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BRIEF COMMUNICATION

SINGLE- VS DUAL-SCALE VOLUME AVERAGING FOR HETEROGENEOUS MULTIPHASE SYSTEMS

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1. INTRODUCTION

At present, the direct theoretical description and numerical simulation of multiphase transport phenomena on a microscopic level are nearly excluded due to the complex geometry of the interphase boundaries and due to limitations in computer capacity. One way of investigating macroscopic aspects of multiphase systems is to use a volume-averaging technique (Drew 1983; Hassanizadeh & Gray 1979a, b, 1980). By this procedure, *point* transport equations valid on the microscopic level are averaged over a representative element volume (REV), to obtain an averaged formulation of the dynamic behavior of each phase at any point in space. The resulting averaged or macroscopic equations contain the phase fractions as well as products of deviations from mean values and terms accounting for interphase transport. These terms are expressed by appropriate constitutive relationships obtained from microscopic considerations; hence, the micro–macroscopic couplings are fully reflected in the averaged transport equations.

Averaging theorems that relate an average of a spatial or temporal derivative to the derivative of the average are a key mathematical tool used to perform volume averaging. A number of studies have been devoted to developing these theorems and applying them to multiphase transport problems (Whitaker 1967; Slattery 1967; Gray & Lee 1977; Cushman 1982). Gray (1983) further derived averaging theorems for a nonconstant averaging volume. However, all previous studies are formally restricted to homogeneous multiphase systems with only a single microscopic length scale. In this case it is sufficient to perform single-step volume averaging to transform the microscopic equations into the corresponding macroscopic equations. This conventional volume-averaging technique is referred to from now on as single-scale volume averaging, so as to distinguish it from dual-scale volume averaging for multiscale heterogeneous systems, which is the subject of the present paper.

This brief communication considers a heterogeneous multiphase system where disparate multiple length scales associated with various phases exist. Such heterogeneous systems arise from a wide range of applications in chemical, civil, geological, mechanical, materials, hydrological and petroleum engineering. Typical examples include solid–gas flows with nonuniform particles, dual-porosity flows in a naturally fractured reservoir (Douglas & Arbogast 1990), solute transport in aggregated porous media (van Genuchten & Wierenga 1976), diffusion and dispersion in packed beds consisting of porous catalysts (Plumb & Whitaker 1990) and transport during dendritic solidification of metallic alloys (Beckermann & Viskanta 1992). There is great interest in developing meaningful transport equations for heterogeneous systems with multiple length scales, in order to capture the various interesting phenomena occurring on different length scales.

Basically, two different volume-averaging approaches to the modeling of transport processes in heterogeneous multiphase systems have been utilized. One approach treats the fluid associated with a smaller microscopic length scale (micropore fluid) and the fluid in a microstructure of a larger length scale (macropore fluid) as ordinary distinct phases, and then directly applies the conventional volume-averaging procedure, referred to as single-scale volume averaging in this paper (e.g. Hassanizedeh 1988). Despite the fact that this approach has appealing advantages in

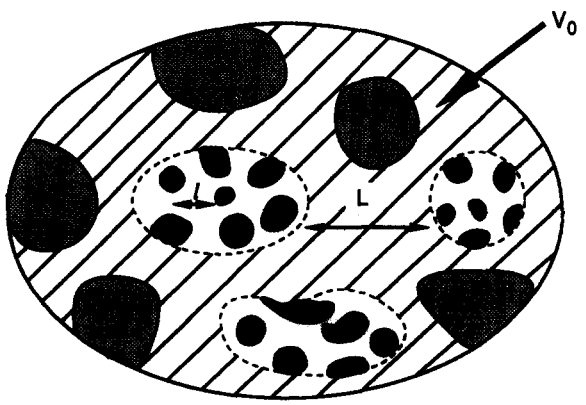
terms of simplicity and straightforwardness, fundamental questions remain with regard to its validity for multiscale heterogeneous systems. In the other approach, a two-step volume-averaging procedure, consisting of local volume averaging and large-scale averaging, is performed in order to include the effect of local heterogeneities (Quintard & Whitaker 1988; Plumb & Whitaker 1988, 1990). In local-volume averaging, the *point* equations and interfacial boundary conditions are averaged to form the local-volume-averaged equations. Then, the large-scale averaging further homogenizes these local-volume-averaged equations over a higher scale volume, whose size is large compared to the length scale of the local heterogeneities. We refer to this procedure as dual-scale volume averaging. Apparently, the latter approach does more justice to the multiscale nature of a heterogeneous system and provides more physical insight.

