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Transport Phenomena in Heterogeneous Media Based on Volume Averaging Theory

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I. Introduction

Determination of flow variables and scalar transport for problems involving heterogeneous (and porous) media is difficult, even when the problem is subject to simplifications allowing the specification of medium periodicity or regularity. Linear or linearized models fail to intrinsically account for transport phenomena, requiring dynamic coefficient models to correct for shortcomings in the governing models. Allowing inhomogeneities to adopt random or stochastic character further confounds the already daunting task of properly identifying pertinent transport mechanisms and predicting transport phenomena.

This problem is presently treated by procedures that are mostly heuristic in nature because sufficiently detailed descriptions are not included in the description of the problem and consequently are not available. The ability to describe the details, and features, of a proposed material with precision will help reduce the need for a heuristic approach.

Some aspects of the development of the needed theory are now well understood and have seen substantial progress in the thermal physics and in fluid mechanics sciences, particularly in porous media transport phenomena. The basis for this progress is the so-called volume averaging theory (VAT), which was first proposed in the 1960s by Anderson and Jackson [1], Slattery [2], Marle [3], Whitaker [4], and Zolotarev and Radushkevich [5].

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Further advances in the use of VAT are found in the work of Slattery [6], Kaviany [7], Gray *et al.* [8], and Whitaker [9, 10]). Many of the important details and examples of application are found in books by Kheifets and Neimark [11], Dullien [12], and Adler [13].

Publications on turbulent transport in porous media based on VAT began to appear in 1986. Primak *et al.* [14], Shcherban *et al.* [15], and later studies by Travkin and Catton [16, 18, 20, 21], etc., Travkin *et al.* [17, 19, 22], Gratton *et al.* [26, 27] and Catton and Travkin [28] present a generalized development of VAT for heterogeneous media applicable to nonlinear physical phenomena in thermal physics and fluid mechanics.

In most physically realistic cases, highly complex integral–differential equations result. When additional terms in the two- and three-phase statements are encountered, the level of difficulty in attempting to obtain closure and, hence, effective coefficients, increases greatly. The largest challenge is surmounting problems associated with the consistent lack of understanding of new, advanced equations and insufficient development of closure theory, especially for integral–differential equations. The ability to accurately evaluate various kinds of medium morphology irregularities results from the modeling methodology once a porous medium morphology is assigned. Further, when attempting to describe transport processes in a heterogeneous media, the correct form of the governing equations remains an area of continuously varying methods among researchers (see some discussion in Travkin and Catton [16, 21]).

An important feature of VAT is being able to consider specific medium types and morphologies, lower-scale fluctuations of variables, cross-effects of different variable fluctuations, interface variable fluctuations effects, etc. It is not possible to include all of these characteristics in current models using conventional theoretical approaches. The VAT approach has the following desirable features:

1. Effects of interfaces and grain boundaries can be included in the modeling.
2. The effect of morphology of the different phases is incorporated. The morphology decription is directly incorporated into the field equations.
3. Separate and combined fields and their interactions are described exactly. No assumptions about effective coefficients are required.
4. Effective coefficients correct mathematical description — those "theories" presently used for that purpose are only approximate description, and often simply wrong.
5. Correct description of experiments in heterogeneous media — again, at present the homogeneous presentation of medium properties is used for this purpose, and explanation of experiments is done via bulk features. Those bulk features describe the field as by classical homogeneous medium differential equations.
6. Deliberate design and optimization of materials using hierarchical physical descriptions based on the VAT governing equations can be used to connect properties and morphological characteristics to component features. What is usually done is to carry out an experimental search by adding a third or a fourth component to the piezoelectric material, for example. This can be done in a more direct, more observable way, and with a more correct understanding of the effects of adding additional components and, of course, of the morphology of the fourth component.

In this work we restrict ourselves to a brief analysis of previous work and show that the best theoretical tool is the nonlocal description of hierarchical, multiscaled processes resulting from application of VAT. Application of VAT to radiative transport in a porous medium is based on our advances in electrodynamics and microscale energy transport phenomena in two-phase heterogeneous media. Some other governing conservation equations for transport in porous media can be found in Travkin and Catton [21] and the references therein.

One of the aims of this work is to outline the possibilities for a method for optimizing transport in heterogeneous as well as porous structures that can be used in different engineering fields. Applications range from heat and mass exchangers and reactors in mechanical engineering design to environmental engineering usage (Travkin *et al.* [19]). A recent application is in urban air pollution, where optimal control of a pollutant level in a contaminated area is determined, along with the design of an optimal control point network for the control of constituent dispersion and remediation actions. Using second-order turbulent models, equation sets were obtained for turbulent filtration and two-temperature or two-concentration diffusion in nonisotropic porous media and interphase exchange and microroughness. Previous work has shown that the flow resistance and heat transfer over highly rough surfaces or in a rough channel or pipe can be properly predicted using the technique of averaging the transport equations over the near surface representative elementary volume (REV). Prescribing the statistical structure of the capillary or globular porous medium morphology gives the basis for transforming the integral–differential transport equations into differential equations with probability density functions governing their coefficients and source terms. Several different closure models for these terms for some uniform, nonuniform, nonisotropic, and specifically random nonisotropic highly porous layers were developed. Quite

different situations arise when describing processes occuring in irregular or random morphology. The latest results, obtained with the help of exact closure modeling for canonical morphologies, open a new field of possibilities for a purposeful search for optimal design of spacial heterogeneous transport structures. A way to find and govern momentum transport through a capillary nonintersecting medium by altering its morphometrical characteristics is given as validation of the process.

II. Fundamentals of Hierarchical Volume Averaging Techniques

Since the porosity in a porous medium is often anisotropic and randomly inhomogeneous, the random porosity function can be decomposed into additive components: the average value of $\langle m(x)\rangle$ in the REV and its fluctuations in various directions,

$$m_1(\vec{x}) = \langle m_1(\vec{x})\rangle + \hat{m}_1(\vec{x}), \qquad \langle m_1\rangle = \frac{\Delta\Omega_1}{\Delta\Omega}.$$

The averaged equations of turbulent filtration for a highly porous medium are similar to those in an anisotropic porous medium. Five types of averaging over an REV function f are defined by the following averaging operators arranged in their order of seniority (Primak *et al.* [14]): average of f over the whole REV,

$$\langle f\rangle = \langle f\rangle_1 + \langle f\rangle_2 = \langle m_1\rangle \tilde{f}_1 + (1 - \langle m_1\rangle)\tilde{f}_2, \tag{1}$$

phase averages of f in each component of the medium,

$$\langle f\rangle_1 = \langle m_1\rangle \frac{1}{\Delta\Omega_1}\int_{\Delta\Omega_1} f(t, \vec{x})\, d\omega = \langle m_1\rangle \tilde{f}_1 \tag{2}$$

$$\langle f\rangle_2 = \langle m_2\rangle \frac{1}{\Delta\Omega_2}\int_{\Delta\Omega_2} f(t, \vec{x})\, d\omega = \langle m_2\rangle \tilde{f}_2 \tag{3}$$

and intraphase averages,

$$\{f\}_1 = \tilde{f}_1 = \frac{1}{\Delta\Omega_1}\int_{\Delta\Omega_1} f(t, \vec{x})\, d\omega \tag{4}$$

$$\{f\}_2 = \tilde{f}_2 = \frac{1}{\Delta\Omega_2}\int_{\Delta\Omega_2} f(t, \vec{x})\, d\omega. \tag{5}$$

When the interface is fixed in space, the averaged functions for the first and second phase (as liquid and solid) within the REV and over the entire REV fulfill the conditions

$$\{f + g\}_1 = \{f\}_1 + \{g\}_1 \qquad \text{and} \qquad \{a_1\} = a = \text{const} \tag{6}$$

for steady-state phases and

$$\left\{\frac{\partial f}{\partial t}\right\}_1 = \frac{\partial\{f\}_1}{\partial t}, \qquad \{\tilde{f}\tilde{g}\}_1 = \tilde{f}\tilde{g} \tag{7}$$

except for the differentiation condition,

$$\{\nabla f\}_1 = \nabla\tilde{f} + \frac{1}{\Delta\Omega_f}\int_{\partial S_w} \hat{f}\vec{ds}_1$$

$$\hat{f} = f - \tilde{f}, \qquad f \forall \Delta\Omega_f, \tag{8}$$

where ∂S_w is the inner surface in the REV, and $\vec{ds}$ is the solid-phase, inward-directed differential area in the REV ($\vec{ds} = \vec{n}dS$). The fourth condition implies an unchanging porous medium morphology.

The three types of averaging fulfill all four of the preceding conditions as well as the following four consequences:

$$\{\tilde{f}\}_1 = \tilde{f}, \quad \{\tilde{f}\}_1 = \{f - \tilde{f}\}_1 = 0 \tag{9}$$

$$\{\tilde{f}\tilde{g}\}_1 = \tilde{f}\tilde{g}, \quad \{\tilde{f}\hat{g}\}_1 = \tilde{f}\tilde{\hat{g}} = 0 \tag{10}$$

Meanwhile, $\langle f\rangle_1$ and $\langle f\rangle_2$ fulfill neither the third of the conditions,

$$\langle a\rangle_1 \neq a, \qquad \langle a\rangle_1 = \langle m_1\rangle a, \tag{11}$$

nor all the consequences of the other averaging conditions. Futher, the differential condition becomes

$$\langle\nabla f\rangle_1 = \nabla\langle f\rangle_1 + \frac{1}{\Delta\Omega}\int_{\partial S_{12}} f\vec{ds}_1, \tag{12}$$

in accordance with one of the major averaging theorems—the theorem of averaging the ∇ operator (Slattery [6]; Gray *et al.* [8]; Whitaker [10]).

If the statistical characteristics of the REV morphology and the averaging conditions with their consequences lead to the following special ergodic hypothesis: the spacial averages, ($\langle f\rangle_1$, $\tilde{f}$, and $\{f\}_2$), then this theorem converges with increases in the averaging volume to the appropriate probability (statistical) average of the function f of a random value with probability density distribution p. This hypothesis is stated mathematically as follows:

$$\tilde{f}^b(\vec{x}) = \int_{-\infty}^{\infty} f(\vec{x}, \alpha)p_\alpha\{\alpha, \vec{x}\}\, d\alpha$$

$$\lim_{\Delta\Omega\to\infty} \tilde{f} = \tilde{f}^b. \tag{13}$$

Quintard and Whitaker [29] expressed some concern about the connection between different scale volume averaged variables, for example,

$$\langle T_f \rangle_f = \frac{1}{\Delta\Omega} \int_{\Delta\Omega_f} T_f \, d\omega \tag{14}$$

$$\{T_f\}_f = \frac{1}{\Delta\Omega_f} \int_{\Delta\Omega_f} T_f \, d\omega. \tag{15}$$

In a truly periodic system it is known that the steady temperature in phase f can be written as

$$T_f(\mathbf{r}_f) = \mathbf{h} \cdot \mathbf{r}_f + \mathring{T}_f(\mathbf{r}_f) + T_{f0}, \tag{16}$$

where $\mathbf{h}$ and T_{f0} are constants and $\mathring{T}_f(\mathbf{r}_f)$ is a periodic function of zero mean over the f-phase. Applying the phase averaging operator $\langle \, \rangle_f$ to this function, one finds

$$\langle T_f(\mathbf{x}) \rangle_f = \mathbf{h} \cdot \langle \mathbf{r}_f(\mathbf{x}) \rangle_f + \langle \mathring{T}_f(\mathbf{r}_f) \rangle_f + \langle m \rangle T_{f0},$$

while Quintard and Whitaker [29] obtain (their Eq. (13))

$$\langle T_f(\mathbf{r}_f) \rangle_f = \langle T_f(\langle \mathbf{r}_f \rangle_f) \rangle_f = \mathbf{h} \cdot \langle \mathbf{r}_f \rangle_f + \langle m \rangle T_{f0}, \tag{17}$$

meaning that

$$\langle \mathring{T}_f(\mathbf{r}_f) \rangle_f = 0. \tag{18}$$

The parameter $\langle \mathring{T}_f(\mathbf{r}_f) \rangle_f$ cannot always be equal to zero, because it depends on the peculiarities of the chosen REV. In some instances, when the REV is not the volume that contains the known number of exact function periods, the averaged function $\langle \mathring{T}_f(\mathbf{r}_f) \rangle_f$ value should not be zero. If it is assumed, however, that the REV volume $\Delta\Omega$ contains the exact number of spacial periods, then

$$\langle \mathring{T}_f(\mathbf{r}_f) \rangle_f = 0.$$

Averaging the fluid temperature, T_f, over $\Delta\Omega_f$ yields the intrinsic average

$$\{T_f(\mathbf{x})\}_f = \mathbf{h} \cdot \{\mathbf{r}_f\}_f + T_{f0} = \mathbf{h} \cdot \mathbf{x} + \mathbf{h} \cdot \{\mathbf{y}_f\}_f + T_{f0}, \tag{19}$$

because the averaging of $\mathbf{r}_f$ (see Fig. 1) results in

$$\{\mathbf{r}_f\}_f = \mathbf{x} + \{\mathbf{y}_f\}_f, \tag{20}$$

while Quintard and Whitaker [29] obtain (their Eq. (15))

$$\{T_f\}_f = \{T_f(\{\mathbf{r}_f\}_f)\}_f = \mathbf{h} \cdot \{\mathbf{r}_f\}_f + T_{f0} \tag{21}$$

