A model of turbulent flow and two-temperature heat transfer in a highly porous medium was evaluated numerically for a layer of regular packed particles (Travkin and Catton [16, 20]; Gratton *et al.* [26, 27]) with heat exchange from the side surfaces. Nonlinear two-temperature heat and momentum turbulent transport equations were developed on the basis of VAT, requiring the evaluation of transport coefficient models. This approach required that the coefficients in the equations, as well as the form of the equations themselves, be consistent to accurately model the processes and morphology of the porous medium. The integral terms in the equations were dropped or transformed in a rigorous fashion consistent with physical arguments regarding the porous medium structure, flow and heat transfer regimes (Travkin and Catton [20]; Travkin *et al.* [17]). The form of the Darcy term as well as the quadratic term was shown to depend directly on the assumed version of the convective and diffusion terms. More importantly, both diffusion (Brinkman) and drag resistance terms in the final forms of the flow equations were proven to be directly connected. These relations follow naturally from the closure process. The resulting necessity for transport coefficient models for forced, single phase fluid convection led to their development for nonuniformly and randomly structured highly porous media.

A regular morphology structure was used to determine the characteristic morphology functions, (porosity $\langle m \rangle$, and specific surface S_w) that were used in the equations in the form of analytically calculable functions. A first approximation for the coefficients, for example, drag resistance or heat transfer, was obtained from experimentally determined coefficient correlations. Existing models for variable morphology functions such as porosity and specific surface were used by Travkin and Catton [20] and Gratton *et al.* [27] to obtain comparisons with other work in a relatively high Reynolds number range.

All the coefficient models they used were strictly connected to assumed (or admitted) porous medium morphology models, meaning that the coefficient values are determined in a manner consistent with the selected geometry. Comparison of modeling results was sometimes difficult because other models utilized mathematical treatments or models that do not allow a complete description of the medium morphology; see Travkin and Catton [16]. Closures were developed for capillary and globular medium morphology models (Travkin and Catton [16, 17, 20]; Gratton *et al.* [26, 27]). It was shown that the approach taken to close the integral resistance terms in the momentum equation for a regular structure allows the second-order terms for the laminar and turbulent regimes to naturally occur. These terms were taken to be analogous to the Darcy or Forchheimer terms for different flow velocities. Numerical evaluations of the models show distinct differences in the overall drag coefficent among the straight capillary and globular models for both the regular and simple cubic morphologies.

IV. Microscale Heat Transport Description Problems and VAT Approach

Study of energy transport at different scales in a heterogeneous media or system emphasizes the importance of transport phenomena at subcrystalline and atomic scales. Among many works addressing subcrystalline transport phenomena (see Fushinobu *et al.* [91]; Caceres and Wio [92]; Tzou *et al.* [93]; Majumdar [94]; Peterson [95], etc.), the governing energy transport equations, whether they are of differential type or integrodifferential, are for homogeneous or homogenized matter. This idealization significantly reduces the value of the physical description that results. VAT shows great promise as a tool for development of models for this type of phenomena because it becomes possible to include the inherent nonlinearity and heterogeneity found at the subcrystalline level and reflect the impact at the upper levels or scales.

A heuristic approach suggested by Tzou [96] lumps all the atomic and subcrystalline scale phenomena "into the delayed response in time in the macroscopic formulation." This approach was proposed by author to close the existing gap in knowledge and to help engineers develop applications. Unfortunately, the coupling between the characteristics of the subscale phenomena and delayed response time is lost. There is an ongoing search for the transport equations describing many-body systems that exhibit highly nonequilibrium behavior, including non-Markovian diffusion. The more exact the description of a physical phenomenon provided by a mathematical model, the more possibilities there are for innovative improvements in the function of a particular material or device. Our contribution to the effort is an extensive analysis of existing approaches to the development of theories for the subcrystalline and atomic scale levels. We have also made progress in the development of VAT-based tools applicable at the atomic and nanoscale level for description of transport of heat, mass, and charge in SiC and superconductive ceramics.

At the subcrystalline scale, we will consider energy transport using a VAT description for effects of crystal defects and impurities on phonon–phonon scattering, which has a substantial impact on thermal conductivity. At the crystal scale, the importance of thermal resistance (different models) due to various mechanisms—lattice unharmonic resistance and crystal boundary defects—will be treated. Including these phenomena shows that they have a major impact on the transport characteristics in critical applications such as optical ceramics and superconductive ceramics.

A. Traditional Descriptions of Microscale Heat Transport

Kaganov *et al.* [97] first developed a theory to describe energy exchange between electrons and the lattice of a solid for arbitrary temperatures using earlier advances in this field by Ginzburg and Shabanskii [98] and by Akhiezer and Pomeranchuk [99]. In their work, they assumed that the electron gas was in an equilibrium state. After a brief summary of this early work, an analysis leading to a method for estimating the relaxation processes between the electron fluid temperature T_e and the phonon temperature T_l will be presented.