The current paper accomplishes two tasks in progressing toward a macroscopic description of heterogeneous multiphase systems. First, we develop dual-scale volume-averaging theorems for spatial and temporal derivatives of physical variables. These theorems will allow for a direct and easy use of the dual-scale volume-averaging method in various transport processes. In contrast, Whitaker and coworkers performed the dual-scale volume-averaging procedure each time for a particular equation. The other difference between this work and that of Whitaker lies in the fact that we relax the assumption that the small-scale averaging volume (or local averaging volume, in Whitaker's terminology) is independent of space and time. Therefore, interchanging the order of integration and differentiation in the large-scale averaging is not trivial. This relaxation becomes critical in applications involving a change of phase, where a phase having a small microscopic length scale undergoes appreciable growth or decay. Thus, the work extends the technique of dual-scale volume averaging. Also, we compare both volume-averaging methods, in order to examine the validity of single-scale volume averaging as applied to heterogeneous multiphase systems.

2. SINGLE-SCALE VOLUME AVERAGING

For comparison with the dual-scale volume-averaging theory, the single-scale averaging theorems are briefly reviewed.

As an example, let us consider a two-scale, four-phase system as illustrated in figure 1. The four phases contained within the averaging volume V_0 are characterized by either of the two length scales. Here it must be stressed that the phases are not required to be physically different, but may represent the same physical phase if that phase has different length scales. For instance, a liquid of a smaller length scale is considered to be a phase different from the same liquid having a larger length scale.



l small microscale length

L large microscale length

Figure 1. Illustration of a dual-scale four-phase heterogeneous system.

Each phase k in V_0 occupies a total volume V_k and is bounded by the interfacial areas A_k and A^k. Here the subscript and superscript are especially devised to denote the interface of phase k with another phase having the same length scale and with a phase having a different scale, respectively. The reason for dividing the total interfacial area into two parts, which are characterized by their length scales, is to facilitate the comparison with the dual-scale volume-averaging theory.

The definition of a volume-averaged quantity Ψ in phase k is

$$\langle \Psi_k \rangle = \frac{1}{V_0} \int_{V_0} X_k \Psi_k \, dV, \tag{1}$$

where X_k is the distribution function, being equal to unity in phase k and zero elsewhere. The intrinsic phase average is defined as

$$\langle \Psi_k \rangle^k = \frac{1}{V_k} \int_{V_0} X_k \Psi_k \, dV \tag{2}$$

and this leads to the definition of the volume fraction ε_k as

$$\varepsilon_k = \frac{V_k}{V_0}. \tag{3}$$

Clearly, ε_k is constrained by

$$\sum_k \varepsilon_k = 1 \quad \text{and} \quad 0 < \varepsilon_k \leqslant 1. \tag{4}$$

Also, it follows that

$$\langle \Psi_k \rangle = \varepsilon_k \langle \Psi_k \rangle^k. \tag{5}$$

The fluctuating component of Ψ_k is defined as

$$\hat{\Psi}_k = \Psi_k - \langle \Psi_k \rangle^k \tag{6}$$

and the average of the product of two quantities Ψ_k and Φ_k is thus given by

$$\langle \Psi_k \Phi_k \rangle^k = \langle \Psi_k \rangle^k \langle \Phi_k \rangle^k + \langle \hat{\Psi}_k \hat{\Phi}_k \rangle^k. \tag{7}$$

Finally, we need two important averaging theorems which relate the average of a derivative to the derivative of the average (Whitaker 1967; Slattery 1967):

$$\left\langle \frac{\partial \Psi_k}{\partial t} \right\rangle = \frac{\partial \langle \Psi_k \rangle}{\partial t} - \frac{1}{V_0} \int_{A_k} \Psi_k \mathbf{w} \cdot \mathbf{n} \, dA - \frac{1}{V_0} \int_{A^k} \Psi_k \mathbf{w} \cdot \mathbf{n} \, dA \tag{8}$$

and

$$\langle \nabla \Psi_k \rangle = \nabla \langle \Psi_k \rangle + \frac{1}{V_0} \int_{A_k} \Psi_k \mathbf{n} \, dA + \frac{1}{V_0} \int_{A^k} \Psi_k \mathbf{n} \, dA \tag{9}$$

or, alternatively,

$$\langle \nabla \Psi_k \rangle = \varepsilon_k \nabla \langle \Psi_k \rangle^k + \frac{1}{V_0} \int_{A_k} \hat{\Psi}_k \mathbf{n} \, dA + \frac{1}{V_0} \int_{A^k} \hat{\Psi}_k \mathbf{n} \, dA, \tag{10}$$

where $\mathbf{n}$ is the outwardly directed normal vector at an interface moving at a velocity $\mathbf{w}$.

3. DUAL-SCALE VOLUME AVERAGING

In order to develop a macroscopic model that fully accounts for the multiscale nature of the system under consideration, a more rigorous and fundamental procedure is needed. As shown in figure 2, spatial smoothing over the large-scale (macroscopic) volume, V_0, requires knowledge of the transport equations averaged first over the small-scale volume, δV, while the latter is obtained from another averaging process. In other words, we must spatially smooth the corresponding *point* equations successively over the volumes δV and V_0. In the following, this dual-scale volume-averaging procedure will be developed for each phase k with the small length scale.