They note (see p. 375), "now represent $\mathbf{r}_f$ in terms of the position vector, $\mathbf{x}$, that locates the centroid of the averaging volume, and the relative

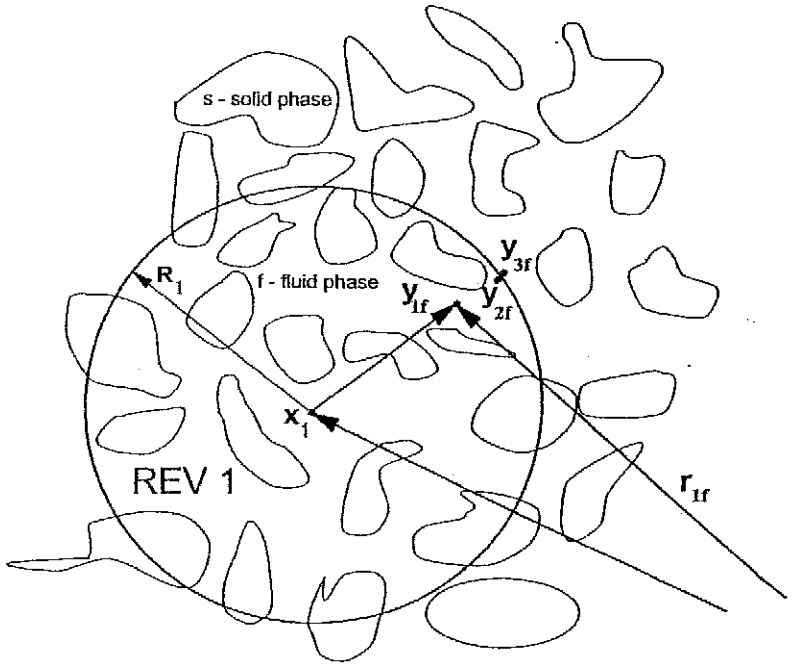

FIG. 1. Representative elementary averaging volume with the "virtual" points of representation inside of the REV (Carbonell and Whitaker [31]; Quintard and Whitaker [29]).

position vector $\mathbf{y}_f$ as indicated in Fig. 3" (see Fig. 1), or

$$\mathbf{r}_f = \mathbf{x} + \mathbf{y}_f \Rightarrow \{\mathbf{r}_f(\mathbf{x}, \mathbf{y}_f)\}_f = \mathbf{x} + \{\mathbf{y}_f(\mathbf{r}_f, \mathbf{x})\}_f, \tag{22}$$

so that Eq. (21) can be written with dependence on both $\mathbf{x}$ and $\mathbf{r}_f$,

$$\{T_f(\mathbf{x}, \mathbf{r}_f)\}_f = \{T_f(\mathbf{x}, \{\mathbf{y}_f\}_f)\}_f = \mathbf{h} \cdot \mathbf{x} + \mathbf{h} \cdot \{\mathbf{y}_f(\mathbf{r}_f, \mathbf{x})\}_f + T_{f0}, \tag{23}$$

meaning that after averaging, $T_f(\mathbf{r}_f)$ continues to be dependent on the position of the "virtual" point $\mathbf{r}_f$, which may have changed location within the $\Delta\Omega_f$.

To do this, they introduce a so-called "virtual REV" allowing the averaged value inside of the REV to be variable (see the remark on p. 354 of Quintard and Whitaker [30]: "In all our previous studies of multiphase transport phenomena, we have always assumed that averaged quantities could be treated as constants *within the averaging volume* and that the *average of the spatial deviations was zero*. We now wish to avoid these assumptions..."), and the result is a "virtual" averaged variable that is not

constant within the fixed volume of the REV. When Quintard and Whittaker derive the gradient of the average of the function (23), they use its dependence on $\mathbf{x}$ for the two right-hand-side terms in (23) to obtain

$$\nabla\{T_f(\mathbf{x}, \mathbf{r}_f)\}_f = \mathbf{h} + \mathbf{h}\cdot\nabla_{\mathbf{x}}\{\mathbf{y}_f(\mathbf{r}_f, \mathbf{x})\}_f. \tag{24}$$

Several comments about the Quintard and Whittaker treatment that need to be considered are the following:

1. How the communication of the variables from different spaces $\mathbf{r}_f$ at the lower scale space and $\mathbf{x}$ at the upper scale space is established is not meaningful. Their connection must be determined at the beginning of the averaging process and their communication is very limited.

2. One should only connect a value at a point at the higher level to the lower level REV, not only to a point within the lower level REV. When one considers an averaged variable at any point other than the representative point $\mathbf{x}$ for a particular REV, then

$$\nabla\{T_f(\mathbf{x})\}_f = \nabla(\mathbf{h}\cdot\mathbf{x} + \{\mathring{T}_f(\mathbf{x})\}_f + T_{f0}),$$

and for the upper scale, the exact result is

$$\nabla\{T_f(\mathbf{x})\}_f = \nabla(\mathbf{h}\cdot\mathbf{x} + T_{f0}) = \mathbf{h}. \tag{25}$$

3. If a function and its gradient are periodic, then the averaged function should be periodic. The VAT-based answer should be seen by determination of the averaged values, which are not averaged, only the REV being used at the lower scale.

The work by Quintard and Whittaker and the improving of understanding of some basic principles of averaging has led us to state the following lemma and then point out differences from the work of Whittaker and his colleagues.

Lemma. *If a function ψ, representing any continuous physical field, is averaged over the subdomain $\Delta\Omega_{1f}$, which is the subregion occupied by phase f (fluid phase) of the REV $\Delta\Omega_1$ in the heterogeneous two-phase medium (Fig. 1), and the averaged function $\{\psi(\mathbf{x})\}_f$ is assumed to have different values at different locations $\mathbf{x}_i$ within the $\Delta\Omega_{1f}$, then the averaged function $\{\psi(\mathbf{x})\}_f$ can have discontinuities of the first kind at the boundary $\partial\Delta\Omega_1$ of the REV $\Delta\Omega_1$.*

Proof. Consider the situation where the point $\mathbf{y}_{2f}$ (Fig. 1; see also Fig. 3, p. 375, in the paper by Quintard and Whitaker [29]) is located an infinitely distance from the boundary of the REV $\Delta\Omega_1$ within $\partial\Delta\Omega_1$. It represents the intrinsic phase averaged value $\{\psi_{2f}\}_f$ of variable ψ averaged in the REV $\Delta\Omega_1$. According to Carbonell and Whitaker [31] and Quintard and Whitaker [29], its value can be different from $\{\psi_{1f}\}_f$ or $\{\psi_x\}_f$.

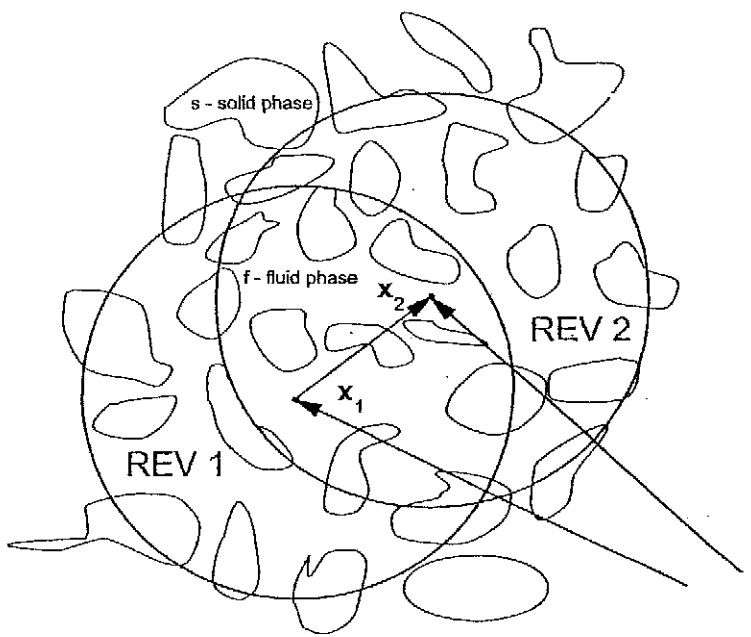

FIG. 2. Representative elementary averaging volumes with the fixed points of representation.

Next, consider a point $\mathbf{y}_{3f}$ located an infinitely small distance outside of the initial REV $\Delta\Omega_1$ within a boundary $\partial\Delta\Omega_1$. The point $\mathbf{y}_{3f}$ represents the averaged value $\{\psi_{3f}\}_f$ which belongs to some REV $\Delta\Omega_3$, as shown in Fig. 2, with its center at the point $\mathbf{x}_3 = (\mathbf{y}_{3f} - \varepsilon) + (R_1/2)$, with ε being an infinitely small constant.

Following arguments of Carbonell and Whitaker [31], this point $\mathbf{y}_{3f}$ is allowed to be in at least one more REV, $\Delta\Omega_2$, which has its center $\mathbf{x}_2$ just shifted from the point $\mathbf{x}_1$ an infinitely small distance, as does $\mathbf{y}_{3f}$ from the boundary $\partial\Delta\Omega_1$.

Further, suppose that one is approaching the boundary $\partial\Delta\Omega_1$ from both sides by points $\mathbf{y}_{2f}$ and $\mathbf{y}_{3f}$. According to Carbonell and Whitaker [31] and Quintard and Whitaker [29], the values $\{\psi_{2f}\}_f$ and $\{\psi_{3f}\}_f$ can be different when $\partial\Delta\Omega_1$ is reached, which means that the averaged value $\{\psi\}_f$ experiences (can have) a discontinuity at each and every point of the boundary $\partial\Delta\Omega_1$.

As long as the boundary $\partial\Delta\Omega_1$ of the REV can be arbitrarily moved, changed or assigned, then the consequence of this change is that $\{\psi_f\}_f$ can have discontinuities at each point of a REV.

The relationships between different scale variables and their points of representation can be found by noting the following points:

1. There is a fixed relationship between the location of the point $\mathbf{x}_1$ of the upper scale field and averaging within the REV $\Delta\Omega_1$. In other words, for each determined $\Delta\Omega_1$ there is only one $\mathbf{x}_1$ that represents the value $\{\psi_f(\mathbf{x}_1)\}_f$ on the upper field level (macroscale field) if both are mapped on the same region (excluding close to boundary regions).

