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BRIEF COMMUNICATION

LOCAL VOLUME AVERAGING OF MULTIPHASE SYSTEMS USING A NON-CONSTANT AVERAGING VOLUME

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INTRODUCTION

The technique of local volume averaging of continuum equations of motion and transport has been used by many authors to obtain equations applicable to multiphase systems (e.g. Whitaker 1967; Bear 1972; Hassanizadeh & Gray 1979a, b). In performing averaging of this sort, it is necessary to make use of theorems which relate averages of derivatives to derivatives of average quantities. Slattery (1967) and Whitaker (1967) developed this relation for spatial derivatives by analogy with the transport theorem. Bachmat (1972) proved the averaging theorems for both spatial and temporal derivatives. Gray & Lee (1977) provided a simple proof which makes use of a distribution function which behaves as a multidimensional extension to the Dirac delta function concept. Cushman (1982) has also presented a very rigorous proof of these theorems making use of distribution theory. In a somewhat related work, Gray (1982) has developed averaging theorems which are local in only two of the dimensions while being global in the third dimension.

When averaging point equations, it is necessary to use an averaging volume of a size large enough that the averaged quantities obtained are meaningful and suitable for the flow under consideration. However this averaging volume should not be so large that macroscopic inhomogeneities affect the average values. For example, in analyzing porous media flows, one typically assumes that an averaging volume exists of length scale l such that (Whitaker 1969)

$$d \ll l \ll L \qquad [1]$$

where d is characteristic length of the pore; and L is some macroscopic dimension representative of the process under consideration. Currently used averaging theorems require that an averaging volume which is independent of time and space be applicable at every point in the region under consideration. Within this framework, many problems are adequately described by the equations obtained.

Nevertheless, there are a few types of problems which may be more amenable to analysis if the averaging volume may be formulated as a function of time and space. For example, in a porous medium composed of a well-sorted soil, the grain size gradient may require that the averaging volume not be constant in space. At each point in such a system it is still necessary to identify an averaging volume of characteristic length l which satisfies [1] and produces meaningful averages. Other problems where the added flexibility of a variable averaging volume may be useful include analysis of a swelling soil where the solid phase volume is a function of time and space, and infiltration problems where large gradients in water fraction may exist.

In the present work, currently used averaging theorems are extended to allow for averaging volumes which vary in space and time. This derivation, done in the context of the ideas presented by Gray & Lee (1977), makes use of a spherical averaging volume with a radius which varies continuously in space and time.

DEFINITIONS FOR AVERAGING

In an earlier work, Gray & Lee (1977) defined a function γ_α which is a multi-dimensional extension of the unit step function and allows for great simplification in developing proofs of the averaging theorems for multiphase systems. This function is defined such that it has a value of unity in phase α, but is zero in all other phases. Furthermore, arguments were presented which show that

$$\nabla\gamma_\alpha = -\mathbf{n}_\alpha\delta(\mathbf{x}-\mathbf{x}_{\alpha\beta}) \qquad [2]$$

where $\mathbf{x}_{\alpha\beta}$ is the location of the α–β interface; $\mathbf{n}_\alpha$ is a unit normal pointing out of the α-phase; and $\delta(\mathbf{x}-\mathbf{x}_{\alpha\beta})$ is a multi-dimensional analogue to the Dirac delta function. It must be emphasized that $\delta(\mathbf{x}-\mathbf{x}_{\alpha\beta})$ is not simply the classical point Dirac delta function in multi-dimensional space, but is an extension of the concept of a point delta function to a distributed version.

The notation and definitions to be used follow that of Gray & Lee (1977) but will be repeated here in brief form. For averaging, we locate the center of the averaging volume by the position vector $\mathbf{x}$. At this center a $\boldsymbol{\xi}$ coordinate system is defined such that a point within an averaging volume is located by

$$\mathbf{r} = \mathbf{x} + \boldsymbol{\xi}. \qquad [3]$$

The averaging is done over the $\boldsymbol{\xi}$-space and the following averages are defined

phase average

$$\langle\psi_\alpha\rangle(\mathbf{x}, t) = \frac{1}{\delta V}\int_{\delta V}\psi(\mathbf{x}+\boldsymbol{\xi}, t)\gamma_\alpha(\mathbf{x}+\boldsymbol{\xi}, t)\,\mathrm{d}v_\xi \qquad [4]$$

intrinsic phase average

$$\langle\psi_\alpha\rangle^\alpha(\mathbf{x}, t) = \frac{1}{\delta V_\alpha}\int_{\delta V}\psi(\mathbf{x}+\boldsymbol{\xi}, t)\gamma_\alpha(\mathbf{x}+\boldsymbol{\xi}, t)\,\mathrm{d}v_\xi \qquad [5]$$

where δV is the averaging volume; and δV_α is the volume of α-phase within the averaging volume. Note that in the above equations, the effective volume over which the integrations are performed is δV_α because $\gamma_\alpha = 0$ when a point is not in the α-phase.