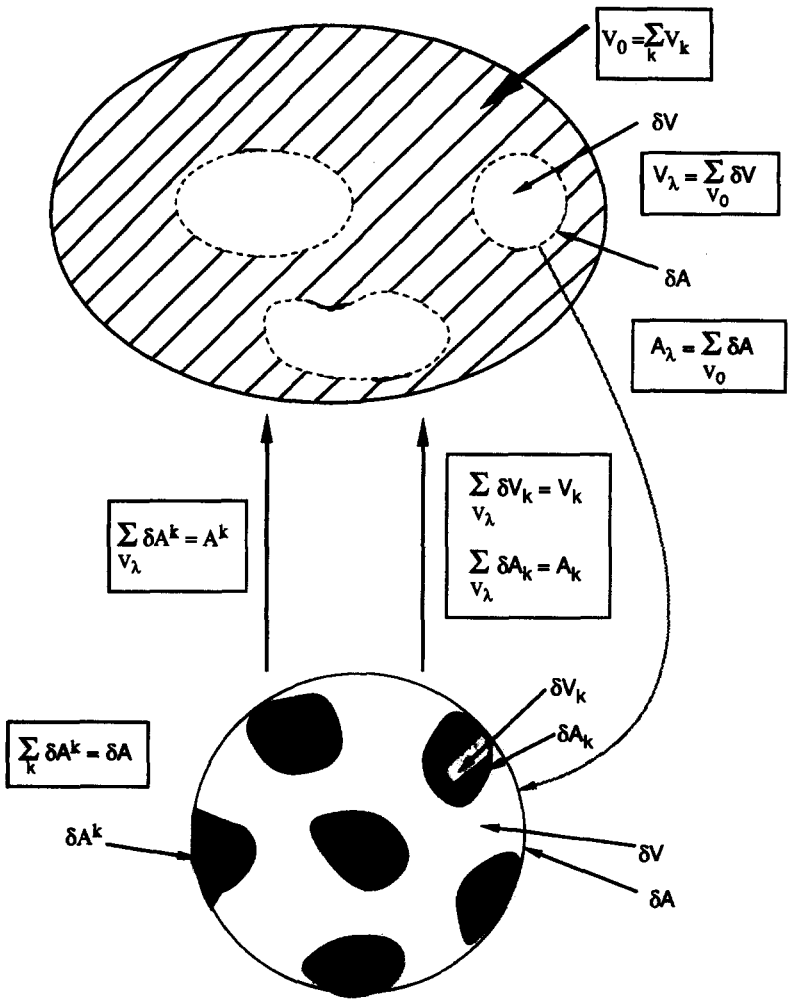


Figure 2. Illustration of the large- and small-scale averaging volumes.

3.1. Averaging volumes and areas

The large-scale volume V_0 contains a network of small scale volumes, δV, which are bounded by the area, δA, as shown in figure 2. The volume δV contains smaller scale phases, each occupying a volume δV_k. The size of a small scale volume, δV, is assumed to be much smaller than the size of the large-scale volume, V_0, but still larger than the length scale of the phases within δV. Hence, the representative radius of the small-scale averaging volume, δV, can be of the same order of magnitude as the larger length scale of the phases in the system. Because the small-scale volume and area represent quantities which are infinitesimally small with respect to the macroscopic scale but finite when compared to the smallest length scale, it is indeed appropriate to denote them as δV and δA, respectively. Thus, we denote all geometrical quantities inside δV with the δ-prefix. The interfacial area of phase k with the other phases within δV is denoted by δA_k, since this interface is between phases with the same length scale. In contrast, the area δA^k is the portion of the outer boundary of the small-scale averaging volume, δA, where phase k exists. Hence,

$$\sum_k \delta A^k = \delta A. \qquad [11]$$

In addition, we define a summation operator by which a geometrical or physical quantity in a small-scale volume, δV, can be integrated over the large-scale volume, V_0, i.e.

$$\sum_{V_0} \Phi \delta V = \int_{V_\lambda} \Phi \, dV, \qquad [12]$$

where Φ is a constant quantity inside each small-scale volume and the subscript λ denotes the region occupied by all phases with the smaller length scale. Thus, [12] simplifies the integration into a summation of Φ over all discrete small-scale volumes contained in V_0. For instance,

$$\sum_{V_0} \delta V = V_\lambda. \tag{13}$$

Similarly, we have

$$\sum_{V_0} \delta A = A_\lambda, \tag{14}$$

$$\sum_{V_0} \delta V_k = V_k, \tag{15}$$

$$\sum_{V_0} \delta A_k = A_k \tag{16}$$

and

$$\sum_{V_0} \delta A^k = A^k; \quad \sum_k A^k = A_\lambda; \tag{17}$$

where A_λ denotes the total boundary area of all small-scale averaging volumes inside V_0. A schematic illustration of the above nomenclature and most geometrical relations is also provided in figure 2.