2. If there is the value $\{\psi_f(\mathbf{x}_2)\}_f$, $(\mathbf{x}_2 - \mathbf{x}_1) \leqslant \varepsilon$, then there is another $\Delta\Omega_2 \neq \Delta\Omega_1$, and in it

$$\{\psi_f(\mathbf{x}_2)\}_f = \frac{1}{\Delta\Omega_{f2}} \int_{\Delta\Omega_{f2}} \psi_f(\mathbf{r}_f)\, d\omega \neq \frac{1}{\Delta\Omega_{f1}} \int_{\Delta\Omega_{f1}} \psi_f(\mathbf{r}_f)\, d\omega, \qquad (26)$$

where $\psi_f(\mathbf{r}_f) \neq const.$

A. Theoretical Verification of Central VAT Theorem and Its Consequences

When the coefficient of thermal conductivity k_f is a constant value, the fluid stedy-state conduction regime is described by

$$k_f \nabla^2(\langle m\rangle \tilde{T}_f) + \nabla\cdot\left[\frac{k_f}{\Delta\Omega}\int_{\partial S_w} T_f \vec{d}s\right] + \frac{k_f}{\Delta\Omega}\int_{\partial S_w} \nabla T_f \cdot \vec{d}s = 0. \qquad (27)$$

The full 1D Cartesian coordinates version of this equation, without any source, for a fixed solid matrix in is

$$\frac{\partial}{\partial x}\left[\langle m\rangle \frac{\partial \tilde{T}_f}{\partial x}\right] + \frac{\partial}{\partial x}\left[\frac{1}{\Delta\Omega}\int_{\partial S_w} \hat{T}_f \vec{d}s\right] + \frac{1}{\Delta\Omega}\int_{\partial S_w} \frac{\partial T_f}{\partial x_i}\cdot \vec{d}s = 0, \qquad (28)$$

$$\frac{\partial}{\partial x}\left[\langle m\rangle \frac{\partial \tilde{T}_f}{\partial x}\right] + MD_2 + MD_3 = 0, \qquad (29)$$

where the second and third terms on the right-hand side are the so-called morphodiffusive terms, MD_2 and MD_3, respectively (see also, for example, Travkin and Catton [21]),

The solid-phase equation with constant k_s equation is of the same form,

$$\frac{\partial}{\partial x}\left(\langle s\rangle \frac{\partial\{T_s\}_s}{\partial x}\right) + \frac{\partial}{\partial x}\left[\frac{1}{\Delta\Omega}\int_{\partial S_w} \hat{T}_s \vec{d}s_1\right] + \frac{1}{\Delta\Omega}\int_{\partial S_w} \frac{\partial T_s}{\partial x_i}\cdot \vec{d}s_1 = 0, \qquad (30)$$

which can also be written in terms of the fluctuating variable,

$$\langle s\rangle \frac{\partial^2 \tilde{T}_s}{\partial x^2} + \frac{\partial}{\partial x}\left[\frac{1}{\Delta\Omega}\int_{\partial S_w} \hat{T}_s \vec{d}s_1\right] + \frac{1}{\Delta\Omega}\int_{\partial S_w} \frac{\partial \hat{T}_s}{\partial x_i}\cdot \vec{d}s_1 = 0. \qquad (31)$$

Travkin and Catton [16, 18, 20] suggested that the integral heat transfer terms in Eqs. (28, (30), and (31) be closed in a natural way by a third (III) kind of heat transfer law. The second integral term reflects the changing averaged surface temperature along the x coordinate. Equations (28) and (30) can be treated using heat transfer correlations for the heat exchange integral term (the last term). Regular dilute arrangements of pores, spherical particles, or cylinders have been studied much more than random morphologies. Using separate element or "cell" modeling methods (Sangani and Acrivos [32] and Gratton *et al.* [26]) to find the interface temperature field allows one to close the second, "surface" diffusion integral terms in (28), (30), and (27).

Many forms of the energy equation are used in the analysis of transport phenomena in porous media. The primary difference between such equations and those resulting from a more rigorous development based on VAT are certain additional terms. The best way to evaluate the need for these additional more complex terms is to obtain an exact mathematical solution and compare the results with calculations using the VAT equations. This will clearly display the need for using the more complex VAT mathematical statements.

Consider a two-phase heterogeneous medium consisting of an isotropic continuous (solid or fluid) matrix and an isotropic discontinuous phase (spherical particles or pores). The volume fraction of the matrix, or f-phase, is $\langle m\rangle = m_f = \Delta\Omega_f/\Delta\Omega$, and the volume fraction of filler, or s-phase, is $m_s = 1 - m_f = \Delta\Omega_s/\Delta\Omega$, where $\Delta\Omega = \Delta\Omega_f + \Delta\Omega_s$ is the volume of the REV. The constant properties (phase conductivities, k_f and k_s), stationary (time-independent) heat conduction differential equations for T_f and T_s, the local phase temperatures, are

$$-\nabla\cdot\mathbf{q}_f = k_f\nabla^2 T_f = 0, \quad -\nabla\cdot\mathbf{q}_s = k_s\nabla^2 T_s = 0,$$

with the fourth (IVth) kind interfacial (f–s) thermal boundary conditions

$$T_f = T_s, \quad \mathbf{ds}_1\cdot\mathbf{q}_f|_{\partial S_w} = \mathbf{ds}_1\cdot\mathbf{q}_s|_{\partial S_w}.$$

Here $\mathbf{q}_f = -k_f\nabla T_f$ and $\mathbf{q}_s = -k_s\nabla T_s$ are the local heat flux vectors, ∂S_w is the interfacial surface, and $\mathbf{ds}_1$ is the unit vector outward to the s-phase. No internal heat sources are present inside the composite sample, so the temperature field is determined by the boundary conditions at the external surface of the sample. After correct formulation of these conditions, the problem is completely stated and has a unique solution.

Two ways to realize a solution to this problem were compared (Travkin and Kushch [33, 34]). The first is the conventional way of replacing the actual composite medium by an equivalent homogeneous medium with an effective thermal conductivity coefficient, $k = k_{eff}(\langle s\rangle, k_f, k_s)$, assuming one

knows how to obtain or calculate it. The exact effective thermal coefficient was obtained using direct numerical modeling (DNM) based on the mathematical theory of globular morphology multiphase fields developed by Kushch (see, for example, [35–38]).

Averaging the heat flux, $\langle \mathbf{q} \rangle$, and temperature, $\langle T \rangle$, over the REV yields $\langle \mathbf{q} \rangle = k_{eff} \nabla \langle T \rangle$, and for the stationary case there results

$$\nabla \cdot (k_{eff} \nabla \langle T \rangle) = 0. \tag{32}$$

The boundary conditions for this equation are formulated in the same manner as for a homogeneous medium.

The second way is to solve the problem using the VAT two-equation, three-term integrodifferential equations (28) and (30). To evaluate and compare solutions to these equations with the DNM results, one needs to know the local solution characteristics, the averaged characteristics over the both phases in each cell, and, in this case, the additional morphodiffusive terms.

An infinite homogeneous isotropic medium containing a three-dimensional (3D) array of spherical particles is chosen for analysis. The particles are arranged so that their centers lie at the nodes of a simple cubic lattice with period a. The temperature field in this heterogeneous medium is caused by a constant heat flux $\mathbf{Q}_z$ prescribed at the sample boundaries, which, because of the absence of heat sources, leads to the equality of averaged internal heat flux $\langle q \rangle = \mathbf{Q}_z$.

When all the particles have the same radii, the result is the triple periodic structure used widely, beginning from Rayleigh's work [39], to evaluate the effective conductivity of particle-reinforced composites.

The composite medium model consists of the three regions shown in Fig. 3. The half-space lying above the A–A plane has a volume content of the disperse phase $m_s = m_A$, and for the half-space below the B–B plane $m_s = m_B$. To define the problem, let $m_A > m_B$. The third part is the composite layer between the plane boundaries A–A and B–B containing N double periodic lattices of spheres (screens) with changing diameters.

Solutions to the VAT equations (28) and (30) for a composite with varying volume content of disperse phase with accurate DNM closure of the micro model VAT integrodifferential terms were obtained implicitly, meaning that each term was calculated independently using the results of DNM calculations.

For the one-dimensional case, Eq. (32) becomes

$$\frac{\partial}{\partial z}\left(k_{eff} \frac{\partial T}{\partial z}\right) = 0, \quad (z_1 \leqslant z \leqslant z_2), \quad m_s = m_s(z),$$

where $k_{eff}(m_s)$ is the effective conductivity coefficient.

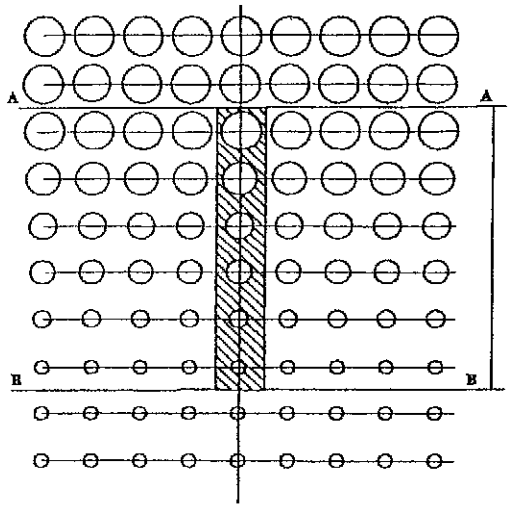

FIG. 3. Model of two-phase medium with variable volume fraction of disperse phase.

The normalized solution of the both models (VAT and DNM) for the case of linearly changing porosity $m_s = m_s^{(1)} + z(m_s^{(2)} - m_s^{(1)})$, where $m_s(z_1) = m_s^{(1)}$, $m_s(z_2) = m_s^{(2)}$, $z_1 = 0$, $z_2 = 1$, between A–A and B–B and with effective conductivity coefficients of $k_{eff} = 0$, 0.2, 1, 10, and 10,000, are presented in Fig. 4. There is practically no difference (less than 10^{-3}) between the solutions, and what there is is probably because of numerical error accumulation (Travkin and Kushch [34]).

Lines 1–5 represent solutions of the one-term equation, respectively, whereas the points (circles, triangles, etc.) represent the solutions of the VAT equations with accurate DNM closure of the micro model VAT integrodifferential terms MD_2 and MD_3 for the composite with varying volume content of disperse phase. Here the number of screens is nine, corresponding to a relatively small particle phase concentration gradient.

The coincidence of the results of the exact calculation of the two-equation, three-term conductive-diffusion transport VAT model (28) and (30) with the exact DNM solution and with the one-temperature effective coefficient model for heterogeneous media with nonconstant spatial morphology clearly demonstrates the need for using all the terms in the VAT equations. The need for the morphodiffusive terms in the energy equation is further demonstrated by noting that their magnitudes are all of the same order.

Confirmation of the fact that there is no difference in solutions between the correct one-term, one-temperature effective diffusivity equation and the

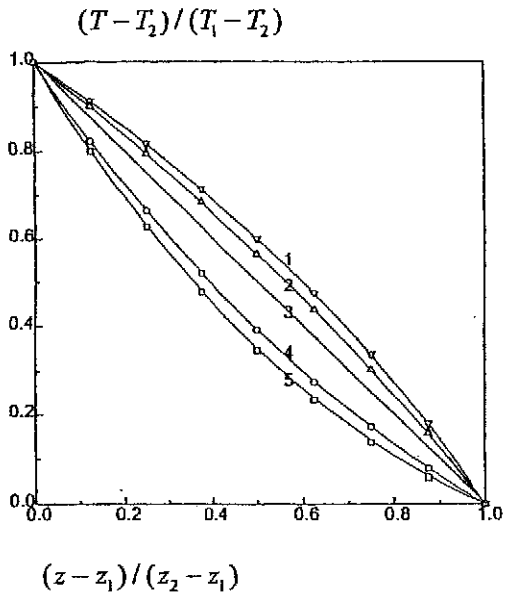

FIG. 4. Comparison of VAT three-term equation particle temperature (symbols) with the exact analytical based on the effective conductance coefficient obtained by exact DNM (solid lines).

three-terms, two-temperature VAT equations does not mean that it is better to take for modeling and analysis the effective diffusivity one-term, one-temperature equation (see Subsection VI, E and arguments in Sections VII and VIII). Among other issues one needs to analyze goals of modeling and to understand that the good solution of the effective diffusivity one-term one-temperature equation as it was found and described in the preceding statements means nothing less than the ground of the exact solution of the VAT problem. Also, it is important that for the exact (or accurate) solution of conventional diffusivity equation, the effective coefficient needs to be found, and this means in turn that finding the solution of the two-field problem is imperative and consequently appears to be the major problem. Meanwhile, this is the problem that was posed just at the beginning as the original one.