The heat balance equation for the electron temperature is

$$c_e(T)\,\frac{\partial T_e}{\partial t} = -\bar{U} + Q, \tag{97}$$

where Q is the heat source, $c_e(T)$ is the electronic specific heat,

$$c_e(T) = \left(\frac{\pi}{2}\right)^2 k_B n_e \frac{k_B T_1}{\varepsilon_0},$$

and

$$\varepsilon_0 = (3n_e/8\pi)^{2/3}(2\pi\hbar)^2/(2m^*).$$

$\bar{U}$ is the heat exchange term,

$$\bar{U} = \frac{2\pi^2}{3}\,\frac{m^* c_s^2 n_e (T_e - T_l)}{\tau(T_l)}\,\frac{(T_e - T_l)}{T_l}, \quad T_l \ll T_D;\ (T_e - T_l) \ll T_l \tag{98}$$

$$\bar{U} = \frac{\pi^2}{6}\,\frac{m^* c_s^2 n_e}{\tau(T_l)}\,\frac{(T_e - T_l)}{T_l}, \quad T_l \gg T_D;\ (T_e - T_l) \ll T_l, \tag{99}$$

where m^* is the effective electronic mass, c_s is the sound velocity, n_e is the number of electrons per unit volume, $\tau(T_l)$ is the time to traverse a mean free path of electrons under the condition that the lattice temperature coincides with the electron temperature and is equal respectively to T_l.

When the lattice temperature is assumed to be much less than the temperature of the electrons (an assumption later found to be weak), then

$$\bar{U} = \begin{cases} \dfrac{2\pi^2}{15}\,\dfrac{m^* c_s^2 n_e}{\tau(T_e)}, & (T_e \ll T_D;\ T_l \ll T_e); \\[2ex] \dfrac{\pi^2}{6}\,\dfrac{m^* c_s^2 n_e}{\tau(T_e)}, & (T_e \gg T_D;\ T_l \ll T_e). \end{cases} \tag{100}$$

Kaganov *et al.* [97] used an equation for elastic lattice vibration of the form

$$\frac{\partial^2 U_l}{\partial r^2} = c_s^2 \Delta U_l - \left(\frac{U}{\rho}\right)\nabla\delta(\mathbf{r} - \mathbf{V}t). \tag{101}$$

This also allowed them to develop the heat exchange term (here U_l is the displacement vector). In this equation, $\rho = M/d^3$ is the density of lattice, M is the mass of the lattice atom, V is the lattice volume, and U is the interaction constant of the electron with the lattice that appears in the expression for the time to travel the mean free path.

It was nearly 20 years before needs in different physical fields (namely, intense short-timespan energy heating in laser applications) brought attention to this phenomenon and to use it for further technological advances. Anisimov *et al.* [100, 101] introduced a simplified two-fluid temperature model for heat transport in solids,

$$C_e(T_e)\,\frac{\partial T_e}{\partial t} = \chi \Delta T_e - \alpha_{ep}(T_e - T_l) + f(\mathbf{r}, t) \tag{102}$$

$$C_l\,\frac{\partial T_l}{\partial t} = \alpha_{ep}(T_e - T_l), \quad \alpha_{ep} = \frac{\pi^2}{6}\,\frac{m^* c_s^2 n_e}{\tau(T_e)}. \tag{103}$$

Further development of the idea of a two-field two-temperature model for energy transport in metals by Qiu and Tien [102–104] used this model. They modified the energy exchange rate coefficent (heat transfer) model in a way that uses the coefficient of conductivity K_e in the following formula instead of time between collisions $\tau(T_e)$:

$$\bar{U} = G = \frac{\pi^4 (n_e c_s k_B)^2}{K_e}. \tag{104}$$

Tzou *et al.* [93] used the two-fluid model with two equations for the electron–phonon transport in metals based on previous works by Anisimov *et al.* [101], Fujimoto *et al.* [105], Elsayed-Ali [106], and others. The equation for diffusion in an electron gas is a parabolic heat conduction equation with an exchange term

$$C_e\,\frac{\partial T_e}{\partial t} = \nabla\cdot(K_e \nabla T_e) - G_{ep}(T_e - T_l), \tag{105}$$

with phonon transport (phonon–electron interactions) for the metal lattice (just simplified equation) being described by

$$C_l\,\frac{\partial T_l}{\partial t} = G_{ep}(T_e - T_l), \tag{106}$$

where K_e is the thermal conductivity of the electron gas. Using the Wiedermann–Franz law for the electron–phonon interaction, Qiu and Tien [102, 103] show that the coupling factor G_{ep} can be approximated by

$$G_{ep} = \frac{\pi^4 (n_e c_s k_B)^2}{K_e}, \tag{107}$$

where c_s, the speed of sound in solid, is

$$c_s = \frac{k_B}{2\pi\hbar} (6\pi^2 n_a)^{-1/3} T_D, \tag{108}$$

T_D is the Debye temperature, $\hbar$ is Planck's constant, and n_e and n_a are the electronic and atomic volumetric number densities. Assuming constant thermal properties, the two equations can be combined, yielding a one-temperature equation

$$\frac{\partial^2 T_l}{\partial x^2} + \frac{\alpha_e}{C_T^2} \frac{\partial^3 T_l}{\partial x^2 \partial t} = \frac{1}{\alpha_T} \frac{\partial T_l}{\partial t} + \frac{1}{C_T^2} \frac{\partial^2 T_l}{\partial t^2}, \tag{109}$$

where the thermal diffusivity of electron gas α_e, equivalent thermal diffusivity α_T, and thermal wave speed C_T are defined by

$$\alpha_e = \frac{K_e}{C_e}, \quad \alpha_T = \frac{K_e}{C_e + C_l}, \quad C_T^2 = \frac{K_e G}{C_e C_l}. \tag{110}$$