3.2. Averaging operators and averaged quantities

Averaged quantities are related to microscopic quantities through a properly defined averaging operator. In the present work, two-level averaging operators are required: one for the small-scale volume which is denoted by $\{\cdot\}$; and the other over the large-scale volume which is denoted by $\langle\cdot\rangle$. Therefore, we have

$$\{\Psi_k\} = \frac{1}{\delta V}\int_{\delta V} X_k \Psi_k \, \mathrm{d}V, \tag{18}$$

where X_k is again the phase function, being equal to the unity in phase k and zero elsewhere within δV. The large-scale averaging operator is conventionally defined as

$$\langle \Psi_k \rangle = \frac{1}{V_0}\int_{V_0} X_k \Psi_k \, \mathrm{d}V. \tag{19}$$

Here, X_k means more than a phase function. When phase k has a higher length scale, X_k has the same meaning as before. However, when phase k has a smaller length scale, X_k is equal to unity in phase k within the λ-region and zero elsewhere within the large-scale volume, V_0; i.e. $X_k = X_\lambda$.

Combining the two definitions of the averaging operators for the two length scales, a dual-scale averaging operator can be written as

$$\langle \{\Psi_k\} \rangle = \frac{1}{V_0}\int_{V_0} X_\lambda \{\Psi_k\} \, \mathrm{d}V = \frac{1}{V_0}\int_{V_0} X_\lambda \left(\frac{1}{\delta V}\int_{\delta V} X_k \Psi_k \, \mathrm{d}V \right) \mathrm{d}V. \tag{20}$$

The intrinsic volume average is defined only for the dual scale:

$$\langle \{\Psi_k\} \rangle^k = \frac{1}{V_k}\int_{V_0} X_\lambda \{\Psi_k\} \, \mathrm{d}V. \tag{21}$$

Then, it follows that

$$\langle \{\Psi_k\} \rangle = \varepsilon_k \langle \{\Psi_k\} \rangle^k. \tag{22}$$

For the special case, $\Psi_k = 1$, we obtain the definitions of two types of volume fractions for each phase based on either δV or V_0. First, [18] yields

$$\delta\varepsilon_k = \frac{\delta V_k}{\delta V}, \tag{23}$$

which is constrained by

$$\sum_k \delta\varepsilon_k = 1. \tag{24}$$

The quantity, $\delta\varepsilon_k$, can be referred to as the internal volume fraction of phase k within the small-scale volume. Second, substitution of $\Psi_k = 1$ into [20] leads to

$$\varepsilon_k = \frac{1}{V_0}\int_{V_0} X_\lambda \delta\varepsilon_k \, dV. \tag{25}$$

To gain a simple physical interpretation of the volume fractions, we further assume that $\delta\varepsilon_k$ can be treated as a constant with respect to the above integration. Then the following relationship between the two kinds of volume fractions is obtained:

$$\varepsilon_k = \delta\varepsilon_k \cdot \varepsilon_\lambda, \tag{26}$$

where ε_λ is defined as

$$\varepsilon_\lambda = \frac{V_\lambda}{V_0} \tag{27}$$

which can be interpreted as the global volume fraction of all small scale phases within V_0. Therefore, in terms of [26], the total volume fraction of a small-scale phase in the large-scale averaging volume is equal to the product of the global small-scale fraction and the internal phase fraction. However, it should be pointed out that the above assumption regarding the constant $\delta\varepsilon_k$ is not implied in the following derivation.

Again, the dual-scale intrinsic phase average can be related to the volume average by

$$\langle\{\Psi_k\}\rangle^k = \frac{\langle\{\Psi_k\}\rangle}{\varepsilon_k}. \tag{28}$$

The small-scale fluctuating component of Ψ_k is conventionally defined as

$$\hat{\Psi}_k = \Psi_k - \{\Psi_k\}^k \tag{29}$$

and the large-scale one as

$$\{\Psi_k\}' = \{\Psi_k\}^k - \langle\{\Psi_k\}\rangle^k. \tag{30}$$

Combining [29] and [30], we get

$$\{\Psi_k\}' + \hat{\Psi}_k = \Psi_k - \langle\{\Psi_k\}\rangle^k. \tag{31}$$

This equation simply implies that two fluctuating components appear in dual-scale volume averaging. One is between the microscopic- and small-scale volume averages, and the other arises from the second volume averaging due to local heterogeneities.

The dual-scale volume average of the product of two quantities Ψ_k and Φ_k is then expressed by

$$\begin{aligned}\langle\{\Psi_k\Phi_k\}\rangle^k &= \langle\{\Psi_k\}\{\Phi_k\} + \{\hat{\Psi}_k\hat{\Phi}_k\}\rangle^k \\ &= \langle\{\Psi_k\}\rangle^k\langle\{\Phi_k\}\rangle^k + \langle\{\Psi_k\}'\{\Phi_k\}'\rangle^k + \langle\{\hat{\Psi}_k\hat{\Phi}_k\}\rangle^k.\end{aligned} \tag{32}$$

Note that in dual-scale volume averaging, dispersion arises from two sources: one is from microscopic fluctuations while the other is due to the nonhomogeneity of a small-scale volume-averaged quantity within the large-scale volume.