III. Nonlinear and Turbulent Transport in Porous Media

To a great extent, the analysis of porous media linear transport phenomena are given in the numerous studies by Whitaker and coauthors; see, for

example, [10, 30, 31, 40–46], as well as by studies by Gray and coauthors [8, 47–50]. Our present work is mostly devoted to the description of other physical fields, along with development of their physical and mathematical models. Still, the connection to linear and partially linear problem statements needs to be outlined.

The linear Stokes equations are

$$\nabla V = 0,$$
$$0 = -\nabla p + \mu \nabla^2 V + \rho_f \vec{g}, \tag{33}$$

and although the Stokes equation is adequate for many problems, linear as well as nonlinear processes will result in different equations and modeling features.

The general averaged form of the transport equations will be developed for permeable interface boundaries between the phases. Two forms of the right-hand-side Laplacian term will be considered. First, one can have two forms of the diffusive flux in gradient form that can be written

$$\langle \mu \nabla V \rangle_f = \mu \nabla \langle V \rangle_f + \frac{\mu}{\Delta\Omega} \int_{\partial s_w} V \vec{d}s \tag{34}$$

or

$$\langle \mu \nabla V \rangle_f = \mu \langle m \rangle \nabla \tilde{V} + \frac{\mu}{\Delta\Omega} \int_{\partial s_w} \hat{V} \vec{d}s. \tag{35}$$

It was pointed out first by Whitaker [42, 43] that these forms allow greater versatility in addressing particular problems. Using the two averaged forms of the velocity gradient, (34) and (35), one can obtain two averaged versions of the diffusion term in Eq. (33), namely,

$$\langle \mu \nabla (\nabla V) \rangle_f = \mu \nabla \cdot (\nabla \langle m \rangle \tilde{V}) + \mu \nabla \cdot \left[\frac{1}{\Delta\Omega} \int_{\partial s_w} V \vec{d}s \right] + \frac{\mu}{\Delta\Omega} \int_{\partial s_w} \nabla V \cdot \vec{d}s, \tag{36}$$

where the production term $\nabla V \cdot \vec{d}s$ is a tensorial variable, and the version with fluctuations in the second integral term

$$\langle \mu \nabla (\nabla V) \rangle_f = \mu \nabla \cdot (\langle m \rangle \nabla \tilde{V}) + \mu \nabla \cdot \left[\frac{1}{\Delta\Omega} \int_{\partial s_w} \hat{V} \vec{d}s \right] + \frac{\mu}{\Delta\Omega} \int_{\partial s_w} \nabla V \cdot \vec{d}s, \tag{37}$$

Using these two forms of the momentum viscous diffusion term, one can write two versions of the averaged Stokes equations. The first version is

$$\nabla\langle V\rangle_f + \frac{1}{\Delta\Omega}\int_{\partial S_w} U_i\cdot\vec{d}s = 0, \quad U_i \equiv V \tag{38}$$

and

$$0 = -\nabla\langle p\rangle_f - \frac{1}{\Delta\Omega}\int_{\partial S_w} p\vec{d}s + \mu\nabla\cdot(\nabla\langle m\rangle\tilde{V}) + \mu\nabla\cdot\left[\frac{1}{\Delta\Omega}\int_{\partial S_w} V\vec{d}s\right] + \frac{\mu}{\Delta\Omega}\int_{\partial S_w}\nabla V\cdot\vec{d}s + \langle m\rangle\rho_f\vec{g}, \tag{39}$$

and the second version is found by using the following relation for the pressure gradient:

$$-\nabla\langle p\rangle_f - \frac{1}{\Delta\Omega}\int_{\partial S_w} p\vec{d}s = -\langle m\rangle\nabla\tilde{p} - \frac{1}{\Delta\Omega}\int_{\partial S_w}\hat{p}\vec{d}s. \tag{40}$$

Using the averaging rules developed by Primak *et al.* [14], Shcherban *et al.* [15] and Travkin and Catton [16, 18] facilitated the development of the momentum equation. By combining equations (37) and (40), one is able to write the momentum transport equations in the second form with velocity fluctuations

$$\nabla\langle V\rangle_f - \{V\}_f\nabla\langle m\rangle + \frac{1}{\Delta\Omega}\int_{\partial S_w}\hat{U}_i\cdot\vec{d}s = 0, \tag{41}$$

obtained using

$$V = \{V\}_f + \hat{V}$$

$$\frac{1}{\Delta\Omega}\int_{\partial S_w} V\vec{d}s = -\{V\}_f\nabla\langle m\rangle + \frac{1}{\Delta\Omega}\int_{\partial S_w}\hat{U}_i\cdot\vec{d}s, \tag{42}$$

and the momentum equation

$$0 = -\langle m\rangle\nabla\tilde{p} - \frac{1}{\Delta\Omega}\int_{\partial S_w}\hat{p}\vec{d}s + \mu\nabla\cdot(\langle m\rangle\nabla\tilde{V}) + \mu\nabla\cdot\left[\frac{1}{\Delta\Omega}\int_{\partial S_w}\hat{V}\vec{d}s\right] + \frac{\mu}{\Delta\Omega}\int_{\partial S_w}\nabla V\cdot\vec{d}s + \langle m\rangle\rho_f\vec{g}. \tag{43}$$

The third version of these equations is almost never used but can be found in [21].

A. Laminar Flow with Constant Coefficients

The transport equations for a fluid phase with linear diffusive terms are

$$\frac{\partial U_i}{\partial x_i} = 0 \tag{44}$$

$$\frac{\partial U_i}{\partial t} + U_j\frac{\partial U_i}{\partial x_j} = -\frac{1}{\rho_f}\frac{\partial p}{\partial x_j} + \nu\frac{\partial}{\partial x_j}\left(\frac{\partial U_i}{\partial x_j}\right) + S_u \tag{45}$$

$$\frac{\partial\Phi_f}{\partial t} + U_j\frac{\partial\Phi_f}{\partial x_j} = D_f\frac{\partial}{\partial x_j}\left(\frac{\partial\Phi_f}{\partial x_j}\right) + S_{\Phi_f}. \tag{46}$$

Here Φ represents any scalar field (for example, concentration C) that might be transported into either of the porous medium phases, and the last terms on the right-hand side of (45) and (46) are source terms. In the solid phase, the diffusion equation is

$$\frac{\partial\Phi_s}{\partial t} = D_s\frac{\partial}{\partial x_j}\left(\frac{\partial\Phi_s}{\partial x_j}\right) + S_{\Phi_s}. \tag{47}$$

The averaged convective operator term in divergence form becomes, after phase averaging,

$$\left\langle\frac{\partial}{\partial x_j}(U_jU_i)\right\rangle_f = \langle\nabla(U_jU_i)\rangle_f = \nabla\langle U_jU_i\rangle_f + \frac{1}{\Delta\Omega}\int_{\partial S_w} U_jU_i\cdot\vec{d}s = \nabla[\langle m\rangle\tilde{U}_j\tilde{U}_i + \langle m\rangle\{\hat{u}_j\hat{u}_i\}_f] + \frac{1}{\Delta\Omega}\int_{\partial S_w} U_jU_i\cdot\vec{d}s. \tag{48}$$

Decomposition of the first term on the right-hand side of (48) yields fluctuation types of terms that need to be treated in some way.

The nondivergent version of the averaged convective term in the momentum equation is

$$\left\langle\frac{\partial}{\partial x_j}(U_jU_i)\right\rangle_f = \langle m\rangle\tilde{U}_j\nabla\tilde{U}_i + \tilde{U}_i\nabla\langle U_j\rangle_f + \nabla\langle\hat{u}_j\hat{u}_i\rangle_f + \frac{1}{\Delta\Omega}\int_{\partial S_w} U_jU_i\cdot\vec{d}s = \langle m\rangle\tilde{U}_j\frac{\partial}{\partial x_j}\tilde{U}_i - \tilde{U}_i\frac{1}{\Delta\Omega}\int_{\partial S_w} U_j\cdot\vec{d}s + \nabla\langle\hat{u}_j\hat{u}_i\rangle_f + \frac{1}{\Delta\Omega}\int_{\partial S_w} U_jU_i\cdot\vec{d}s. \tag{49}$$

The divergent and nondivergent forms of the averaged convective term in

the diffusion equation are

$$\langle \nabla(C\vec{U}_i)\rangle_f = \nabla\langle C\vec{U}_i\rangle_f + \frac{1}{\Delta\Omega}\int_{\partial S_w} C\vec{U}_i\cdot\vec{d}s$$

$$= \nabla[\langle m\rangle\tilde{C}\tilde{\vec{U}}_i + \langle m\rangle\{\hat{c}\hat{\vec{u}}_i\}_f] + \frac{1}{\Delta\Omega}\int_{\partial S_w} C\vec{U}_i\cdot\vec{d}s$$

$$= \langle m\rangle\tilde{\vec{U}}_i\frac{\partial}{\partial x_i}\tilde{C} - \tilde{C}\frac{1}{\Delta\Omega}\int_{\partial S_w}\vec{U}_i\cdot\vec{d}s + \nabla\langle\hat{c}\hat{\vec{u}}_i\rangle_f + \frac{1}{\Delta\Omega}\int_{\partial S_w} C\vec{U}_i\cdot\vec{d}s. \tag{50}$$

Other averaged versions of this term can be obtained using impermeable interface conditions (see also Whitaker [42] and Plumb and Whitaker [44]). For constant diffusion coefficient D, the averaged diffusion term becomes

$$\langle\nabla\cdot(D\nabla C)\rangle_f = D\nabla\cdot\nabla(\langle m\rangle\tilde{C}) + D\nabla\cdot\left[\frac{1}{\Delta\Omega}\int_{\partial S_w} C\vec{d}s\right] + \frac{D}{\Delta\Omega}\int_{\partial S_w}\nabla C\cdot\vec{d}s, \tag{51}$$

or

$$\langle\nabla\cdot(D\nabla C)\rangle_f = D\nabla\cdot(\langle m\rangle\nabla\tilde{C}) + D\nabla\cdot\left[\frac{1}{\Delta\Omega}\int_{\partial S_w}\hat{c}\vec{d}s\right] + \frac{D}{\Delta\Omega}\int_{\partial S_w}\nabla C\cdot\vec{d}s, \tag{52}$$

or

$$\langle D\cdot(D\nabla C)\rangle_f = D\langle m\rangle\nabla^2\tilde{C} + D\nabla\cdot\left[\frac{1}{\Delta\Omega}\int_{\partial S_w}\hat{c}\vec{d}s\right] + \frac{D}{\Delta\Omega}\int_{\partial S_w}\nabla\hat{c}\cdot\vec{d}s. \tag{53}$$

Other forms of Eq. (52), using the averaging operator for constant diffusion coefficient, constant porosity, and absence of interface surface permeability and transmittivity, can be found in works by Whitaker [42] and Plumb and Whitaker [44], as well as by Levec and Carbonell [46].