The phase averages are related to the intrinsic phase averages by

$$\langle\psi_\alpha\rangle = \epsilon_\alpha\langle\psi_\alpha\rangle^\alpha \qquad [6]$$

where

$$\epsilon_\alpha = \frac{\delta V_\alpha}{\delta V} = \frac{1}{\delta V}\int_{\delta V}\gamma_\alpha(\mathbf{x}+\boldsymbol{\xi}, t)\,\mathrm{d}v_\xi. \qquad [7]$$

In the subsequent portion of the paper, the nabla operator will be used with the conventions that: ∇_x refers to derivatives taken with respect to $\mathbf{x}$ holding $\boldsymbol{\xi}$ constant; ∇_ξ refers to derivatives taken with respect to $\boldsymbol{\xi}$ holding $\mathbf{x}$ constant; ∇ refers to either ∇_x or ∇_ξ.

AVERAGING THEOREMS FOR NON-CONSTANT AVERAGING VOLUME

In this section we will derive theorems which relate the average of a derivative to the derivative of an average for multi-phase systems when the averaging volume may vary in space and time. To develop these theorems, we will make use of two different indicator functions. The first is $\gamma_\alpha(\mathbf{x}+\boldsymbol{\xi}, t)$ which has a value of unity in the α-phase and is zero in all other phases. The second generalized function is $\kappa(\mathbf{x}, \boldsymbol{\xi}, t)$ which has a value of 1 in δV located at $\mathbf{x}$ and is zero outside this averaging volume. Thus if $\mathbf{b}(\mathbf{x}, \boldsymbol{\xi}, t)$ is the position vector of the surface of the averaging volume located at x,

$$\kappa(\mathbf{x}, \boldsymbol{\xi}, t) = 1 - M[(\boldsymbol{\xi} - \mathbf{b})\cdot\mathbf{n}] \qquad [8a]$$

where $\mathbf{n}$ is the outward unit vector at the boundary δV

$$M = \begin{cases} 0 & \text{if} \quad (\boldsymbol{\xi} - \mathbf{b})\cdot\mathbf{n} < 0 \\ 1 & \text{if} \quad (\boldsymbol{\xi} - \mathbf{b})\cdot\mathbf{n} > 0 \end{cases} \qquad [8b]$$

and the geometry of δV has been assumed to be such that a line drawn from $\boldsymbol{\xi} = 0$ radially outward in any direction will intersect the boundary of the averaging volume at only one point. Note that if the averaging volumes are spheres, b will not depend on $\boldsymbol{\xi}$. Also if V is constant in space or time, b will not depend on $\mathbf{x}$ or t respectively. We will assume here that the variation of δV in space and time is continuous such that the first derivatives of b are finite.

Because the product $\kappa\gamma_\alpha$ has the value of 1 in δV_α within δV but is zero everywhere else in space,

$$\delta V\langle\nabla\psi_\alpha\rangle = \int_{\delta V} (\nabla\psi)\gamma_\alpha\, \mathrm{d}v = \int_{V_\infty} (\nabla\psi)\gamma_\alpha\kappa\, \mathrm{d}v \qquad [9]$$

where $\psi(\mathbf{x}+\boldsymbol{\xi}, t)$ is a property of interest; and V_∞ is a volume which encompasses the entire $\mathbf{x}$ domain and does not depend on space or time. The rightmost term in [9] may be rearranged using the chain rule to the form

$$\int_{V_\infty} (\nabla\psi)\gamma_\alpha\kappa\, \mathrm{d}v = \int_{V_\infty} \nabla(\psi\gamma_\alpha\kappa)\, \mathrm{d}v - \int_{V_\infty} \psi(\nabla\gamma_\alpha)\kappa\, \mathrm{d}v - \int_{V_\infty} \psi\gamma_\alpha(\nabla\kappa)\, \mathrm{d}v. \qquad [10]$$