Tzou [96] later proposed a unified two-fluid model to derive the general hyperbolic equation with two relaxation times τ_T and τ_q,

$$\nabla^2 T + \tau_T \frac{\partial}{\partial t} (\nabla^2 T) = \frac{1}{\alpha} \frac{\partial T}{\partial t} + \frac{\tau_q}{\alpha} \frac{\partial^2 T}{\partial t^2}, \tag{111}$$

which he argues is the same equation derived from two-step models in metals. A more complex two-temperatures model was obtained by Gladkov [107] using parabolic equations

$$\frac{\partial T_1}{\partial t} + V \frac{\partial T_1}{\partial x} = \chi_1 \frac{\partial^2 T_1}{\partial x^2} - \alpha_{12}(T_1 - T_2) \tag{112}$$

and

$$\frac{\partial T_2}{\partial t} = \chi_2 \frac{\partial^2 T_2}{\partial x^2} + \alpha_{21}(T_1 - T_2), \tag{113}$$

It can be seen from his work that the coefficients of heat transfer α_{12} and α_{21} are not equal. After combining the two equations into one, an equation for a mobile (liquid) medium results:

$$\left(1 + \frac{\alpha_{21}}{\alpha_{12}}\right) \frac{\partial T_1}{\partial t} + \frac{1}{\alpha_{12}} \frac{\partial^2 T_1}{\partial t^2} + \frac{V}{\alpha_{12}} \frac{\partial^2 T_1}{\partial t \partial x} + \frac{\alpha_{21} V}{\alpha_{12}} \frac{\partial T_1}{\partial x} = \chi_2 \frac{V}{\alpha_{12}} \frac{\partial^3 T_1}{\partial x^3} - \frac{\chi_1 \chi_2}{\alpha_{12}} \frac{\partial^4 T_1}{\partial x^4} + \chi_1 \frac{\partial^2 T_1}{\partial x^2}. \tag{114}$$

There are other works (see, for example, Joseph and Preziosi [108]) treating the two-fluid heat transport and obtaining the same kind of hyperbolic equation.

1. *Equation of Phonon Radiative Transfer*

Majumdar [94] suggested an equation for phonon radiative transfer (EPRT). In three dimensions the equation is

$$\frac{\partial \mathbf{L}_\omega}{\partial t} + (V_{ph} \cdot \nabla \mathbf{I}_\omega) = \frac{\mathbf{I}_\omega^0(T(\mathbf{x})) - \mathbf{I}_\omega}{\tau(\omega,\ T)}, \tag{115}$$

where $\mathbf{I}_\omega$ is the directional-spectral phonon intensity, V_{ph} is the phonon propagation speed, and $\mathbf{I}_\omega^0(T(\mathbf{x}))$ is the equilibrium intensity corresponding to a blackbody intensity at temperatures below the Debye temperature. To make matters more complex, it should be noted that as stressed by Peterson [95], "However, fundamental differences exist between phonon and photon behavior in the regime where scattering and collisional processes are important. . . . Even in perfect crystals, the so-called unklapp processes that are responsible for finite thermal conductivity do not obey momentum conservation."

2. *Hyperbolic Heat Conduction Equations*

The work by Vernotte, Cattaneo, Morse, and Feshbach that led to the hyperbolic heat conduction equation was primarily heuristic in nature (without a first principle physical basis). The final form is often presented as a telegraph equation (see Joseph and Preziosi [108]),

$$\frac{\partial^2 T}{\partial t^2} + \frac{1}{\tau} \frac{\partial T}{\partial t} = \frac{k}{(\tau\gamma)} \nabla^2 T, \tag{116}$$

or

$$\tau \frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} = \frac{1}{\gamma} \nabla \cdot (K \nabla T), \tag{117}$$

for nonconstant thermal conductivity K; γ here is the heat capacity.

Majumdar *et al.* [109] produced microphotographs of thermal images that show the grain structure, visible in the topographical image, and notes that "the grain boundaries appear hotter than within the grain. It is at present not clear why this occurs.... The hot electrons collide with the lattice and transfer energy by the emission of phonons." The governing equations for a nonmagnetic medium they use are conservation of electrons,

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{V}_e) = 0; \tag{118}$$

conservation of electron momentum,

$$\frac{\partial \mathbf{V}_e}{\partial t} + (\mathbf{V}_e \cdot \nabla)\mathbf{V}_e = -\frac{e}{m^*}\,\mathbf{E} - \frac{k_B}{m^* n}\,\nabla(nT_e) - \left(\frac{\mathbf{V}_e}{\tau_m}\right); \tag{119}$$

where the last term "is the collision and scattering **term analogous to the Darcy** term in porous media flow"; conservation of electron energy,

$$\begin{aligned}\frac{\partial W_e}{\partial t} + \nabla \cdot (W_e\mathbf{V}_e) &= -e(n\mathbf{V}_e \cdot \mathbf{E}) - \mathrm{k}_B\nabla \cdot (n\mathbf{V}_e T_e)\\ &\quad + \nabla \cdot (k_e \nabla T_e) - \left(\frac{(W_e - (3/2)k_B T_o)}{\tau_{e-o}}\right);\end{aligned} \tag{120}$$

conservation of lattice optical phonon energy,

$$C_o\frac{\partial T_o}{\partial t} = \frac{(W_e - (3/2)k_B T_o)}{\tau_{e-o}} - \left(C_o\,\frac{(T_o - T_a)}{\tau_{o-a}}\right); \tag{121}$$

and conservation of acoustical energy,

$$C_a\frac{\partial T_a}{\partial t} = \nabla \cdot (k_a \nabla T_a) + \left(C_o\,\frac{(T_o - T_a)}{\tau_{o-a}}\right). \tag{122}$$

The last four equations have terms, the last term on the right-hand side, that qualitatively reflect the collision and scattering rates in each process. Here τ_m is the electron momentum relaxation time, τ_{e-o} is the electron optical relaxation time, τ_{o-a} is the optical acoustical relaxation time, and k_B is Boltzmann's constant. In those equations assumed a scalar effective mass for the electrons m^*.