A similar derivation can be carried out for the momentum equation to treat cases where Stokes flow is invalid. Two versions of the momentum equation will result. The equation without the fluctuation terms is

$$\rho_f\left(\langle m\rangle\frac{\partial\tilde{\vec{V}}}{\partial t} + \langle m\rangle\tilde{\vec{V}}\cdot\nabla\tilde{\vec{V}} - \tilde{\vec{V}}\frac{1}{\Delta\Omega}\int_{\partial S_w}\vec{V}\cdot\vec{d}s + \nabla\langle\hat{\vec{v}}\hat{\vec{v}}\rangle_f + \frac{1}{\Delta\Omega}\int_{\partial S_w}\vec{V}\vec{V}\cdot\vec{d}s\right)$$

$$= -\nabla(\langle m\rangle\tilde{p}) - \frac{1}{\Delta\Omega}\int_{\partial S_w} p\vec{d}s + \mu\nabla\cdot\nabla(\langle m\rangle\tilde{\vec{V}})$$

$$+ \mu\nabla\cdot\left[\frac{1}{\Delta\Omega}\int_{\partial S_w}\vec{V}\vec{d}s\right] + \frac{\mu}{\Delta\Omega}\int_{\partial S_w}\nabla\vec{V}\cdot\vec{d}s + \langle m\rangle\rho_f\vec{g}. \tag{54}$$

with the fluctuation diffusion terms it becomes

$$\rho_f\left(\langle m\rangle\frac{\partial\tilde{\vec{V}}}{\partial t} + \langle m\rangle\tilde{\vec{V}}\cdot\nabla\tilde{\vec{V}} - \tilde{\vec{V}}\frac{1}{\Delta\Omega}\int_{\partial S_w}\vec{V}\cdot\vec{d}s + \nabla\langle\hat{\vec{v}}\hat{\vec{v}}\rangle_f + \frac{1}{\Delta\Omega}\int_{\partial S_w}\vec{V}\vec{V}\cdot\vec{d}s\right)$$

$$= -\langle m\rangle\nabla\tilde{p} - \frac{1}{\Delta\Omega}\int_{\partial S_w}\hat{p}\vec{d}s + \mu\nabla\cdot(\langle m\rangle\nabla\tilde{\vec{V}})$$

$$+ \mu\nabla\cdot\left[\frac{1}{\Delta\Omega}\int_{\partial S_w}\hat{\vec{v}}\vec{d}s\right] + \frac{\mu}{\Delta\Omega}\int_{\partial S_w}\nabla\vec{V}\cdot\vec{d}s + \langle m\rangle\rho_f\vec{g}. \tag{55}$$

The steady-state momentum transport equations for systems with impermeable interfaces can readily be derived from Eq. (54) and (55). They are

$$\rho_f(\langle m\rangle\tilde{\vec{V}}\cdot\nabla\tilde{\vec{V}} + \nabla\langle\hat{\vec{v}}\hat{\vec{v}}\rangle_f) = -\nabla(\langle m\rangle\tilde{p}) - \frac{1}{\Delta\Omega}\int_{\partial S_w} p\vec{d}s + \mu\nabla\cdot\nabla(\langle m\rangle\tilde{\vec{V}})$$

$$+ \frac{\mu}{\Delta\Omega}\int_{\partial S_w}\nabla\vec{V}\cdot\vec{d}s + \langle m\rangle\rho_f\vec{g}, \tag{56}$$

or

$$\rho_f(\langle m\rangle\tilde{\vec{V}}\cdot\nabla\tilde{\vec{V}} + \nabla\langle\hat{\vec{v}}\hat{\vec{v}}\rangle_f) = -\langle m\rangle\nabla\tilde{p}) - \frac{1}{\Delta\Omega}\int_{\partial S_w}\hat{p}\vec{d}s + \mu\nabla\cdot\nabla(\langle m\rangle\tilde{\vec{V}})$$

$$+ \frac{\mu}{\Delta\Omega}\int_{\partial S_w}\nabla\vec{V}\cdot\vec{d}s + \langle m\rangle\rho_f\vec{g}. \tag{57}$$

B. Nonlinear Fluid Medium Equations in Laminar Flow

To properly account for Newtonian fluid flow phenomena within a porous medium in a general way, modeling should begin with the Navier–Stokes equations for variable fluid properties,

$$\rho_f\left(\frac{\partial V}{\partial t} + V\cdot\nabla V\right) = -\nabla p + \nabla\cdot[\mu(\nabla V + (\nabla V)^*)] + \rho_f\vec{g} \tag{58}$$

$$\mu = \mu(V, C_i, T),$$

rather than the constant viscosity Navier–Stokes equations. The following form of the momentum equation will be used in further developments:

$$\rho_f\left(\frac{\partial V}{\partial t} + V\cdot\nabla V\right) = -\nabla p + \nabla\cdot(2\mu S) + \rho_f\vec{g} \tag{59}$$

$$\mu = \mu(V, C_i, T).$$

The negative stress tensor σ_{ij} in this equation is

$$N_{ij} = -\sigma_{ij} = 2\mu(\nabla V)^s = 2\mu S, \tag{60}$$

and the symmetric tensor S is the deformation tensor

$$S = (\nabla V)^s = \frac{1}{2}(\nabla V + (\nabla V)^*), \tag{61}$$

with $(\nabla V)^*$ being the transposed diad ∇V.

The homogeneous phase diffusion equations are

$$\frac{\partial \Phi_f}{\partial t} + U_j \frac{\partial \Phi_f}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\lambda_f(\vec{x}, \Phi_f, V)\frac{\partial \Phi_f}{\partial x_j}\right) + S_{\Phi_f} \tag{62}$$

and

$$\frac{\partial \Phi_s}{\partial t} = \frac{\partial}{\partial x_j}\left(\lambda_s \frac{\partial \Phi_s}{\partial x_j}\right) + S_{\Phi_s}. \tag{63}$$

Here Φ_f and λ are scalar fields and nonlinear diffusion coefficients for these fields. The averaging procedures for transport equation convective terms were established earlier. The averaged nonlinear diffusion term yields

$$\langle \nabla\cdot(D\nabla C)\rangle_f = \nabla\cdot(\langle m\rangle \tilde{D}\nabla\tilde{C}) + \nabla\cdot\left[\tilde{D}\frac{1}{\Delta\Omega}\int_{\partial S_w}\hat{c}\vec{d}s\right]$$
$$+\nabla\cdot(\langle\tilde{D}\nabla\hat{c}\rangle_f) + \frac{1}{\Delta\Omega}\int_{\partial S_w} D\nabla C\cdot\vec{d}s. \tag{64}$$

The other version of the diffusive terms with the full value of concentration on the interface surface is

$$\langle \nabla\cdot(D\nabla C)\rangle_f = \nabla\cdot(\tilde{D}\nabla(\langle m\rangle\tilde{C})) + \nabla\cdot\left[\tilde{D}\frac{1}{\Delta\Omega}\int_{\partial S_w} C\vec{d}s\right]$$
$$+\nabla\cdot(\langle\hat{D}\nabla\hat{c}\rangle_f) + \frac{1}{\Delta\Omega}\int_{\partial S_w} D\nabla C\cdot\vec{d}s. \tag{65}$$

General forms of the nonlinear transport equations can be derived for impermeable and permeable interface surfaces. The averaged momentum diffusion term is

$$\left\langle\frac{\partial}{\partial x_j}(2\mu S)\right\rangle_f = \langle\nabla\cdot(2\mu S)\rangle_f = \nabla\cdot(\langle 2\mu S\rangle_f) + \frac{1}{\Delta\Omega}\int_{\partial S_w} 2\mu S\cdot\vec{d}s$$
$$= \nabla\cdot 2(\langle m\rangle\tilde{\mu}\tilde{S} + \langle m\rangle\{\hat{\mu}\hat{S}\}_f) + \frac{2}{\Delta\Omega}\int_{\partial S_w}\mu S\cdot\vec{d}s. \tag{66}$$

The general nonlinear averaged momentum equation for a porous medium is

$$\rho_f\left(\langle m\rangle\frac{\partial\tilde{V}}{\partial t} + \langle m\rangle\tilde{V}\cdot\nabla\tilde{V} - \tilde{V}\frac{1}{\Delta\Omega}\int_{\partial S_w} V\cdot\vec{d}s + \nabla\langle\hat{v}\hat{v}\rangle_f + \frac{1}{\Delta\Omega}\int_{\partial S_w} VV\cdot\vec{d}s\right)$$
$$= -\nabla(\langle m\rangle\tilde{p}) - \frac{1}{\Delta\Omega}\int_{\partial S_w} p\vec{d}s + \nabla\cdot 2(\langle m\rangle\tilde{\mu}\tilde{S} + \langle m\rangle\{\hat{\mu}\hat{S}\}_f)$$
$$+\frac{2}{\Delta\Omega}\int_{\partial S_w}\mu S\cdot\vec{d}s + \langle m\rangle\rho_f\vec{g}. \tag{67}$$

The steady-state momentum transport equations for systems with impermeable interfaces follows from Eq. (67),

$$\rho_f(\langle m\rangle\hat{V}\cdot\nabla\tilde{V} + \nabla\langle\hat{v}\hat{v}\rangle_f)$$
$$= -\nabla(\langle m\rangle\tilde{p}) - \frac{1}{\Delta\Omega}\int_{\partial S_w} p\vec{d}s + \nabla\cdot 2(\langle m\rangle\tilde{\mu}\tilde{S} + \langle m\rangle\{\hat{\mu}\hat{S}\}_f)$$
$$+\frac{\mu}{\Delta\Omega}\int_{\partial S_w}\mu S\cdot\vec{d}s + \langle m\rangle\rho_f\vec{g}. \tag{68}$$

The averaged nonlinear mass transport equation in porous medium follows

$$\langle m\rangle\frac{\partial\tilde{C}_f}{\partial t} + \langle m\rangle\tilde{U}_i\nabla\tilde{C}_f - \frac{\tilde{C}_f}{\Delta\Omega}\int_{\partial S_w} U_i\cdot\vec{d}s + \nabla\langle\hat{c}_f\hat{u}_i\rangle_f + \frac{1}{\Delta\Omega}\int_{\partial S_w} C_f U_i\cdot\vec{d}s$$
$$= \nabla\cdot(\tilde{D}\nabla(\langle m\rangle\tilde{C})) + \nabla\cdot\left[\tilde{D}\frac{1}{\Delta\Omega}\int_{\partial S_w} C\vec{d}s\right]$$
$$+\nabla\cdot(\langle\hat{D}\nabla\hat{c}\rangle_f) + \frac{1}{\Delta\Omega}\int_{\partial S_w} D\nabla C\cdot\vec{d}s + \langle m\rangle S_{c_f}. \tag{69}$$

A few simpler transport equations that can be readily used while maintaining fundamental relationships in heterogeneous medium transport are given by Travkin and Catton [21].

C. Porous Medium Turbulent VAT Equations

Turbulent transport processes in highly structured or porous media are of great importance because of the large variety of heat- and mass-exchange equipment used in modern technology. These include heterogeneous media for heat exchangers and grain layers, packed columns, and reactors. In all cases there occurs a jet or stalled flow of fluids in channels or around the

obstacles. There are, however, few theoretical developments for flow and heat exchange in channels of complex configuration or when flowing around nonhomogeneous bodies with randomly varied parameters. The advanced forms of laminar transport equations in porous media were developed in a paper by Crapiste *et al.* [41]. For turbulent transport in heterogeneous media, there are few modeling approaches and their theoretical basis and final modeling equations differ.

The lack of a sound theoretical basis affects the development of mathematical models for turbulent transport in the complex geometrical environments found in nuclear reactors subchannels where rod-bundle geometries are considered to be formed by subchannels. Processes in each subchannel are calculated separately (see Teyssedou *et al.* [51]). The equations used in this work has often been obtained from two-phase transport modeling equations [52] with heterogeneity of spacial phase distributions neglected in the bulk. Three-dimensional two-fluid flow equations were obtained by Ishii [52] using a statistical averaging method. In his development, he essentially neglected nonlinear phenomena and took the flux forms of the diffusive terms to avoid averaging of the second power differential operators. Ishii and Mishima [53] averaged a two-fluid momentum equation of the form

$$\frac{\partial \alpha_k \rho_k v_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k v_k v_k) = -\alpha_k \nabla p_k + \nabla \cdot \alpha_k (\bar{\bar{\tau}} + \tau_k^t) + \alpha_k \rho_k \mathbf{g} + v_{ki} \Gamma_k + \mathbf{M}_{ik} - \nabla \alpha_k \cdot \tau_i, \qquad (70)$$

where α_k is the local void fraction, τ_i is the mean interfacial shear stress, τ_k^t is the turbulent stress for the kth phase, $\bar{\bar{\tau}}$ is the averaged viscous stress for the kth phase, Γ_k is the mass generation, and $\mathbf{M}_{ik}$ is the generalized interfacial drag. Using the area average in the second time averaging procedure, Ishii and Mishima [53] introduced a distribution of parameters to take into consideration the nonlinearity of convective term averaging. This approach cannot strictly take into account the stochastic character of various kinds of spatial phase distributions. The equations used by Lahey and Lopez de Bertodano [54] and Lopez de Bertodano *et al.* [55] are very similar, with the momentum equation being

$$\alpha_k \rho_k \frac{D_k u_{jk}}{Dt} = -\alpha_k \nabla p_k + \nabla \cdot \alpha_k [\mu_k \nabla u_{jk} - \rho_k (\overline{u'_{jk} u'_{jk}})] - \alpha_k \rho_k \mathbf{g} + \mathbf{M}_{ik} - \mathbf{M}_{wk} - \tau_i \cdot \nabla \alpha_k + (p_{ki} - p_k) \nabla \alpha_k. \qquad (71)$$

Here the index i denotes interfacial phenomena and M_{wk} is the volumetric wall force on phase k. Additional terms in Eq. (70) and (71) are usually based on separate micro modeling efforts and experimental data.