In the first term on the right, because V_∞ does not depend on $\mathbf{x}$, we can change ∇ to ∇_x, interchange the order of differentiation and integration, and rearrange to obtain

$$\int_{V_\infty} \nabla(\psi\gamma_\alpha\kappa)\, \mathrm{d}v = \nabla_x \int_{V_\infty} \psi\gamma_\alpha\kappa\, \mathrm{d}v = \nabla_x \int_{\delta V} \psi\gamma_\alpha\, \mathrm{d}v = \nabla_x[\delta V\langle\psi_\alpha\rangle]. \qquad [11]$$

The second term on the right side of [10] reduces to an integral over the interface between the α- and β-phases (Gray & Lee 1977) such that

$$\int_{V_\infty} \psi(\nabla\gamma_\alpha)\kappa\, \mathrm{d}v = \int_{\delta V} \psi(\nabla\gamma_\alpha)\, \mathrm{d}V = -\int_{\delta A_{\alpha\beta}} \psi\mathbf{n}\, \mathrm{d}a. \qquad [12]$$

The final term in [10] simplifies most easily when the REV is spherical. In this case b does not depend on ξ and

$$\nabla_x \kappa = \delta(\xi - b)\nabla_x b \quad [13]$$

where $\delta(\xi - b)$ is the multidimensional analogue to the Dirac function. Thus the last term in [10] becomes an area integral over the bounding surface of the REV, denoted δA, and

$$\int_{V_\infty} \psi\gamma_\alpha(\nabla_x \kappa)\,\mathrm{d}v = \int_{\delta A} \psi\gamma_\alpha \nabla_x b\,\mathrm{d}a = \nabla_x b \int_{\delta A} \psi\gamma_\alpha\,\mathrm{d}a \quad [14]$$

where $\nabla_x b$ is removed from the integral because b depends only on x. Substitution of [11], [12] and [14] into [10] and then reference back to [9] yields

$$\delta V\langle\nabla\psi_\alpha\rangle = \nabla_x[\delta V\langle\psi_\alpha\rangle] + \int_{\delta A_{\alpha\beta}} \psi\mathbf{n}\,\mathrm{d}a - \nabla_x b \int_{\delta A} \psi\gamma_\alpha\,\mathrm{d}a \quad [15]$$

where $\delta V = (4/3)\pi b^3$.

This equation can be rearranged to obtain the averaging theorem in the form

$$\langle\nabla\psi_\alpha\rangle = \frac{1}{\delta V}\nabla_x[\delta V\langle\psi_\alpha\rangle] + \frac{1}{\delta V}\int_{\delta A_{\alpha\beta}} \psi\mathbf{n}\,\mathrm{d}a - \frac{\nabla_x(\delta V)}{\delta V}\frac{1}{\delta A}\int_{\delta A_\alpha} \psi\,\mathrm{d}a \quad [16]$$

where δA_α is the portion of δA which is the α-phase.

When δV is constant, this identity reduces to the classical averaging theorem. Defining

$$\tilde{\psi}(\mathbf{x}, \boldsymbol{\xi}, t) = \psi(\mathbf{x} + \boldsymbol{\xi}, t) - \langle\psi_\alpha\rangle^\alpha(\mathbf{x}, t) \quad [17]$$

we can rearrange [16] to an alternate form

$$\langle\nabla\psi_\alpha\rangle^\alpha = \nabla_x\langle\psi_\alpha\rangle^\alpha + \frac{1}{\delta V_\alpha}\int_{\delta A_{\alpha\beta}} \tilde{\psi}\mathbf{n}\,\mathrm{d}a - \frac{\nabla_x(\delta V)}{\delta V}\frac{1}{\delta A_\alpha}\int_{\delta A_\alpha} \tilde{\psi}\,\mathrm{d}a. \quad [18]$$

The development of averaging theorems for time derivatives is also straightforward in the context of the indicator function. First

$$\delta V\left\langle\frac{\partial\psi_\alpha}{\partial t}\right\rangle = \int_{\delta V} \frac{\partial\psi}{\partial t}\gamma_\alpha\,\mathrm{d}v = \int_{V_\infty} \frac{\partial\psi}{\partial t}\gamma_\alpha\kappa\,\mathrm{d}v. \quad [19]$$

Application of the chain rule to the third term in [19] yields

$$\delta V\left\langle\frac{\partial\psi_\alpha}{\partial t}\right\rangle = \int_{V_\infty} \frac{\partial}{\partial t}(\psi\gamma_\alpha\kappa)\,\mathrm{d}v - \int_{V_\infty} \psi\gamma_\alpha\frac{\partial\kappa}{\partial t}\,\mathrm{d}v - \int_{V_\infty} \psi\frac{\partial\gamma_\alpha}{\partial t}\kappa\,\mathrm{d}v. \quad [20]$$