The electric field is determined using the Gauss law equation written in terms of electric potential ($\mathbf{E} = -\nabla\Phi$),

$$\begin{aligned}\nabla \cdot (\varepsilon\nabla\Phi) &= -e(N_n - N_p - n + p) = -eN_{\#}\\ N_{\#} &= (N_n - N_p - n + p),\end{aligned} \tag{123}$$

where ε is the dielectric constant of Si, N_n is the n-doping concentration, N_p is the p-doping concentration, and p is the hole number density.

B. VAT-Based Two-Temperature Conservation Equations

Conservation equations derived using VAT enable one to capture all of the physics associated with transport of heat at the micro scale with more rigor than any other method. VAT allows one to avoid the ad hoc assumptions that are often required to close an equation set. The resulting equations will have sufficient generality for one to begin to optimize material design from the nanoscale upward. The theoretical development is briefly outlined in what follows.

The nonlinear paraboic VAT-based heat conduction equation in one of the phases of the superstructure (where superstructure is to be determined as the micro- or nanoscale material's organized morphology along with its local characteristics) is

$$\begin{aligned}\langle s_1\rangle(\rho c_p)_1\frac{\partial\{T_1\}_1}{\partial t} &= \nabla \cdot [\langle s_1\rangle\{K_1\}_1\nabla\{T_1\}_1] + \nabla \cdot [\langle s_1\rangle\{\hat{K}_1\nabla\hat{T}_1\}_1]\\ &\quad + \nabla \cdot \left[\frac{\{K_1\}_1}{\Delta\Omega}\int_{\partial S_{12}} \hat{T}_1 \vec{d}s_1\right] + \frac{1}{\Delta\Omega}\int_{\partial S_{12}} K_1\frac{\partial T_1}{\partial x_i}\cdot\vec{d}s_1 + \langle s_1\rangle\{S_{T_1}\}_1.\end{aligned} \tag{124}$$

For constant thermal conductivity, the averaged equation for heat transfer in the first phase can be written

$$\begin{aligned}\langle s_1\rangle(\rho c_p)_1\frac{\partial\tilde{T}_1}{\partial t} &= k_1\nabla^2(\langle s_1\rangle\tilde{T}_1) + k_1\nabla \cdot \left[\frac{1}{\Delta\Omega}\int_{\partial S_{12}} T_1\vec{d}s_1\right]\\ &\quad + \frac{k_1}{\Delta\Omega}\int_{\partial S_{12}} \nabla T_1 \cdot \vec{d}s_1 + \langle s_1\rangle\langle S_{T_1}\}_1.\end{aligned} \tag{125}$$

These VAT equations (124) and (125), written for the two phases, will be seen to yield the same pair of parabolic equations derived by researchers such as Gladkov [107], but with quite different arguments. Closure to Eq. (125) is needed for the second and third terms on the right-hand side. The steps to closure are

$$\begin{aligned}\frac{1}{\Delta\Omega}\int_{\partial S_{12}} k_1\frac{\partial T}{\partial x_i}\cdot\vec{d}s_1 &= -\frac{1}{\Delta\Omega}\int_{\partial S_{12}} k_1\frac{\partial T}{\partial \mathbf{n}_2}\,ds\cdot\mathbf{n}_2\\ &= \frac{1}{\Delta\Omega}\int_{\partial S_{12}} \mathbf{q}_2\cdot\vec{d}s_2 = \tilde{\alpha}_{21}S_{12}(\{T\}_2 - \{T\}_1),\end{aligned} \tag{126}$$

with the heat transfer coefficient, $\tilde{\alpha}_{21}(\partial S_{12})$, defined in phase 2. This closure procedure is appropriate for description of fluid–solid medium heat exchange and might be considered as the analog to solid–solid heat exchange found in many works. A more precise integration of the heat flux over the interface surface, ∂S_{12}, yields exact closure for that term in governing equations for both neighboring phases.

Industry needs to lead one to attempt to estimate, or simulate by numerical calculation or other methods, the effective transport properties of heterogenous material. Among the many diverse methods used to do this, VAT presents itself as an effective tool for evaluating and bringing together different methods and is useful in providing a basis for comparative validation of techniques. To demonstrate the value of a VAT-based process, the effective thermal conductivity will be determined within the VAT framework. The averagd energy equation in phase 1 of a medium is

$$k_1\nabla^2(\langle s_1\rangle\tilde{T}_1) + k_1\nabla\cdot\left[\frac{1}{\Delta\Omega}\int_{\partial S_{12}} T_1\vec{d}s_1\right] = \nabla\cdot[-\vec{q}_1].$$

The right-hand-side ("diffusive"-like) flux is different from that conventionally found,

$$\vec{q}_1 = [-k_{eff,1}\nabla\tilde{T}_1] = -k_1\nabla(\langle s_1\rangle\tilde{T}_1) - \frac{k_1}{\Delta\Omega}\int_{\partial S_{12}} T_1\vec{d}s_1, \qquad (127)$$

where

$$k_{eff,1} = \left[k_1\nabla(\langle s_1\rangle\tilde{T}_1) + \frac{k_1}{\Delta\Omega}\int_{\partial S_{12}} T_1\vec{d}s_1\right](\nabla\tilde{T}_1)^{-1}. \qquad (128)$$

After these transformations, the heat transfer equation for phase 1 becomes

$$\langle s_1\rangle(\rho c_p)_1\frac{\partial\tilde{T}_1}{\partial t} = \nabla\cdot[k_{eff,1}\nabla\tilde{T}_1] + \tilde{\alpha}_{21}S_{12}(\{T\}_2 - \{T\}_1) + \langle s_1\rangle\{S_{T_1}\}. \qquad (129)$$

This is the same type of heat transport equation routinely used in two-fluid models. The equation for heat transport in the second phase (if any) would be the same, and one can easily obtain the hyperbolic type two-fluid temperature model.