3.3. Averaging theorems

At this point we are ready to develop the macroscopic transport equations. A natural way to do this is to apply the single-scale volume-averaging procedure twice to the microscopic equations. However, this procedure turns out to be extremely tedious and has to be performed for each individual conservation equation. In addition, the second volume averaging over the large-scale volume has to deal with the complicated terms that arise from the first volume-averaging process over the small-scale volume. Instead, a more efficient way to derive the macroscopic equations is

to develop dual-scale averaging theorems, and then directly apply them to the microscopic equations once. This is the aim of the development that follows.

The single-scale volume-averaging theorems will be used as the basis for the derivation of dual-scale theorems. The former have been developed elsewhere (Whitaker 1967; Slattery 1967; Hassanizadeh & Gray 1979a, b). For the sake of generality, it is assumed that the small-scale volume δV is time-dependent and spatially varying. Hence, we utilize Gray's averaging theorems for a nonconstant averaging volume (Gray 1983). In our terminology the temporal theorem can be stated as

$$\left\{\frac{\partial \Psi_k}{\partial t}\right\} = \frac{1}{\delta V}\frac{\partial}{\partial t}[\delta V\{\Psi_k\}] - \frac{1}{\delta V}\int_{\delta A_k} \Psi_k \mathbf{w}\cdot\mathbf{n}\,dA - \frac{1}{\delta V}\int_{\delta A^k} \Psi_k \mathbf{w}\cdot\mathbf{n}\,dA. \quad [33]$$

Note that if δV does not vary with time, the interfacial velocity on δA^k vanishes and [33] reduces to the standard form of the time-averaging theorem.

Averaging all terms in the above equation over the large-scale volume V_0 yields

$$\left\langle\left\{\frac{\partial \Psi_k}{\partial t}\right\}\right\rangle = \frac{1}{V_0}\int_{V_0}\frac{X_\lambda}{\delta V}\frac{\partial}{\partial t}[\delta V\{\Psi_k\}]\,dV - \frac{1}{V_0}\int_{V_0}\left(\frac{X_\lambda}{\delta V}\int_{\delta A_k}\Psi_k \mathbf{w}\cdot\mathbf{n}\,dA\right)dV$$

$$-\frac{1}{V_0}\int_{V_0}\left(\frac{X_\lambda}{\delta V}\int_{\delta A^k}\Psi_k \mathbf{w}\cdot\mathbf{n}\,dA\right)dV. \quad [34]$$

We are going to treat each of the terms on the RHS of [34] separately. Application of the chain rule to the first one yields

$$\frac{1}{V_0}\int_{V_0}\frac{X_\lambda}{\delta V}\frac{\partial}{\partial t}[\delta V\{\Psi_k\}]\,dV = \frac{1}{V_0}\int_{V_0}\frac{\partial}{\partial t}[X_\lambda\{\Psi_k\}]\,dV - \frac{1}{V_0}\int_{V_0}\delta V\{\Psi_k\}\frac{\partial}{\partial t}\left(\frac{X_\lambda}{\delta V}\right)dV. \quad [35]$$

Because V_0 is independent of time, the order of differentiation and integration in the first term on the RHS can be interchanged and the last term can be further decomposed. Then

$$\frac{1}{V_0}\int_{V_0}\frac{X_\lambda}{\delta V}\frac{\partial}{\partial t}[\delta V\{\Psi_k\}]\,dV = \frac{\partial}{\partial t}\langle\{\Psi_k\}\rangle - \frac{1}{V_0}\int_{V_0}\{\Psi_k\}\frac{\partial X_\lambda}{\partial t}\,dV + \frac{1}{V_0}\int_{V_0}X_\lambda\{\Psi_k\}\frac{1}{\delta V}\frac{\partial(\delta V)}{\partial t}\,dV. \quad [36]$$

Making use of the following property of the distribution function, X_λ (Gray & Lee 1977):

$$\frac{\partial X_\lambda}{\partial t} = \mathbf{w}\cdot\mathbf{n}\delta(x - x_{A_\lambda}), \quad [37]$$

where $\mathbf{n}$ is a unit vector normal to the surface pointing to the side where $X_\lambda = 0$, $\mathbf{w}$ is the velocity of the interface, A_λ, and δ is the Dirac function. The second term on the RHS can be reduced to an area integral such that

$$\frac{1}{V_0}\int_{V_0}\{\Psi_k\}\frac{\partial X_\lambda}{\partial t}\,dV = \frac{1}{V_0}\int_{A_\lambda}\{\Psi_k\}\mathbf{w}\cdot\mathbf{n}\,dA = \frac{1}{V_0}\sum_{V_0}\{\Psi_k\}\int_{\delta A}\mathbf{w}\cdot\mathbf{n}\,dA. \quad [38]$$