But $(\partial\kappa/\partial t) = \mathbf{w}\cdot\mathbf{n}\delta(\xi - b)$ and $(\partial\gamma_\alpha/\partial t) = \mathbf{w}\cdot\mathbf{n}\delta(\mathbf{x} - \mathbf{x}^{\alpha\beta})$ where $\mathbf{w}$ is the velocity of the boundaries δA and $\delta A_{\alpha\beta}$. Thus

$$\left\langle\frac{\partial\psi_\alpha}{\partial t}\right\rangle = \frac{1}{\delta V}\frac{\partial}{\partial t}[\langle\psi_\alpha\rangle\delta V] - \frac{1}{\delta V}\int_{\delta A_\alpha} \psi\,\mathbf{w}\cdot\mathbf{n}\,\mathrm{d}a - \frac{1}{\delta V}\int_{\delta A_{\alpha\beta}} \psi\mathbf{w}\cdot\mathbf{n}\,\mathrm{d}a. \quad [21]$$

Note that if δV does not vary with time such that $(\partial b/\partial t) = \mathbf{w}\cdot\mathbf{n} = 0$ on δA, theorem [21] reduces to the standard form of the time averaging theorem. Making use of $\tilde{\psi}$ as defined in [20] we can rearrange [21] to the alternative form

$$\left\langle \frac{\partial \psi_\alpha}{\partial t} \right\rangle^\alpha = \frac{\partial \langle \psi \rangle^\alpha}{\partial t} - \frac{1}{\delta V_\alpha}\int_{\delta A_\alpha} \tilde{\psi}\mathbf{w}\cdot\mathbf{n}\,\mathrm{d}a - \frac{1}{\delta V_\alpha}\int_{\delta A_{\alpha\beta}} \tilde{\psi}\mathbf{w}\cdot\mathbf{n}\,\mathrm{d}a. \quad [22]$$

It may prove useful in application of theorem [21] and [22] to balance equations that for the case of spherical averaging volumes considered here, $\mathbf{w}\cdot\mathbf{n}$ on δA is independent of ξ and thus may be replaced by $\partial b/\partial t$ and brought outside the integral over δA_α. Of course the velocity of the $\delta A_{\alpha\beta}$ interface within an averaging volume will be typically dependent upon position and therefore $\mathbf{w}\cdot\mathbf{n}$ should not be removed from the integral over $\delta A_{\alpha\beta}$.

APPLICATION

We will now apply averaging theorems [16] and [21] or [18] and [22] to the general balance equation for some property ψ

$$\frac{\partial(\rho\psi)}{\partial t} + \nabla\cdot(\rho\mathbf{v}\psi) - \nabla\cdot\mathbf{i} - \rho f = \rho G \quad [23]$$

where $\mathbf{i}$ is the diffusive flux, f is an external supply term, and G is the production rate. We will also make use of mass averaged quantities defined as

$$\bar{\psi}^\alpha = \int_{\delta V} \rho(\mathbf{x}+\xi, t)\psi(\mathbf{x}+\xi, t)\gamma_\alpha(\mathbf{x}+\xi, t)\,\mathrm{d}v_\xi \Big/ \langle\rho_\alpha\rangle(\mathbf{x}, t). \quad [24]$$

The deviation term defined relative to this quantity is

$$\hat{\psi}(\mathbf{x}, \xi, t) = \psi(\mathbf{x}+\xi, t) - \bar{\psi}^\alpha(\mathbf{x}, t). \quad [25]$$

Application of [16] and [21]–[23] yields

$$\begin{aligned}&\frac{\partial(\langle\rho_\alpha\rangle\bar{\psi}^\alpha)}{\partial t} + \nabla_x\cdot(\langle\rho_\alpha\rangle\bar{\mathbf{v}}^\alpha\bar{\psi}^\alpha) - \epsilon_\alpha\nabla_x\cdot\bar{\mathbf{i}}^\alpha - \langle\rho_\alpha\rangle\bar{f}^\alpha \\ &\quad + \frac{1}{\delta V}\int_{\delta A_{\alpha\beta}} \rho\psi(\mathbf{v}-\mathbf{w})\cdot\mathbf{n}\,\mathrm{d}a - \frac{1}{\delta V}\int_{\delta A_{\alpha\beta}} (\mathbf{i}-\bar{\mathbf{i}}^\alpha)\cdot\mathbf{n}\,\mathrm{d}a \\ &\quad - \frac{1}{\delta A}\int_{\delta A_\alpha} \frac{1}{\delta V}\left[\rho\psi\frac{D\delta V}{Dt} - \langle\rho_\alpha\rangle^\alpha\bar{\psi}^\alpha\frac{D^\alpha\delta V}{Dt} - (\mathbf{i}-\bar{\mathbf{i}}^\alpha)\cdot\nabla\delta V\right]\mathrm{d}a \\ &\quad = \langle\rho_\alpha\rangle\bar{G}^\alpha \end{aligned} \quad [26]$$