A similar VAT-based equation can be obtained for the heat transfer in phase 1 when the heat conductivity coefficient is a function of the temperature or other scalar field (nonlinear) (Eq. (124)), but the effective conductivity will have an additional term reflecting the mean surface temperature over the interface surface inside of the REV,

$$K_{eff,1} = \left[\{K_1\}_1\nabla(\langle s_1\rangle\tilde{T}_1) + \langle s_1\rangle\{\hat{K}_1\nabla\hat{T}_1\}_1 + \frac{\{K_1\}_1}{\Delta\Omega}\int_{\partial S_{12}} T_1\vec{d}s_1\right](\nabla\tilde{T}_1)^{-1}. \qquad (130)$$

Equation (124) simplifies to

$$\langle s_1\rangle(\rho c_p)_1\frac{\partial\tilde{T}_1}{\partial t} = \nabla\cdot[K_{eff,1}\nabla\tilde{T}_1] + \tilde{\alpha}_{21}S_{12}(\{T\}_2 - \{T\}_1) + \langle s_1\rangle\{S_{T_1}\}_1. \qquad (131)$$

The third term on the right-hand side of (124) plays a different role when the interface between two phases is only a mathematical surface without thickness neglecting the transport within the surface means there is no need to consider this medium separately. When this is the case, this term can be equal for the both phases, simplifying the closure problem. The problem becomes significantly more complicated when transport within the interface must be accounted for.

C. Subcrystalline Single Crystal Domain Wave Heat Transport Equations

Some features of energy transport, including electrodynamics, that are above the scale of close capture quantum phenomena are considered next. Limiting the scope of the problem allows us to concentrate on the description of heat transport phenomena in the medium above the quantum scale where there are at least the three substantially different physical and spatial scales to consider. Within this scope, the heat transport equation in a single grain (crystalline) can be written in the form

$$\tau\frac{\partial^2 T_g}{\partial t^2} + \frac{\partial T_g}{\partial t} = \frac{1}{\gamma}\nabla\cdot(K\nabla T_g) + \frac{1}{\gamma}S_{T_g}. \qquad (132)$$

Comparing this equation with the equation developed by Tzou [96] with two relaxation times, τ_T and τ_q,

$$\tau_q\frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} = \alpha\nabla^2 T + \tau_T\alpha\frac{\partial}{\partial t}(\nabla^2 T) + \alpha S_{T_g}, \qquad (133)$$

and the parabolic equation obtained by Gladkov [107] for the model with two temperatures for constant coefficients,

$$\left(1 + \frac{\alpha_{21}}{\alpha_{12}}\right)\frac{\partial T_1}{\partial t} + \frac{1}{\alpha_{12}}\frac{\partial^2 T_1}{\partial t^2} + \frac{V}{\alpha_{12}}\frac{\partial^2 T_1}{\partial t\partial x} + \frac{\alpha_{21}V}{\alpha_{12}}\frac{\partial T_1}{\partial x}$$
$$= \chi_2\frac{V}{\alpha_{12}}\frac{\partial^3 T_1}{\partial x^3} - \frac{\chi_1\chi_2}{\alpha_{12}}\frac{\partial^4 T_1}{\partial x^4} + \chi_1\frac{\partial^2 T_1}{\partial x^2}, \qquad (134)$$

one can see that all belong to the family of VAT two-temperature conduction problems with nonconstant effective coefficients for the charged carriers,

$$\frac{\partial \tilde{T}_c}{\partial t} = a_c \nabla \cdot [K_c \nabla \tilde{T}_c] + b_c(\{T\}_l - \{T\}_c) + S_{T_c}, \tag{135}$$

and for phonon temperature transport,

$$\frac{\partial \tilde{T}_l}{\partial t} = a_l \nabla \cdot [K_l \nabla \tilde{T}_l] - b_l(\tilde{T}_l - \tilde{T}_c) + S_{T_l}. \tag{136}$$

This pair of equations is the wave transport equations shown in previous sections.

Our current interest, however, is not to justify past assumptions made to develop appropriate scale level energy transport equations, but to develop mathematical models for heat transport and electrodynamics in multiscale microelectronics superstructures.

D. NONLOCAL ELECTRODYNAMICS AND HEAT TRANSPORT IN SUPERSTRUCTURES

Many microscale heterogeneous heat transport equations and some of the solutions provided elsewhere (see, for example, [110, 111, 112, 113, 109]) required substantial analysis, and many need improvement. Goodson [113], for example, directly addresses the need to model nonhomogeneous medium (diamond CVD layer) thermal transport by accounting for the presence of grains. The Peierls–Boltzmann equation for phonon transport was used along with information on grain structure. In the present work, the goal is to give some insight to situations (and those are substantial in number) where the medium cannot be considered as homogeneous even at the microscale level. For these circumstances, the governing field equations should be based on conservation equations for a heterogeneous medium, for example, the VAT governing equations.