The second equality in [38] transforms the integral over a discrete field into the summation as defined by [12]. The same transformation reduces the third term on the RHS of [36] to

$$\frac{1}{V_0}\int_{V_0}X_\lambda\{\Psi_k\}\frac{1}{\delta V}\frac{\partial(\delta V)}{\partial t}\,dV = \frac{1}{V_0}\sum_{V_0}\{\Psi_k\}\frac{\partial(\delta V)}{\partial t}. \quad [39]$$

Inserting [38] and [39] into [36] yields

$$\frac{1}{V_0}\int_{V_0}\frac{X_\lambda}{\delta V}\frac{\partial}{\partial t}[\delta V\{\Psi_k\}]\,dV = \frac{\partial}{\partial t}\langle\{\Psi_k\}\rangle + \frac{1}{V_0}\sum_{V_0}\{\Psi_k\}\left[\frac{\partial(\delta V)}{\partial t} - \int_{\delta A}\mathbf{w}\cdot\mathbf{n}\,dA\right]. \quad [40]$$

The last term on the RHS of [40] vanishes due to material conservation of the small-scale volume, δV. We can also arrive at the same conclusion, if we set $\Psi_k = 1$ in [33] and then add up the resulting equations for each phase. Hence,

$$\frac{1}{V_0}\int_{V_0}\frac{X_\lambda}{\delta V}\frac{\partial}{\partial t}[\delta V\{\Psi_k\}]\,dV = \frac{\partial}{\partial t}\langle\{\Psi_k\}\rangle. \quad [41]$$

The second term on the RHS of [34] is simplified by employing a similar transformation as in [38], then

$$-\frac{1}{V_0}\int_{V_0}\left\{\frac{X_\lambda}{\delta V}\int_{\delta A_k}\Psi_k\mathbf{w}\cdot\mathbf{n}\,\mathrm{d}A\,\mathrm{d}V\right\}=-\frac{1}{V_0}\sum_{V_0}\frac{1}{\delta V}\left(\int_{\delta A_k}\Psi_k\mathbf{w}\cdot\mathbf{n}\,\mathrm{d}A\right)\delta V$$

$$=-\frac{1}{V_0}\sum_{V_0}\int_{\delta A_k}\Psi_k\mathbf{w}\cdot\mathbf{n}\,\mathrm{d}A$$

$$=-\frac{1}{V_0}\int_{A_k}\Psi_k\mathbf{w}\cdot\mathbf{n}\,\mathrm{d}A. \qquad [42]$$

Likewise,

$$-\frac{1}{V_0}\int_{V_0}\left(\frac{X_\lambda}{\delta V}\int_{\delta A^k}\Psi_k\mathbf{w}\cdot\mathbf{n}\,\mathrm{d}A\right)\mathrm{d}A=-\frac{1}{V_0}\int_{A^k}\Psi_k\mathbf{w}\cdot\mathbf{n}\,\mathrm{d}A. \qquad [43]$$

Substituting [41]–[43] into [34], we finally obtain the dual-scale time-averaging theorem as

$$\left\langle\left\{\frac{\partial\Psi_k}{\partial t}\right\}\right\rangle=\frac{\partial}{\partial t}\langle\{\Psi_k\}\rangle-\frac{1}{V_0}\int_{A_k}\Psi_k\mathbf{w}\cdot\mathbf{n}\,\mathrm{d}A-\frac{1}{V_0}\int_{A^k}\Psi_k\mathbf{w}\cdot\mathbf{n}\,\mathrm{d}A. \qquad [44]$$

The development of the dual-scale averaging theorem for spatial derivatives also begins with the single-scale spatial averaging theorem, which has been derived by Gray (1983) for a nonconstant averaging volume:

$$\{\nabla\Psi_k\}=\frac{1}{\delta V}\nabla[\delta V\{\Psi_k\}]+\frac{1}{\delta V}\int_{\delta A_k}\Psi_k\mathbf{n}\,\mathrm{d}A-\frac{\nabla(\delta V)}{\delta V}\frac{1}{\delta A}\int_{\delta A^k}\Psi_k\mathbf{n}\,\mathrm{d}A. \qquad [45]$$

This is the original form, but in the present terminology. Here, it should be pointed out that the derivation of [45] assumes a spherical volume δV.

