microscopic variables used in its description is impossible, since these variables cannot be resolved in a macroscopic model. Indeed, the availability of such resolving power would render volume-averaging unnecessary. In terms of implementation for macroscopic calculations, it is therefore believed that the continuum and volume-averaged approaches are equally suited.

In describing real systems, it is seldom possible to incorporate all physical mechanisms into a mathematical model of a process, and it is the modeler's task to select those mechanisms which exert a dominant influence on system behavior. With respect to solidification of a binary mixture, the dominant physical mechanisms governing fluid flow in the mushy zone are different than those in the all-liquid region. This condition is evident in existing multidomain solidification models [9, 10], which use different momentum equations in the mushy and all-liquid regions. Single-domain phase-change models [11, 15, 19] have exploited the fact that the governing equations used in the mushy and all-liquid zones are derived, either explicitly or implicitly, from the same fundamental laws of physics, and by ignoring terms which are negligible only in *both* regions, a single set of equations is found to apply in both regions. Criteria for neglecting/retaining terms can also be applied to the all-solid region, so that a single-domain (solid, mush, and liquid) model is obtained.

Equations (16) and (17) are consistent with other mushy zone momentum equations found in the literature [15, 19, 30]. With $u_s = 0$, equation (17) is identical to the momentum equation used by Voller and Prakash [15]. Using volume-averaging procedures, Ganesan and Poirier [30] developed a general momentum equation in vector form, where the solid was considered to be stationary. If the fourth term on the right-hand side of equation (13) is *not* neglected, but $\mathbf{V}_s$ is set equal to zero, equation (16) can be rearranged and expressed as

$$\frac{\partial}{\partial t}(g_l\rho_l u_l)+\nabla\cdot(g_l\rho_l\mathbf{V}_l u_l) = \nabla\cdot(\mu_l\nabla g_l u_l)$$

$$-g_l\frac{\mu_l}{K_x}\frac{\rho}{\rho_l}g_l u_l+g_l\rho_l B_{lx}-g_l\frac{\partial P}{\partial x}. \quad (18)$$

This result is essentially equivalent to the x-component of equation (43) in ref. [30]. Equation (18) and the x-component of equation (43) of ref. [30] differ only in that a higher-order expression for the solid–liquid drag term is used in ref. [30]. The higher-order model for the solid–liquid drag term is appropriate in anisotropic media (columnar dendritic structures) [30], and it may be incorporated into the continuum model as data for its coefficients become available. The relationship between equation (18) and the momentum equation used by Beckermann and Viskanta [19] is discussed by Ganesan and Poirier [30].

4. SUMMARY

The derivation of the continuum momentum equation has been reconsidered in an effort to clarify misconceptions which have arisen since the original development [11]. Key assumptions have been highlighted, as have physical implications and limitations to application of the final result. The most important and distinguishing feature of both the continuum [11, 15, 16] and volume-averaging [19, 30] models is the retention of all terms which may be dominant in some region (solid, mush, or liquid) in the conservation equations. In this respect, the continuum and volume-averaged solidification models are essentially equivalent.

Although equation (17) is limited to situations corresponding to a single, continuous liquid phase and a single, continuous and non-deforming solid phase (a system of primary dendrites and eutectic lamalae would, for example, be considered as one solid phase), the modeling *concept* is not restricted as such. Equation (7) is a more general relation which could be applied to more complicated systems involving, for example, solid precipitating at multiple boundaries with different velocities, void inclusions, and solidification around a matrix of fibers (composite materials). Generally, the continuum approach views a discontinuous solid structure (e.g. free floating crystals) as several *different* phases. However, under conditions for which floating and settling of solid crystals (indeterminate in number) are significant, it becomes advantageous to view the crystals collectively as a single, deformable solid phase. Under such conditions, equation (17) cannot be applied, since it relies on a single, rigid solid phase. Nevertheless, a mixture momentum equation could be developed for situations involving a deforming solid phase by introducing an appropriate (empirically determined) constitutive relation for the solid phase stress into equation (7). Such an approach would require an additional single-phase (solid or liquid) momentum equation for closure. An alternative is to consider separate phase momentum equations, thereby eliminating the need for a mixture equation [29].

Although application of the continuum model to binary mixtures has been extremely successful in predicting important solidification characteristics such as remelting, liquidus interface irregularities, double-diffusive convection in the melt, channeling, and macrosegregation [12–14], quantitative agreement between predicted and measured results has been less satisfactory [14]. Barriers to obtaining good quantitative agreement include uncertainties in requisite thermophysical property data and the permeability associated with the mushy zone. In general, the permeability is a tensor, but with a paucity of permeability data, detailed models are not available. Even in equiaxed regions of the mushy zone, where an isotropic model is appropriate, the permeability is not well known. Also, permeability data are most deficient in the important range corresponding to $0.70 < g_l < 1.0$, where relatively large permeabilities permit significant interdendritic fluid velocities. The permeability depends on several factors related to microscopic morphology, making it difficult to quantify. Moreover, microscopic morphological features, such as dendrite arm spacing, can change significantly during the solidification process [41].