One of the more detailed derivations of the two-phase flow governing equations by Lahey and Drew [56] is based on a volume averaging methodology. Among the problems was that the authors developed their own volume averaging technique without consideration of theoretical advancements developed by Whitaker and colleagues [10, 42] and Gray *et al.* [8] for laminar and half-linear transport equations. The most important weaknesses are the lack of nonlinear terms (apart from the convection terms) that naturally arise and the nonexistence of interphase fluctuations.

Zhang and Prosperetti [57] derived averaged equations for the motion of equal-sized rigid spheres suspended in a potential flow using an equation for the probability distribution. They used the small particle dilute limit approximation to "close" the momentum equations. After approximate resolution of the continuous phase fluctuation tensor $\mathbf{M}_c$, the vector $\mathbf{A}_D(x, t)$, and the fluctuating particle volume flux tensor, $\mathbf{M}_D$, they recognized that (p. 199) "Closure of the system requires an expression for the fluctuating particle volume flux tensor $\mathbf{M}_D$.... This missing information cannot be supplied internally by the theory without a specification of the initial conditions imposed on the particle probability distribution." They also considered the case of "finite volume fractions for the linear problem" where the problem equations were formulated for inviscid and unconvectional media. The development by Zhang and Prosperetti [57] is a good example of the correct application of ensemble averaging. The equations they derive compare exactly with those derived from rigorous volume averaging theory (VAT) [24].

Transport phenomena in tube bundles of nuclear reactors and heat exchangers can be modeled by treating them as porous media [58]. The two-dimensional momentum equations for a constant porosity distribution usually have the form [59]

$$\frac{\partial U}{\partial x} + \frac{\partial V}{\partial y} = 0 \qquad (72)$$

$$\frac{\partial U^2}{\partial x} + \frac{\partial UV}{\partial y} = -\frac{1}{\rho}\frac{\partial P}{\partial x} + \nu_{eff} \nabla^2 U - A_x |\vec{V}|^n U \qquad (73)$$

$$\frac{\partial UV}{\partial x} + \frac{\partial V^2}{\partial y} = -\frac{1}{\rho}\frac{\partial P}{\partial y} + \nu_{eff} \nabla^2 V - A_y |\vec{V}|^n V, \; n > 0, \qquad (74)$$

where the physical quantities are written as averaged values and the solid phase effects are included in two coefficients of bulk resistance, A_x and A_y, and an effective eddy viscosity, ν_{eff}, that is not equal to the turbulent eddy viscosity. These kinds of equations were not designed to deal with non-

linearities induced by the physics of the problem and the medium variable porosity or to take into account local inhomogeneities.

Some of the more interesting applications of turbulent transport in heterogeneous media are to agrometeorology, urban planning, and air pollution. The first significant papers on momentum and pollutant diffusion in urban environment treated as a two-phase medium were those by Popov [60, 61]. In these investigations, an urban porosity function was defined based on statistical averaging of a characteristic function $\eta(x, y, z)$ for the surface roughness that is equal to zero inside of buildings and other structures and equal to unity in an outdoor space. The turbulent diffusion equation for an urban roughness porous medium after ensemble averaging is

$$\frac{\partial m(x_i)\langle \bar{C}_n\rangle}{\partial t} + \frac{\partial}{\partial x_i}\left(m(x_i)\langle \bar{V}_i\rangle\langle \bar{C}_n\rangle\right) = -\frac{\partial}{\partial x_i}\langle(\bar{v}_i)'(\bar{c}_n)'\rangle - \frac{\partial}{\partial x_i}\langle\overline{v_i' c_n'}\rangle + \frac{\partial}{\partial x_i}\left(D_n \frac{\partial\langle C_n\rangle}{\partial x_i}\right), \quad n = 1, 2, 3, 4\ldots, \tag{75}$$

where $\langle\ \rangle$ means porous volume ensemble averaging, and $m(x_i)$ is porosity. Closure of the two "morphological" terms, the first and the second terms on the right-hand side, was obtained using a Boussinesque analogy,

$$\frac{\partial}{\partial x_i}\langle(\bar{v}_i)'(\bar{c}_n)'\rangle + \frac{\partial}{\partial x_i}\langle\overline{v_i' c_n'}\rangle = -K_{ij}\frac{\partial\langle \bar{C}_n\rangle}{\partial x_j}. \tag{76}$$

A descriptive analysis of the deviation variables $(\bar{v}_i)'$, $(\bar{c}_n)'$ and the effective diffusion coefficient K_{ij} was not given. In many studies of meteorology and agronomy, the only modeling of the increase in the volume drag resistance is by addition of a nonlinear term as done by Yamada [62],

$$\frac{\partial \bar{U}}{\partial t} = f_k \bar{V} - \frac{1}{\rho}\frac{\partial \bar{P}}{\partial x} + \frac{\partial}{\partial z}\left(-\overline{u'w'}\right) - (1 - m_s)c_d S(z)|\bar{U}|\bar{U} \tag{77}$$

$$\frac{\partial \bar{V}}{\partial t} = -f_k \bar{U} - \frac{1}{\rho}\frac{\partial \bar{P}}{\partial y} + \frac{\partial}{\partial z}\left(-\overline{v'w'}\right) - (1 - m_s)c_d S(z)|\bar{V}|\bar{V},$$

where $(1 - m_s)$ is the fraction of the earth surface occupied by forest, m_s is the area porosity due to a tree volume, and f_k is a Coriolis parameter.

The averaging technique used by Raupach and Shaw [63] to obtain a turbulent transport equation for a two-phase medium of agro- and forest

cultures is a plain surface 2D averaging procedure where the averaged function is defined by

$$\langle f\rangle_{pf} = \frac{1}{\Delta\Omega_{pf}}\int_{\Delta\Omega_{pf}} f\vec{d}\omega, \tag{78}$$

with $\Delta\Omega_{pf}$ being the area within the volume $\Delta\Omega_p$ occupied by air. Raupach *et al.* [64] and Coppin *et al.* [65] assumed that the dispersive covariances were unimportant,

$$\langle \bar{u}_i''\bar{u}_j''\rangle_{pf}, \tag{79}$$

where $\bar{u}_i''$ is a fluctuation value within the canopy and $\bar{u}_i'' \neq u_i'$. The contribution of these covariances was found by Raupach *et al.* [64] to be small in the region just above the canopy from experiments with a regular rough morphology. This finding has been explained by Scherban *et al.* [15], Primak *et al.* [14], and Travkin and Catton [16, 20] for regular porous (roughness) morphology. Covariances are, however, the result of irregular or random two-phase media. When the surface averaging used by Raupach and Shaw [64] is used instead of volume averaging, especially in the case of nonisotropic media, the neglect of one of the dimensions in the averaging process results in an incorrect value. This result should be called a 2D averaging procedure, particularly when 3D averaging procedures are replaced by 2D for nonisotropic urban rough layer (URL) when developing averaged transport equations.

Raupach *et al.* [64–66] later introduced a true volume averaging procedure within an air volume $\Delta\Omega_f$ that yielded the averaged equation for momentum conservation

$$\frac{\partial \tilde{\bar{U}}_i}{\partial t} + \tilde{\bar{U}}_j\frac{\partial}{\partial x_j}\left(\tilde{\bar{U}}_i\right) = -\frac{1}{\rho_f}\frac{\partial}{\partial x_i}\tilde{\bar{P}} + \frac{\partial}{\partial x_j}\left\{-\overline{u_i' u_j'}\right\}_f + \nu\Delta\tilde{\bar{U}}_i + \frac{\nu}{\Delta\Omega_f}\int_{\partial S_w}\frac{\partial}{\partial x_j}\bar{U}_i\cdot\vec{d}s - \frac{\partial}{\partial x_j}\left\{\bar{u}_i''\bar{u}_j''\right\}_f - \frac{1}{\rho_f\Delta\Omega_f}\int_{\partial S_w}\bar{P}\vec{d}s, \quad i, j = 1 - 3, \tag{80}$$

where ∂S_w is interfacial area. Development of this equation is based on intrinsic averaged values of $\{\ \}_f$ or $\tilde{\bar{U}}_i$, whereas averages of vector field variables over the entire REV are more correct (Kheifets and Neimark [11]). Raupach *et al.* [64] next simplified all the closure requirements by developing a bulk overall drag coefficient. The second, third, and fifth terms on the right-hand side of Eq. (80) are represented by a common drag resistance term. For a stationary fully developed boundary layer, they write

$$\frac{\partial}{\partial z}\left[\{\overline{u'w'}\}_f\{\bar{u}''\bar{w}''\}_f - \nu\frac{\partial\bar{\bar{U}}}{\partial z}\right] = -\frac{1}{2}C_{de}S_{pe}\bar{\bar{U}}^2, \tag{81}$$

where C_{de} is an element drag coefficient and S_{pe} is an element area density—frontal area per unit volume.

A wide range of flow regimes is reported in papers by Fand *et al.* [67] and Dybbs and Edwards [68]. The latter work revealed that there were four regimes for regular spherical packing, and that only when the Reynolds number based on pore diameter, Re_{ch}, exceeded 350 could the flow regime be considered to be turbulent flow. The Fand *et al.* [67] investigation of a randomnly packed porous medium made up of single size spheres showed that the fully developed turbulent regime occurs when $Re_p > 120$, where Re_p is particle Reynolds number.

Volume averaging procedures were used by Masuoka and Takatsu [69] to derive their volume-averaged turbulent transport equations. As in numerous other studies of multiphase transport, the major difficulties of averaging the terms on the right-hand side were overcome by using assumed closure models for the stress components. As a result, the averaged turbulent momentum equation, for example, has conventional additional resistance terms such as the averaged momentum equation developed by Vafai and Tien [70] for laminar regime transport in porous medium. A major assumption is the linearity of the fluctuation terms obtained, for example, by neglect of additional terms in the momentum equation.

A meaningful experimental study by Howle *et al.* [71] confirmed the importance of the role of randomness in the enhancement of transport processes. The results show the very distinct patterns of flow and heat transfer for two cases of regular and nonuniform 2D structured nonorthogonal porous media. Their experimental results clearly demonstrate the influence of nonuniformity of the porous structure on the enhancement of heat transfer.

D. Development of Turbulent Transport Models in Highly Porous Media

Fluid flow in a porous layer or medium can be characterized by several modes. Let us single out from among them the three modes found in a highly porous media. The first is flow around isolated ostacle elements, or inside an isolated pore. The second is interaction of traces or a hyperturbulent mode. The third is fluid flow between obstacles or inside a blocked interconnected swarm of channels (filtration mode). The models developed by Scherban *et al.* [15], Primak *et al.* [14], and Travkin and Catton [16–21] are primarily for nonlinear laminar filtration and hyperturbulent modes in nonlinear transport.

Specific features of flows in the channels of filtered media include the following:

1. Increased drag due to microroughness on the channel boundary surfaces
2. Gravity effects
3. Free convection effects
4. The effects of secondary flows of the second kind and curved streamlines
5. Large-scale vortex effects
6. The anisotropic nature of turbulent transfer and resulting anisotropy of turbulent viscosity

It is well known that in spacial boundary flows, an important role is played by the gradients of normal Reynolds stresses and that this is the case for flows in porous medium channels as well. As a rule, flow symmetry is not observed in these channels. Therefore, in channel turbulence models, the shear components of the Reynolds stress tensors have a decisive effect on the flow characteristics. At present, however, turbulence models that are less than second-order can not be successfully employed for simulating such flows (Rodi [72], Lumley [73], and Shvab and Bezprozvannykh [74]).