For convenience, we first transform [45] into an alternate form as

$$\{\nabla\Psi_k\}=\nabla\{\Psi_k\}+\frac{1}{\delta V}\int_{\delta A_k}\Psi_k\mathbf{n}\,\mathrm{d}A+\frac{\nabla(\delta V)}{\delta V}\left(\{\Psi_k\}-\frac{1}{\delta A}\int_{\delta A^k}\Psi_k\mathbf{n}\,\mathrm{d}A\right). \qquad [46]$$

Then, by performing the second averaging to the above equation, the following results:

$$\langle\{\nabla\Psi_k\}\rangle=\frac{1}{V_0}\int_{V_0}X_\lambda\nabla\{\Psi_k\}\,\mathrm{d}V+\frac{1}{V_0}\int_{V_0}\left(\frac{X_\lambda}{\delta V}\int_{\delta A_k}\Psi_k\mathbf{n}\,\mathrm{d}A\right)\mathrm{d}V$$

$$+\frac{1}{V_0}\int_{V_0}\frac{X_\lambda\nabla(\delta V)}{\delta V}\left(\{\Psi_k\}-\frac{1}{\delta A}\int_{\delta A^k}\Psi_k\mathbf{n}\,\mathrm{d}A\right)\mathrm{d}V. \qquad [47]$$

Application of the chain rule to the first term on the RHS of [47] yields

$$\frac{1}{V_0}\int_{V_0}X_\lambda\nabla\{\Psi_k\}\,\mathrm{d}V=\frac{1}{V_0}\int_{V_0}\nabla(X_\lambda\{\Psi_k\})\,\mathrm{d}V-\frac{1}{V_0}\int_{V_0}\{\Psi_k\}\nabla X_\lambda\,\mathrm{d}V. \qquad [48]$$

The first term of the RHS of [48] can be simplified by interchanging the order of differentiation and integration, since V_0 does not depend on spatial coordinates. The second term needs further manipulation.

The following property has widely been used in deriving averaging theorems (Gray & Lee 1977):

$$\nabla X_\lambda=-\mathbf{n}\,\delta(x-x_{A_\lambda},t). \qquad [49]$$

This equation involves the Dirac function, which is zero everywhere except at the interface A_λ. Use of this relation and the mean value theorem simplifies the second term on the RHS of [48], such that

$$-\frac{1}{V_0}\int_{V_0}\{\Psi_k\}\nabla X_\lambda\,\mathrm{d}V=\frac{1}{V_0}\int_{V_0}\mathbf{n}\delta(x-x_{A_\lambda},t)\{\Psi_k\}\,\mathrm{d}V$$

$$=\frac{1}{V_0}\sum_{V_0}\left[\mathbf{n}\delta(x-x_{\delta A},t)\frac{1}{\delta V}\int_{\delta V_k}\Psi_k\,\mathrm{d}V\right]\delta V$$

$$=\frac{1}{V_0}\sum_{V_0}\left[\mathbf{n}\delta(x-x_{\delta A},t)\int_{\delta V_k}\Psi_k\,\mathrm{d}V\right], \qquad [50]$$

where the fact has been employed that $\mathbf{n}$ and δ are both constant within the smaller-scale volumes for the spherical averaging volumes considered here, so that they can be moved out of the integral. Now, moving $\mathbf{n}\delta$ back inside the integral, one obtains

$$\frac{1}{V_0}\sum_{V_0}\int_{\delta V_k}\mathbf{n}\delta(x-x_{\delta A},t)\Psi_k\,\mathrm{d}V=\frac{1}{V_0}\sum_{V_0}\int_{\delta A^k}\Psi_k\mathbf{n}\,\mathrm{d}A$$

$$=\frac{1}{V_0}\int_{A_k}\Psi_k\mathbf{n}\,\mathrm{d}A, \qquad [51]$$

where the integrand is nonzero only at the intersection of δA and δV_k, which turns out to be δA^k. Finally, [48] is reduced to

$$\frac{1}{V_0}\int_{V_0}X_k\nabla\{\Psi_k\}\,\mathrm{d}V=\nabla\langle\{\Psi_k\}\rangle+\frac{1}{V_0}\int_{A^k}\Psi_k\mathbf{n}\,\mathrm{d}A. \qquad [52]$$

Now, we simplify the second term on the RHS of [47] by utilizing the summation transformation as defined by [12]. Hence,

$$\frac{1}{V_0}\int_{V_0}\left(\frac{X_\lambda}{\delta V}\int_{\delta A_k}\Psi_k\mathbf{n}\,\mathrm{d}A\right)\mathrm{d}V=\frac{1}{V_0}\sum_{V_0}\left(\frac{1}{\delta V}\int_{\delta A_k}\Psi_k\mathbf{n}\,\mathrm{d}A\right)\delta V=\frac{1}{V_0}\sum_{V_0}\int_{\delta A_k}\Psi_k\mathbf{n}\,\mathrm{d}A=\frac{1}{V_0}\int_{A_k}\Psi_k\mathbf{n}\,\mathrm{d}A. \qquad [53]$$