The VAT governing equations for heterostructures will be found starting from a set of governing equations for a solid-state electron plasma fluid. Phase averaging of the electron conservation equation (118) yields

$$\left\langle \frac{\partial n}{\partial t} \right\rangle_m + \langle \nabla \cdot (n\mathbf{V}_e) \rangle_m = 0 \tag{137}$$

where $\langle\ \rangle_m$ means averaging over the major phase of the material. The VAT final form for this equation is

$$\frac{\partial \langle n \rangle_m}{\partial t} + \nabla \cdot \langle n\mathbf{V}_e \rangle_m + \frac{1}{\Delta\Omega} \int_{\partial S_{ms}} n\mathbf{V}_e \cdot \vec{d}s = 0, \tag{138}$$

or

$$\frac{\partial \langle n \rangle_m}{\partial t} + \nabla \cdot [\langle s_m \rangle \tilde{n} \tilde{\mathbf{V}}_e + \langle m \rangle \{\hat{n} \hat{\mathbf{V}}_e\}_m] + \frac{1}{\Delta\Omega} \int_{\partial S_{12}} n\mathbf{V}_e \cdot \vec{d}s_m = 0, \tag{139}$$

where ∂S_{ms} is the "interface" (real or imaginary) of phases and scatterers.

It will be assumed that only immobile scatterers produce phase separation. This is not an essential restriction and is only taken to simplify the appearance of the equations and streamline the development. We recognize that defects and other scattering objects where processes are also occuring, such as nonmajor phases, occur, but we are not interested in them at this time because their volumetric fractions are very small and their importance is decreased by scattering of the fields in a major phase.

The electron fluid momentum transport equation can be written in two forms, and the form influences the final appearance of the VAT equations. The first is

$$\left\langle \frac{\partial \mathbf{V}_e}{\partial t} \right\rangle_m + \langle (\mathbf{V}_e \cdot \nabla)\mathbf{V}_e \rangle_m = -\frac{e}{m^*} \langle \mathbf{E} \rangle_m - \frac{k_B}{m^*} \left\langle \frac{1}{n} \nabla(nT_e) \right\rangle_m - \Downarrow \frac{\mathbf{V}_e}{\tau_m} \Downarrow. \tag{140}$$

Using the transformation

$$\begin{aligned} \left\langle \frac{1}{n} \nabla(nT_e) \right\rangle_m &= \left\langle \nabla T_e + T_e \frac{1}{n} \nabla n \right\rangle_m = \langle \nabla T_e + T_e \nabla(\ln n) \rangle_m \\ &= \langle \nabla T_e + T_e \nabla(Z_n) \rangle_m, \quad Z_n = \ln n, \end{aligned} \tag{141}$$

it can be written as

$$\left\langle \frac{\partial \mathbf{V}_e}{\partial t} \right\rangle_m + \langle (\mathbf{V}_e \cdot \nabla)\mathbf{V}_e \rangle_m = -\frac{e}{m^*} \langle \mathbf{E} \rangle_m - \frac{k_B}{m^*} \langle \nabla T_e + T_e \nabla(Z_n) \rangle_m - \Downarrow \frac{\mathbf{V}_e}{\tau_m} \Downarrow, \tag{142}$$

where the brackets $\Downarrow\Downarrow$ define the problem uncertainty in the treatment of this relaxation term. Strictly speaking, this term should not be in this form and may not exist.

The same equation written in conservative form is

$$\left\langle \frac{\partial n\mathbf{V}_e}{\partial t} \right\rangle_m + \langle \nabla \cdot (n\mathbf{V}_e\mathbf{V}_e) \rangle_m = -\frac{e}{m^*} \langle n\mathbf{E} \rangle_m - \frac{k_B}{m^*} \langle \nabla(nT_e) \rangle_m - \Downarrow \frac{n\mathbf{V}_e}{\tau_m} \Downarrow, \tag{143}$$

Using

$$
\begin{aligned}
\langle(\mathbf{V}_e\cdot\nabla)\mathbf{V}_e\rangle_m &= \langle\nabla\cdot(n\mathbf{V}_e\mathbf{V}_e)\rangle_m - \langle\mathbf{V}_e(\nabla\cdot(n\mathbf{V}_e))\rangle_m \\
&= \nabla\cdot\langle n\mathbf{V}_e\mathbf{V}_e\rangle_m + \frac{1}{\Delta\Omega}\int_{\partial S_{ms}}(n\mathbf{V}_e\mathbf{V}_e)\cdot\vec{d}s_m \\
&\quad -\{\langle s_m\rangle\tilde{\mathbf{V}}_e\{\nabla\cdot(n\mathbf{V}_e)\}_m + \langle\hat{\mathbf{V}}_e(\nabla\cdot(n\mathbf{V}_e))^{(\wedge)}\rangle_m\}, \qquad (144)
\end{aligned}
$$