Derivation of the equations of turbulent flow and diffusion in a highly porous medium during the filtration mode is based on the theory of averaging of the turbulent transfer equation in the liquid phase and the transfer equations in the solid phase of a heterogeneous medium (Primak *et al.* [14] and Scherban *et al.* [15]) over a specified REV.

The initial turbulent transport equation set for the first level of the hierarchy, microelement, or pore, was taken to be of the form (see, for example, Rodi [72] and Patel *et al.* [75])

$$\frac{\partial\bar{U}_i}{\partial t} + \bar{U}_j\frac{\partial\bar{U}_i}{\partial x_j} = -\frac{1}{\rho_f}\frac{\partial\bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\nu\frac{\partial\bar{U}_i}{\partial x_j} - \overline{u_i'u_j'}\right) + S_{U_i} \tag{82}$$

$$\frac{\partial\bar{\Phi}_f}{\partial t} + \bar{U}_j\frac{\partial\bar{\Phi}_f}{\partial x_j} = \frac{\partial}{\partial x_j}\left(D_f\frac{\partial\bar{\Phi}_f}{\partial x_j} - \overline{u_i'\varphi_f'}\right) + S_{\Phi_f} \tag{83}$$

$$\frac{\partial\bar{U}_i}{\partial x_i} = 0. \tag{84}$$

Here $\bar{\Phi}_f$ and its fluctuation represent any scalar field that might be transported into either of the porous medium phases, and the last terms on the right-hand side of (82) and (83) are source terms.

Next we introduce free stream turbulence into the hierarchy Let us represent the turbulent values as

$$U = \bar{U} + u' = \bar{U}_k + \tilde{U}_r + u'_k + u'_r \qquad (85)$$
$$\bar{U} = \bar{\tilde{U}} + \hat{\hat{u}},$$

where the index k stands for the turbulent components independent of inhomogeneities of dimensions and properties of the multitude of porous medium channels (pores), and r stands for contributions due to the porous medium inhomogeneity. Being independent of the dimensions and properties of the inhomogeneities of the porous medium configurations, sections, and boundary surfaces does not mean that the distribution of values of $\bar{U}_k$ and u'_k are altogether independent of the distance to the wall, pressure distribution, etc. Thus, the values $\bar{U}_k$ or u'_k stand for the values generally accepted in the turbulence theory, that is, when a plane surface is referred to, these values are those of a classical turbulent boundary layer. When a round-section channel is involved, and even if the cross-section of this channel is not round, but without disturbing nonhomogeneities in the section, then the characteristics of this regular sections (and flow) may be considered to be those that could be marked with index k. Hence, if a channel in a porous medium can be approximately by superposition of smooth regular (of regular shape) channels, it is possible to give such a flow its characteristics and designated them with the index k, which stands for the basic (canonical) values of the turbulent quantities.

Triple decomposition techniques have been used in papers by Brereton and Kodal [76] and Bisset *et al.* [77], among others. The latter utilized triple decomposition, conditional averaging, and double averaging to analyze the structure of large-scale organized motion over the rough plate.

It should be noted that there are problems where $\bar{U}_k$ and u'_k can be found from known theoretical or experimental expressions (correlations) where the definitions of $\bar{U}_k$ and u'_k are equivalent to the solution of an independent problem (for example, turbulent flow in a curved channel). The same thing can be said about flow around a separate obstacle located on a plain surface. In this case one can write

$$\bar{U} = \bar{\tilde{U}} = \bar{U}_k + \tilde{U}_r, \quad u' = u'_k. \qquad (86)$$

The term $u'_r = \hat{\hat{u}}$ appears if the flow is through a nonuniform array of obstacles. If all the obstacles are the same and ordered, then $\hat{\hat{u}}$ can be taken equal to 0. Naturally, the term u'_k in this particular case does not equal the fluctuation vector u'_{ks} over a smooth, plain surface.

The following hypothesis about the additive components is developed to correct the foregoing deficiencies:

$$\bar{U} = \bar{\tilde{U}} + \hat{\tilde{u}} = \{\bar{U}_k + \tilde{U}_r\}_f + u'_r, \quad u' = u'_k$$
$$\bar{\tilde{U}} = \bar{\tilde{U}}_k + \bar{\tilde{U}}_r - \bar{U}_k + \tilde{U}_r, \quad \hat{\tilde{u}} = u'_r$$
$$(\overline{u'_k}) = 0, \quad \{\tilde{\tilde{u}}\}_f = \{u'_r\}_f = 0. \qquad (87)$$

It should be noted that solutions to the equations for the turbulent characteristics may be influenced by external parameters of the problem, namely, by the coefficients and boundary conditions, which themselves can carry information about porous medium morphological features. The adoption of a hypothesis about the additive components of functions representing turbulent filtration facilitates the problem of averaging the equations for the Reynolds stresses and covariations of fluctuations (flows) in pores over the REV.

After averaging the basic initial set of turbulent transport equations over the REV and using the averaging formalism developed in the works by Primak *et al.* [14], Shcherban *et al.* [15], and Primak and Travkin [78], one obtains equations for mass conservation,

$$\frac{\partial}{\partial x_i}\langle \bar{U}_i \rangle_f + \frac{1}{\Delta\Omega}\int_{\partial S_w} \bar{U}_i \cdot \vec{d}s = 0, \qquad (88)$$

for turbulent filtration (with molecular viscosity terms neglected for simplicity),

$$\langle m\rangle \frac{\partial \bar{\tilde{U}}_i}{\partial t} + \frac{\partial}{\partial x_j}(\langle m\rangle \bar{\tilde{U}}_j \bar{\tilde{U}}_i) = -\frac{1}{\rho_f}\frac{\partial}{\partial x_i}(\langle m\rangle \bar{\tilde{p}}) + \frac{\partial}{\partial x_j}\langle -\overline{u'_j u'_i}\rangle_f + \frac{\partial}{\partial x_j}\langle -\hat{\hat{u}}_j \hat{\hat{u}}_i\rangle_f$$
$$- \frac{1}{\rho_f \Delta\Omega}\int_{\partial S_w} \bar{p}\vec{d}s - \frac{1}{\Delta\Omega}\int_{\partial S_w} \bar{U}_j \bar{U}_i \cdot \vec{d}s$$
$$- \frac{1}{\Delta\Omega}\int_{\partial S_w} \overline{u'_j u'_i}\cdot \vec{d}s + \langle m\rangle \tilde{S}_{U_i}, \quad i,j = 1\text{–}3, \qquad (89)$$

and for scalar diffusion (with molecular diffusivity terms neglected),

$$\langle m\rangle \frac{\partial \bar{\tilde{\Phi}}_f}{\partial t} + \frac{\partial}{\partial x_i}(\langle m\rangle \bar{\tilde{U}}_i \bar{\tilde{\Phi}}_f)$$
$$= \frac{\partial}{\partial x_i}\langle -\overline{u'_i \varphi'_f}\rangle_f + \frac{\partial}{\partial x_i}\langle -\hat{\hat{u}}_i \hat{\tilde{\varphi}}_f\rangle_f - \frac{1}{\Delta\Omega}\int_{\partial S_w} \bar{U}_i \bar{\Phi}_f \cdot \vec{d}s$$
$$- \frac{1}{\Delta\Omega}\int_{\partial S_w} \overline{u'_i \varphi'_f}\cdot \vec{d}s + \langle m\rangle \tilde{S}_{\Phi_f}, \quad i = 1\text{–}3. \qquad (90)$$

Many details and possible variants of the preceding equations with tensorial terms are found in Primak *et al.* [14], Scherban *et al.* [15], and Travkin and Catton [16, 21]. Using an approximation to K-theory in an elementary channel (pore), the equation for turbulent diffusion of nth species takes the following more complex form after being averaged:

$$\langle m\rangle \frac{\partial \tilde{\bar{C}}_n}{\partial t} + \langle \bar{V}\rangle_f \nabla \tilde{\bar{C}}_n = -\nabla\langle \hat{\tilde{v}}_i \hat{\tilde{c}}_n\rangle_f + \nabla\cdot(\tilde{K}_c \nabla(\langle m\rangle \tilde{\bar{C}}_n)) + \nabla\cdot\left[\tilde{K}_c \frac{1}{\Delta\Omega}\int_{\partial S_w} \bar{C}_n \vec{d}s\right] + \nabla\cdot(\langle \hat{k}_c \nabla \hat{\tilde{c}}_n\rangle_f) + \frac{1}{\Delta\Omega}\int_{\partial S_w} K_c \nabla \bar{C}_n \cdot \vec{d}s + \frac{\tilde{\bar{C}}_n}{\Delta\Omega}\int_{\partial S_w} \bar{U}_i \cdot \vec{d}s - \frac{1}{\Delta\Omega}\int_{\partial S_w} \bar{C}_n \bar{U}_i \cdot \vec{d}s + \langle m\rangle \tilde{S}_n, \quad n = 1, 2, 3, 4\ldots. \tag{91}$$

In the more general case, the momentum flux integrals on the right-hand sides of Eq. (89) through (91) do not equal zero, since there could be penetration through the phase transition boundary changing the boundary conditions in the microelement to allow for heat and mass exchange through the interface surface as the values of velocity, concentrations, and temperature at ∂S_w do not equal zero (see also Crapiste *et al.* [41]). The first term on the right-hand side of Eq. (91) is the divergence of the REV averaged product of velocity fluctuations and admixture concentration caused by random morphological properties of the medium being penetrated and is responsible for morphoconvectional dispersion of admixture in this particular porous medium. The third term on the right-hand side of Eq. (91) can be associated with the notion of morphodiffusive dispersion of a substance or heat in a randomly nonhomogeneous medium. The term with $\tilde{S}_n$ may also reflect, specifically, the impact of microroughness from the previous level of the simulation hierarchy. The importance of accounting for this roughness has been demonstrated by many studies. The remaining step is to account for the microroughness characteristics of the previous level.

One-dimensional mathematical statements will be used in what follows for simplicity. Admission of specific types of medium irregularity or randomness requires that complicated additional expressions be included in the generalized governing equations. Treatment of these additional terms becomes a crucial step once the governing averaged equations are written. An attempt to implement some basic departures from a porous medium with

strictly regular morphology descriptions into a method for evaluation of some of the less tractable, additional terms is explained next.

The 1D momentum equation with terms representing a detailed description of the medium morphology is depicted as

$$\frac{\partial}{\partial x}\left(\langle m\rangle(\tilde{K}_m + \nu)\frac{\partial \tilde{\bar{U}}}{\partial x}\right) + \frac{\partial}{\partial x}\left(\left\langle \hat{K}_m \frac{\partial \hat{\tilde{u}}}{\partial x}\right\rangle_f\right) + \frac{\partial}{\partial x}(\langle -\hat{\tilde{u}}\hat{\tilde{u}}\rangle_f) = \langle m\rangle \tilde{\bar{U}}\frac{\partial \tilde{\bar{U}}}{\partial x_j} - \frac{1}{\Delta\Omega}\int_{\partial S_w}(K_m + \nu)\frac{\partial \bar{U}}{\partial x_i}\cdot\vec{d}s + \frac{1}{\rho_f \Delta\Omega}\int_{\partial S_w}\bar{p}\vec{d}s + \frac{1}{\rho_f}\frac{\partial}{\partial x}(\langle m\rangle\tilde{\bar{p}}) = \langle m\rangle\tilde{\bar{U}}\frac{\partial \tilde{\bar{U}}}{\partial x_j} + u^2_{*rk}S_w(x) + \frac{1}{\rho_f\Delta\Omega}\int_{\partial S_w}\bar{p}\vec{d}s + \frac{1}{\rho_f}\frac{\partial}{\partial x}(\langle m\rangle\tilde{\bar{p}}), \tag{92}$$

where K_m is the turbulent eddy viscosity, and u^2_{*rk} is the square friction velocity at the upper boundary of surface roughness layer h_r averaged over interface surface S_w.