An additional uncertainty relates to supplemental closure rules required to implement the continuum model. The momentum equation is coupled to the energy and species conservation equations through the buoyancy term, which is related to the temperature and liquid composition, and less directly through the permeability, which is a strong function of the local liquid volume fraction. If local thermodynamic equilibrium (equal phase temperatures and chemical potentials) is assumed, temperature, liquid composition, and liquid volume fraction can be related to the mixture enthalpy (dependent variable of the energy equation) and mixture composition (dependent variable of the species equation) through the equilibrium phase diagram. Simple thermodynamic relations thereby provide means of relating temperature, enthalpy, concentrations, and phase fractions. However, binary metal systems which exhibit limited solid solubility typically exhibit non-equilibrium, since dendrites are not chemically saturated due to the extremely slow nature of solid state diffusion [41]. The equilibrium freezing assumption may therefore provide inaccurate predictions of local solute segregation between liquid and solid phases and of phase volume fractions. Nevertheless, the equilibrium freezing approximation is a logical starting point in modeling binary solidification, and its use in no way affects the validity of the conservation equations. It is, in fact, a simple matter to incorporate non-equilibrium relationships into the continuum model [16, 40], although such a treatment is not well suited for the remelting of dendrites.

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MODELISATION DES SYSTEMES A SOLIDIFICATION DENDRITIQUE: REVISION DE L'EQUATION DE QUANTITE DE MOUVEMENT DU CONTINUUM

Résumé—Il y a eu ces dernières années un regain d'intérêt dans la modélisation des phénomènes de transport associés à la solidification dendritiques des mélanges binaires. La solidification se fait dans une région biphasique (boue) caractérisée par des géométries complexes interfaciales solide–liquide, et le développement d'un modèle qui conduit à la solution dicte l'usage d'hypothèses de continuum (théorie de mélange) et/ou des procédures de moyenne en volume. Une analyse des articles récents suggère que les modèles de solidification développés à partir des hypothèses de la théorie de mélange sont moins valides et moins généraux que les modèles similaires basés sur les moyennes en volume, particulièrement en considération des équations respectives de la quantité de mouvement qui décrivent l'écoulement fluide interdentrique. Dans cet article, ces différentes approches sont montrées conduire à des équations identiques de conservation macroscopique, et l'équation de quantité de mouvement du continuum est reconsidérée pour lever une confusion concernant la validité du modèle de continuum. On montre la cohérence entre des équations de quantité de mouvement présentées récemment.

DIE MODELLIERUNG DENTRITISCH ERSTARRENDER SYSTEME: NEUFORMULIERUNG DER IMPULSERHALTUNGSGLEICHUNG IM KONTINUUM

Zusammenfassung—In den letzten Jahren entstand ein erneutes Interesse an der Modellierung von Transportvorgängen, die mit der dentritischen Erstarrung in binären Gemischen zusammenhängen. Die Erstarrung tritt in einem Zweiphasengebiet mit Fest–Flüssig-Phasengrenzen von komplizierter Geometrie auf. Die Entwicklung eines geeigneten Modells erfordert die Annahme eines Kontinuums (Mischungstheorie) und/oder Verfahren der Volumenmittelung. Eine Übersicht über die einschlägige Literatur vermittelt den Eindruck, daß Erstarrungsmodelle auf der Grundlage der Mischungstheorie weniger richtig und weniger umfassend seien als solche, die von einer Volumenmittelung ausgehen. Dies gilt insbesondere im Hinblick auf die Impulstransportgleichungen, welche die Fluidströmung zwischen den Dentriten beschreiben. In der vorliegenden Arbeit wird gezeigt, daß die unterschiedlichen Ansätze zu identischen makroskopischen Erhaltungsgleichungen führen. Die Impulstransportgleichung für das Kontinuum wird neu formuliert, um die Diskussionen über die Gültigkeit des Kontinuumsmodells auszuräumen. Die Übereinstimmung mit einer jüngst publizierten Impulstransportgleichung wird dargelegt.

МОДЕЛИРОВАНИЕ СИСТЕМ ДЕНДРИТНОГО ЗАТВЕРДЕВАНИЯ: МОДИФИКАЦИЯ УРАВНЕНИЯ КОЛИЧЕСТВА ДВИЖЕНИЯ В ПРИБЛИЖЕНИИ СПЛОШНОЙ СРЕДЫ

Аннотация—В последние годы возобновился интерес к моделированию явлений переноса, связанных с дендритным затвердеванием бинарных смесей. Затвердевание происходит в двухфазной области, которая характеризуется зсожной геометрией границы раздела твердое тело–жидкость. Разработка соответствующей модели требует допущений об использовании положений теории сплошной среды (теория смесей) и/или применения методов усреднения по объему. Обзор современной литературы позволяет предположить, что модели затвердевания, разработанные с учетом допущений теории смесей, являются менее адекватными, чем простые модели, основанные на усреднении по объему, особенно в отношении соответствующих уравнений количества движения, описывающих течение междендритной жидкости. Уравнение количества движения в приближении теории смесей преобразуется с целью устранения причин неадекватности. Демонстрируется соответствие между различными уравнениями количества движения.