Eq. (142) can be written in the VAT form as

$$
\begin{aligned}
&\frac{\partial\langle\mathbf{V}_e\rangle_m}{\partial t} + \nabla\cdot\langle n\mathbf{V}_e\mathbf{V}_e\rangle_m + \frac{1}{\Delta\Omega}\int_{\partial S_{ms}}(n\mathbf{V}_e\mathbf{V}_e)\cdot\vec{d}s_m \\
&\quad -\{\langle s_m\rangle\tilde{\mathbf{V}}_e\{\nabla\cdot(n\mathbf{V}_e)\}_m + \langle\hat{\mathbf{V}}_e(\nabla\cdot(n\mathbf{V}_e))^{(\wedge)}\rangle_m\} \\
&= -\frac{e}{m^*}\langle\mathbf{E}\rangle_m - \frac{k_B}{m^*}\left(\nabla\langle T_e\rangle_m + \frac{1}{\Delta\Omega}\int_{\partial S_{ms}}T_e\vec{d}s_m\right) \\
&\quad -\frac{k_B}{m^*}\left\{\langle s_m\rangle\tilde{T}_e\left(\nabla\{Z_n\}_m + \frac{1}{\Delta\Omega_m}\int_{\partial S_{ms}}Z_n\vec{d}s_m\right) + \langle\hat{T}_e(\nabla(Z_n))^{(\wedge)}\rangle_m\right\},
\end{aligned}
\tag{145}
$$

where the last term on the right-hand side of (142), the scattering and collision reflection term, has been replaced by a number of terms, each reflecting interface-specific phenomena, including scattering and collision. Some manipulation of the convection terms of the conservative form of the momentum equation has been done to combine the forms of the equations of mass and momentum.

The second conservative form of the momentum equation is derived in the form

$$
\begin{aligned}
&\langle n\rangle_m\frac{\partial\tilde{\mathbf{V}}_e}{\partial t} + (\langle n\mathbf{V}_e\rangle_m\cdot\nabla)\tilde{\mathbf{V}}_e + \frac{\partial}{\partial t}\langle\hat{n}\hat{\mathbf{V}}_e\rangle_m + \nabla\cdot\langle\widehat{n\mathbf{V}}_e\hat{\mathbf{V}}_e\rangle_m \\
&\quad -\tilde{\mathbf{V}}_e\left(\frac{1}{\Delta\Omega}\int_{\partial S_{ms}}n\mathbf{V}_e\cdot\vec{d}s\right) + \frac{1}{\Delta\Omega}\int_{\partial S_{ms}}(n\mathbf{V}_e\mathbf{V}_e)\cdot\vec{d}s_m \\
&= -\frac{e}{m^*}\langle n\mathbf{E}\rangle_m - \frac{k_B}{m^*}\left(\nabla[\langle s_m\rangle\tilde{n}\tilde{T}_e + \langle s_m\rangle\{\hat{n}\hat{T}_e\}_m] + \frac{1}{\Delta\Omega}\int_{\partial S_{ms}}nT_e\vec{d}s_m\right),
\end{aligned}
\tag{146}
$$

where a number of the integral terms are scattering and collision terms. There are other possible forms of the left-hand side of the momentum equation VAT equations that will not be pursued at this time.

The homogeneous volume averaged electron gas energy equation for a heterogeneous polycrystal becomes

$$
\begin{aligned}
\left\langle\frac{\partial W_e}{\partial t}\right\rangle_m + \langle\nabla\cdot(W_e\mathbf{V}_e)\rangle_m &= -e\langle n\mathbf{V}_e\cdot\mathbf{E}\rangle_m - k_B\langle\nabla\cdot(n\mathbf{V}_eT_e)\rangle_m \\
&\quad + \langle\nabla\cdot(k_e\nabla T_e)\rangle_m - \left\Downarrow\frac{(W_e-(3/2)k_BT_o)}{\tau_{e-o}}\right\Downarrow,
\end{aligned}
\tag{147}
$$

or

$$
\begin{aligned}
&\frac{\partial\langle W_e\rangle_m}{\partial t} + \nabla\cdot\langle W_e\mathbf{V}_e\rangle_m + \frac{1}{\Delta\Omega}\int_{\partial S_{ms}}(W_e\mathbf{V}_e)\cdot\vec{d}s_m \\
&\quad = -e\langle n\mathbf{V}_e\cdot\mathbf{E}\rangle_m - k_B\nabla\cdot\langle(n\mathbf{V}_eT_e)\rangle_m - \frac{k_B}{\Delta\Omega}\int_{\partial S_{ms}}(n\mathbf{V}_eT_e)\cdot\vec{d}s_m \\
&\quad + \nabla\cdot[\{k_e\}_m\nabla(\langle s_m\rangle\{T_e\}_m)] + \nabla\cdot[\langle s_1\rangle\{\hat{k}_e\nabla\hat{T}_e\}_m] \\
&\quad + \nabla\cdot\left[\frac{\{k_e\}_m}{\Delta\Omega}\int_{\partial S_{ms}}T_e\vec{d}s_m\right] + \frac{1}{\Delta\Omega}\int_{\partial S_{ms}}k_e\frac{\partial T_e}{\partial x_i}\cdot\vec{d}s_m.
\end{aligned}
\tag{148}
$$

The integral terms again reflect scattering and collision that appear as a result of the heterogeneous medium transport description.