General statements for energy transport in a porous medium require two-temperature treatments. Travkin *et al.* [19, 26] showed that the proper form for the turbulent heat transfer equation in the fluid phase using one-equation K-theory closure with primarily 1D convective heat transfer is

$$c_{pf}\rho_f\langle m\rangle\tilde{\bar{U}}\frac{\partial \tilde{\bar{T}}_f}{\partial x} = \frac{\partial}{\partial x}\left[\langle m\rangle(\tilde{K}_T + k_f)\frac{\partial \tilde{\bar{T}}_f}{\partial x}\right] + \frac{\partial}{\partial x}\left(\left\langle \hat{K}_T\frac{\partial \hat{\tilde{T}}_f}{\partial x}\right\rangle\right) + c_{pf}\rho_f\frac{\partial}{\partial x}(\langle m\rangle\{-\hat{\tilde{T}}_f\hat{\tilde{u}}\}_f) + \frac{\partial}{\partial x}\left[\frac{(\tilde{K}_T + k_f)}{\Delta\Omega}\int_{\partial S_w}\hat{\tilde{T}}_f\vec{d}s\right] + \frac{1}{\Delta\Omega}\int_{\partial S_w}(K_T + k_f)\frac{\partial \bar{T}_f}{\partial x_i}\cdot\vec{d}s, \tag{93}$$

whereas in the neighboring solid phase, the corresponding equation is

$$\frac{\partial}{\partial x}\left((1 - \langle m\rangle)\{K_{sT}\}_s\frac{\partial\{T_s\}_s}{\partial x}\right) + \frac{\partial}{\partial x}\left(\left\langle \hat{K}_{sT}\frac{\partial \hat{T}_s}{\partial x}\right\rangle_s\right) + \frac{\partial}{\partial x}\left[\frac{\{K_{sT}\}_s}{\Delta\Omega}\int_{\partial S_w}\hat{T}_s\vec{d}s_1\right] + \frac{1}{\Delta\Omega}\int_{\partial S_w}K_{sT}\frac{\partial T_s}{\partial x_i}\cdot\vec{d}s_1. \tag{94}$$

The generalized longitudinal 1D mass transport equation in the fluid phase, including description of potential morphofluctuation influence, for a

medium morphology with only 1D fluctuations is written

$$\frac{\partial}{\partial x}\left[\langle m\rangle(\tilde{K}_C + D_f)\frac{\partial \tilde{\bar{C}}_f}{\partial x}\right] + \frac{\partial}{\partial x}\left(\left\langle \hat{K}_C \frac{\partial \hat{\bar{C}}_f}{\partial x}\right\rangle_f\right) + \frac{\partial}{\partial x}\left(\langle m\rangle\{-\hat{c}_f\hat{u}\}_f\right) + \frac{\partial}{\partial x}\left[\frac{(\tilde{K}_C + D_f)}{\Delta\Omega}\int_{\partial S_w}\hat{\bar{c}}_f \vec{d}s\right] + \frac{1}{\Delta\Omega}\int_{\partial S_w}(K_C + D_f)\frac{\partial \bar{C}_f}{\partial x_i}\cdot\vec{d}s + \langle m\rangle\tilde{S}_C = \langle m\rangle\tilde{\bar{U}}\frac{\partial \tilde{\bar{C}}_f}{\partial x}, \tag{95}$$

whereas the corresponding nonlinear equation for the solid phase is

$$\frac{\partial}{\partial x}\left((1-\langle m\rangle)\{D_s\}_s\frac{\partial\{C_s\}_s}{\partial x}\right) + \frac{\partial}{\partial x}\left(\left\langle \hat{D}_s\frac{\partial \hat{c}_s}{\partial x}\right\rangle_s\right) + \frac{\partial}{\partial x}\left[\frac{\{D_s\}_s}{\Delta\Omega}\int_{\partial S_w}\hat{C}_s\vec{d}s_1\right] + \frac{1}{\Delta\Omega}\int_{\partial S_w}D_s\frac{\partial C_s}{\partial x_i}\cdot\vec{d}s_1. \tag{96}$$

E. Closure Theories and Approaches for Transport in Porous Media

Closure theories for transport equations in heterogeneous media have been the primary measure of advancement and for measuring success in research on transport in porous media. It is believed that the only way to achieve substantial gains is to maintain the connection between porous medium morphology and the rigorous formulation of mathematical equations for transport. There are only two well-known types of porous media morphologies for which researchers have had major successes. But even for these morphologies, namely straight parallel pores and equal-size spherical inclusions, not enough evidence is available to state that the closure problems for them are "closed."

One of the few existing studies of closure for VAT type equations is by Hsu and Cheng [79, 80]. They used a one-temperature averaged equation [Equation (40a) in Hsu and Cheng [80]) without the morphodiffusive term

$$\nabla\cdot[(k_f - k_s)\bar{T}(-\nabla\langle m\rangle)] = \nabla\cdot[(k_s - k_f)\bar{T}(\nabla\langle m\rangle)].$$

The reasoning often applied to the morphoconvective term closure problem in averaged scalar and momentum transport equations is that the terms needing closure may be negligible. The basis for this reasoning is (see Kheifets and Neimark [11])

$$\hat{c} \approx |\nabla C| d_{ch}, \quad \text{and} \quad \hat{j} = D|\nabla C|, \quad \text{so } \nabla\langle\hat{c}\hat{j}\rangle_f \approx D\langle|\nabla C|^2\rangle_f \frac{d_{ch}}{l},$$

where l is the characteristic length associated with averaging volume (see, for example, the work of Lehner [81] and others) and d_{ch} the mean diameter of pores in a REV. It is not obvious that the length scale, d_{ch}, taken for the approximation of $\hat{c}$ follows from use of l as a scale for the second derivative. Furthermore, assuming that the variable to be averaged over the REV changes very slowly over the REV does not mean that it changes very slowly in the neighborhood of the primary REV.

Various closure attempts for heterogeneous medium transport equations resulted in various final equations. One needs to know what these equations are all about. Treatment of the one-dimensional heat conduction equation with a stochastic function for the thermal diffusivity in a paper by Fox and Barakat [82] yielded a spatially fourth-order partial differential equation to be solved. Gelhar *et al.* [83], after having eliminated the second-order terms in the species conservation equation for a stochastic media, were able to develop an interesting procedure for deriving a mean concentration transport equation. The equation form includes an infinite series of derivatives on the right-hand side of the equation. Analysis of this equation allows the derivation of the final form of the mass transport equation,

$$\frac{\partial \tilde{C}^*}{\partial t} + U\frac{\partial \tilde{C}^*}{\partial x} = (A + a_l)U\frac{\partial^2 \tilde{C}^*}{\partial x^2} - B\frac{\partial^3 \tilde{C}^*}{\partial t\partial x^2} - BU\frac{\partial^3 \tilde{C}^*}{\partial x^3},$$

where the most important term is the second term on the right-hand side. In the derivation of this equation, the stochastic character of the existing assigned fields of velocity, concentration, and dispersion coefficients were assumed.

A simple form of the advective diffusion equation with constant diffusion coefficients was developed without sorption effects by Tang *et al.* [84]:

$$\frac{\partial\langle m\rangle C}{\partial t} + \langle m\rangle V_i\cdot\nabla C = D\nabla\cdot(\langle m\rangle\nabla C).$$

They transformed the equation with the help of ensemble averaging into a stochastic transport equation,

$$\frac{\partial\langle m\rangle\tilde{C}^*}{\partial t} + \langle m\rangle\bar{u}_j^*\nabla\tilde{C}^* = D\nabla\cdot(\langle m\rangle\nabla\tilde{C}^*) + \langle m\rangle\rho_{jk}\frac{\partial^2\tilde{C}^*}{\partial x_j\partial x_k},$$

where the tensor of the ensemble dispersion coefficient is a correlation function denoted by

$$\rho_{jk} = \frac{1}{2}\frac{\{\overline{u_j'u_k'}\}^*}{\{\bar{u}\}^*\{\bar{u}\}^*}\vec{x}\cdot\{\bar{u}\}^*,$$

with $\{\bar{u}\}^*$ being the ensemble averaged velocity. The additional term,

reflecting the influence of the stochastic or inhomogeneous nature of the spatial velocity and concentration fluctuations in the ensemble averaged stochastic equation developed by Tang *et al.* [84], has the dispersivity coefficient fully dependent on the velocity fluctuations. As can be seen by this equation, the effect of concentration fluctuations was eliminated.

Torquato and coauthors (see, for example, Torquato *et al.* [85], Miller and Torquato [86], Kim and Torquato [87]) have been developing means to characterize the various mathematical dependencies of a composite medium microstructure in a statistically homogeneous medium. Some of the quantities considered by Torquato are useful in obtaining resolution to certain closure problems for VAT developed mathematical models of globular morphologies. In particular, the different near-neighbor distance distribution density functions deserve special mention (Lu and Torquato [88], Torquato *et al.* [85]).

Carbonell and Whitaker [89] combined the methods of volume averaging and the morphology approach to specify the dispersion tensor for the problem of convective diffusion for cases where there is no reaction or adsorption on the solid phase surface,

$$-D\frac{\partial C}{\partial n}=0, \quad \vec{x}\in\partial S_w,$$

and considered a constant diffusion coefficient and constant porosity $\langle m\rangle$, which greatly simplifies the closure problems. They expressed the spatial deviation function as

$$\hat{c}=\hat{f}(\vec{r})\cdot\nabla\tilde{C},$$

where $\vec{f}$ is a vector function of position in the fluid phase. Averaged equations of convective diffusion are the same as the convective heat transfer equation given by Levec and Carbonell [46] with the exclusion of flux surface integral term. The closure technique used in their paper is analogous to a turbulence theory scheme, helping them to derive the closure equation for the spatial deviation function in the form of a partial differential equation,

$$\hat{V}+(\tilde{V}+\hat{V})\nabla\vec{f}=D\nabla^2\vec{f}, \quad -\vec{n}\cdot\nabla\vec{f}=\vec{n}, \quad \vec{x}\in\partial S_w,$$

One should note that the spatial deviation functions defined for a periodic medium are periodic themselves.

Nozad *et al.* [40] suggested that the same closure scheme be used to represent the fluctuation terms $\hat{T}_f$ and $\hat{T}_s$ for a one-temperature model by using

$$\hat{T}_f=\vec{f}\,\nabla\langle T\rangle+\psi, \quad \hat{T}_s=\vec{g}\nabla\langle T\rangle+\xi$$

for a transient heat conduction problem with constant coefficients in a two-phase system (stationary). Partial differential equations for $\vec{f}$, $\vec{g}$, ψ, and ξ are found. They obtained excellent predictions of the effective thermal conductivity for conductivity ratios $k=k_s/k_f<100$.

Carbonell [90] attempted to obtain an averaged convective-diffusion equation for a straight tube morphological model and obtained an equation with three different concentration variables. This demonstrates that the averaging procedures, taken too literally, can result in incorrect expressions or conclusions.

A common form of the averaged governing equations for closure of multiphase laminar transport in porous media was obtained by Crapiste *et al.* [41]. They developed a closure approach that led to a complex integro-differential equation for the spatial deviations of a substance in the void or fluid phase volume of the macro REV. This means that solving the boundary value problem for spatial concentration fluctuations, for example, requires that one obtain a solution to second-order partial differential or coupled integro differential equations in a real complex geometric volume within the porous medium.

For a heterogeneous porous medium, this means that the coupled integrodifferential equation sets for the averaged spatial deviation variables must be solved for at least two scales. For averaged variables the scales are the external scale or L domain, and for the spatial deviations it is the volume of the fluid phase considered at the local (pore) scale. This presents a great challenge and has not yet been resolved by a real mathematical statement.

To close the reaction-diffusion problem Crapiste *et al.* [41] made a series of assumptions: (1) the diffusion coefficient D and the first-order reaction rate coefficient k_r are constant; (2) diffusion is linear in the solid part of the porous medium, (3) the spatial concentration fluctuation is linearly dependent on the gradient of the intrinsic averaged concentration and the averaged concentration itself, (4) the intrinsic averaged concentration and solid surface averaged concentration are equal, (5) the restriction

$$\frac{k_r d_p}{D}\ll 1$$

should be satisfied; and (6) spatial fluctuations of the intrinsic concentration and the surface concentration fluctuations are equal. The fourth and sixth assumptions are equivalent to an equality of surface and intrinsic concentrations, which means that the adsorption mechanisms are taken to be volumetric phenomena.

In our previous efforts we have obtained some results for both morphologies and demonstrated the strength of morphological closure procedures.