where

$$\bar{\mathbf{i}}^\alpha = \langle\mathbf{i}_\alpha\rangle^\alpha - \langle\rho_\alpha\rangle\overline{\hat{\mathbf{v}}\hat{\psi}}^\alpha, \quad [27a]$$

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla, \quad [27b]$$

and

$$\frac{D^\alpha}{Dt} = \frac{\partial}{\partial t} + \bar{\mathbf{v}}^\alpha \cdot \nabla_x. \qquad [27c]$$

Use has been made here of the identities

$$\langle \rho_\alpha \psi_\alpha \rangle = \langle \rho_\alpha \rangle \bar{\psi}^\alpha, \qquad [28a]$$

and

$$\overline{\mathbf{v}\psi}^\alpha = \bar{\mathbf{v}}_\alpha \bar{\psi}^\alpha + \overline{\hat{\mathbf{v}}\hat{\psi}}^\alpha. \qquad [28b]$$

Alternatively, one can use averaging theorems [18] and [22] directly or rearrange [26] to obtain

$$\frac{\partial(\langle \rho_\alpha \rangle^\alpha \bar{\psi}^\alpha)}{\partial t} + \nabla_x \cdot (\langle \rho_\alpha \rangle^\alpha \bar{\mathbf{v}}^\alpha \bar{\psi}^\alpha) - \nabla_x \cdot \mathbf{i}^\alpha - \langle \rho_\alpha \rangle^\alpha \bar{f}^\alpha$$
$$+ \frac{1}{\delta V_\alpha} \int_{\delta A_{\alpha\beta}} \rho\psi(\mathbf{v} - \mathbf{w}) \cdot \mathbf{n}\, \mathrm{d}a - \frac{1}{\delta V_\alpha} \int_{\delta A_{\alpha\beta}} \langle \rho_\alpha \rangle^\alpha \bar{\psi}^\alpha (\bar{\mathbf{v}}^\alpha - \mathbf{w}) \cdot \mathbf{n}\, \mathrm{d}a$$
$$- \frac{1}{\delta V_\alpha} \int_{\delta A_{\alpha\beta}} (\mathbf{i} - \mathbf{i}^\alpha) \cdot \mathbf{n}\, \mathrm{d}a - \frac{1}{\delta A_\alpha} \int_{\delta A_\alpha} \frac{1}{\delta V} \left[\rho\psi \frac{D\delta V}{Dt} \right.$$
$$\left. - \langle \rho_\alpha \rangle^\alpha \bar{\psi}^\alpha \frac{D^\alpha \delta V}{Dt} - (\mathbf{i} - \mathbf{i}^\alpha) \cdot \nabla \delta V \right] \mathrm{d}a = \langle \rho_\alpha \rangle^\alpha \bar{G}^\alpha. \qquad [29]$$

CONCLUSION

Equations [26] and [29] are generalizations of the balance equations found in Hassanizadeh & Gray (1979a) to allow for non-constant averaging volumes. In the special case of δV constant, these equations become identical to those previously found in the literature as explicit dependence of the equations on the averaging volume size drops out. When δV is not constant, [26] and [29] also lose their explicit dependence on δV if

$$\frac{\partial \delta V}{\partial t} \left[\frac{1}{\delta A_\alpha} \int_{\delta A_\alpha} \rho\psi\, \mathrm{d}a - \frac{1}{\delta V_\alpha} \int_{\delta V_\alpha} \rho\psi\, \mathrm{d}v \right] = 0 \qquad [30a]$$

and

$$\nabla \delta V \cdot \left[\frac{1}{\delta A_\alpha} \int_{\delta A_\alpha} (\rho\psi\mathbf{v} - \mathbf{i})\, \mathrm{d}a - \frac{1}{\delta V_\alpha} \int_{\delta V_\alpha} (\rho\psi\mathbf{v} - \mathbf{i})\, \mathrm{d}v \right] = 0. \qquad [30b]$$

Thus if the conditions stipulated in [30] are satisfied, the traditional averaged equations derived for a constant averaging volume will be appropriate even when the system requires a non-constant volume in order to obtain meaningful averages.

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