Rewriting the last term on the RHS of [47] using the special notation for a volume-averaged quantity, we obtain

$$\left\langle\frac{\nabla(\delta V)}{\delta V}\left(\{\Psi_k\}-\frac{1}{\delta A}\int_{\delta A^k}\Psi_k\mathbf{n}\,\mathrm{d}A\right)\right\rangle=\left\langle\frac{\nabla(\delta V)}{\delta V}\right\rangle\cdot\left\langle\{\Psi_k\}-\frac{1}{\delta A}\int_{\delta A^k}\Psi_k\mathbf{n}\,\mathrm{d}A\right\rangle, \qquad [54]$$

where the identity given by [7] has been employed and any fluctuating components have been neglected as a first approximation. It is clear that the fluctuating components arise from the gross nonuniformity of the small-scale volumes within the large-scale averaging volume. They vanish if δV is spatially uniform with V_0. Substitution of [52]–[54] into [47] leads to the following dual-scale volume-averaging theorem for spatial derivatives:

$$\langle\{\nabla\Psi_k\}\rangle=\nabla\langle\{\Psi_k\}\rangle+\frac{1}{V_0}\int_{A_k}\Psi_k\mathbf{n}\,\mathrm{d}A+\frac{1}{V_0}\int_{A_k}\Psi_k\mathbf{n}\,\mathrm{d}A$$

$$+\left\langle\frac{\nabla(\delta V)}{\delta V}\right\rangle\cdot\left\langle\{\Psi_k\}-\frac{1}{\delta A}\int_{\delta A^k}\Psi_k\mathbf{n}\,\mathrm{d}A\right\rangle. \qquad [55]$$

It is worth noting that the second and third terms on the RHS of [55] arise from the first volume-averaging process within δV and account for the boundary conditions at the A^k and A_k interfaces, while the last term on the RHS results from the second volume-averaging step (i.e. from δV to V_0) and is due to local heterogeneities. Therefore, a dual-scale volume-averaged equation includes the effects of local heterogeneities. In contrast, single-scale volume averaging can only reveal the effects of boundary conditions, while local heterogeneities are implicitly ignored.

4. CONCLUSIONS

A heterogeneous multiphase system has been analyzed using a multifluid approach, in which not only various physical phases but also a phase having different length scales are considered as distinct fluids.

For a heterogeneous system consisting solely of different physical planes, a direct comparison can be made between [8] and [44], as well as between [9] and [55]. The only difference between the two kinds of volume-averaging theorems is the appearance of the last term in [55], which is caused by the spatial variation of δV within the large averaging volume, V_0. In the special case where δV is spatially uniform, the dual-scale volume-averaging theorems reduce to the previously derived single-scale volume-averaging theorems. Even when δV is not uniform, [44] and [55] lose their explicit dependence on δV if the last term is negligibly small compared to the other terms in [55]. Thus, provided that this criterion is satisfied, the traditional single-scale volume-averaging technique can be applied to obtain meaningful averages, even when the system is heterogeneous and characterized by several disparate length scales. The above conclusion applies no matter how δV varies with time.

For a system in which one physical phase exhibits both length scales, one needs to first divide the phase into two different phases according to their respective length scales. This involves the definition of A^k, which represents the imaginary interface between the two length scales. Recall that A^k does not need to be stationary, but can evolve with the growth or decay of a particular length scale.

Lastly, a subtle difference between the single- and dual-scale volume averaging should not be ignored. According to [32], the dispersive terms in the dual-scale averaging arise not only from nonuniformities on the microscopic scale but also from the spatial variability in the field quantities on the small scale. Thus, the modeling of the dispersive terms is more complicated than in single-scale volume averaging and requires additional research.

A direct application of the present fundamental work can be found in the modeling of equiaxed dendritic solidification of metallic alloys (Wang & Beckermann 1992). Such a system can be visualized as consisting of growing crystals that have a complicated ("dendritic") internal structure and are uniformly dispersed in the melt. The solid crystal and the interdendritic liquid within the equiaxed grains share a common interfacial structure of the order of 10^{-5}–10^{-4} m, whereas the interface between the extradendritic liquid outside the grains and the interdendritic liquid has a higher length scale (of the order of 10^{-4} and 10^{-3} m). Following the dual-scale volume-averaging procedure, the system is modeled to consist of three different phases: the solid phase and two liquid phases. The solid/interdendritic liquid interface is described by A_k and the dendrite envelope which separates the inter- and extradendritic liquids is identified as A^k. This imaginary envelope is a smooth surface connecting the dendrite tips. In addition, the equiaxed grains can be assumed to be of a uniform size within V_0, so that the spatial variation of δV is negligible and single-scale volume averaging is justified, as shown above. As a result, a multiphase model was developed that is simple in form but can incorporate several important phenomena occurring on various length scales and lead to improved predictions in a number of situations (Wang & Beckermann 1992). Obviously, for crystals nucleating at different times, a spatial variation of δV will exist within V_0 and single-scale volume averaging may not be appropriate.

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