The equation for longitudinal phonon temperature is

$$
\left\langle C_o\frac{\partial T_o}{\partial t}\right\rangle_m = -\left(\frac{\partial W_e}{\partial t}\right)_c + \left(\frac{\partial W_{LO}}{\partial t}\right)_c,
\tag{149}
$$

or

$$
\begin{aligned}
\left\langle C_o\frac{\partial T_o}{\partial t}\right\rangle_m &= \frac{k_B}{\Delta\Omega}\int_{\partial S_{ms}}(n\mathbf{V}_eT_e)\cdot\vec{d}s_m + \frac{1}{\Delta\Omega}\int_{\partial S_{ms}}(W_e\mathbf{V}_e)\cdot\vec{d}s_m \\
&\quad -\nabla\cdot\left[\frac{\{k_e\}_m}{\Delta\Omega}\int_{\partial S_{ms}}T_e\vec{d}s_m\right] - \frac{1}{\Delta\Omega}\int_{\partial S_{ms}}k_e\frac{\partial T_e}{\partial x_i}\cdot\vec{d}s_m \\
&\quad -\nabla\cdot\left[\frac{\{k_e\}_m}{\Delta\Omega}\int_{\partial S_{ms}}T_a\vec{d}s_m\right] - \frac{1}{\Delta\Omega}\int_{\partial S_{ms}}k_a\frac{\partial T_a}{\partial x_i}\cdot\vec{d}s_m.
\end{aligned}
\tag{150}
$$

The equation of acoustical phonon energy is

$$
\left\langle C_a\frac{\partial T_a}{\partial t}\right\rangle_m = \langle\nabla\cdot(k_a\nabla T_a)\rangle_m + \left\Downarrow C_a\frac{(T_o-T_a)}{\tau_{o-a}}\right\Downarrow
\tag{151}
$$

or

$$\left\langle C_a \frac{\partial T_a}{\partial t} \right\rangle_m = \nabla \cdot [\{k_a\}_m \nabla(\langle s_m \rangle \{T_a\}_m)] + \nabla \cdot [\langle s_1 \rangle \{\hat{k}_a \nabla \hat{T}_a\}_m] + \nabla \cdot \left[\frac{\{k_e\}_m}{\Delta\Omega} \int_{\partial S_{ms}} T_a \vec{d}s_m\right] + \frac{1}{\Delta\Omega} \int_{\partial S_{ms}} k_a \frac{\partial T_a}{\partial x_i} \cdot \vec{d}s_m. \tag{152}$$

Describing phonon scattering and collision is an unsolved problem and as noted by Peterson [95], "The complexity of this aspect of the problem precludes the relatively simple solution used in simulating rarefied gas flows."

Another kind of single phase equation for momentum transport of electronic fluid results for magnetized materials:

$$\left\langle \frac{\partial \mathbf{V}_e}{\partial t} \right\rangle_m + \langle (\mathbf{V}_e \cdot \nabla) \mathbf{V}_e \rangle_m = -\frac{e}{m^*} \langle \mathbf{E} + \mathbf{V}_e \times \mathbf{B} \rangle_m - \frac{k_B}{m^*} \left\langle \frac{1}{n} \nabla(nT_e) \right\rangle_m - \left\Downarrow \frac{\mathbf{V}_e}{\tau_m} \right\Downarrow. \tag{153}$$

The VAT form of this equation is

$$\begin{aligned} &\frac{\partial \langle \mathbf{V}_e \rangle_m}{\partial t} + \nabla \cdot \langle n\mathbf{V}_e \mathbf{V}_e \rangle_m + \frac{1}{\Delta\Omega} \int_{\partial S_{ms}} (n\mathbf{V}_e \mathbf{V}_e) \cdot \vec{d}s_m \\ &\quad - \{\langle s_m \rangle \tilde{\mathbf{V}}_e \{\nabla \cdot (n\mathbf{V}_e)\}_m + \langle \hat{\mathbf{V}}_e (\nabla \cdot (n\mathbf{V}_e))^{(\wedge)} \rangle_m\} \\ &= -\frac{e}{m^*} (\langle \mathbf{E} \rangle_m + \langle \mathbf{V}_e \times \mathbf{B} \rangle_m) - \frac{k_B}{m^*} \left(\nabla \langle T_e \rangle_m + \frac{1}{\Delta\Omega} \int_{\partial S_{ms}} T_e \vec{d}s_m \right) \\ &\quad - \frac{k_B}{m^*} \left\{ \langle s_m \rangle \tilde{T}_e \left(\nabla \{z_n\}_m + \frac{1}{\Delta\Omega_m} \int_{\partial S_{ms}} Z_n \vec{d}s_m \right) + \langle \hat{T}_e (\nabla (Z_n))^{(\wedge)} \rangle_m \right\}. \end{aligned} \tag{154}$$

The Maxwell equations for electromagnetic fields used to develop the VAT Maxwell equations for electromagnetic fields are

$$\nabla \cdot (\varepsilon_m \mathbf{E}_m) = \rho_m, \quad \nabla \cdot (\mu_m \mathbf{H}_m) = 0 \tag{155}$$

$$\nabla \times \mathbf{E}_m = -\frac{\partial \mathbf{B}_m}{\partial t} \tag{156}$$

$$\nabla \times \mathbf{H}_m = \mathbf{j}_m + \frac{\partial}{\partial t} (\mathbf{D}_m), \tag{157}$$

with constitutive relationships

$$\mathbf{B}_m = \mu_m \mathbf{H}_m, \quad \mathbf{D}_m = \varepsilon_m \mathbf{E}_m, \quad \mathbf{j}_m = \sigma_m \mathbf{E}_m. \tag{158}$$

A full description of the derivation of the VAT nonlocal electrodynamics governing equations is given by Travkin *et al.* [114, 115] with only a limited number shown here.

For the electric field, the Maxwell equations, after averaging over phase (m) using $\langle\ \rangle_m$, become

$$\nabla \cdot [\langle s_m \rangle \tilde{\varepsilon}_m \tilde{\mathbf{E}}_m] + \nabla \cdot [\langle s_m \rangle \{\hat{\varepsilon}_m \hat{\mathbf{E}}_m\}_m] + \frac{1}{\Delta\Omega} \int_{\partial S_{12}} (\varepsilon_m \mathbf{E}_m) \cdot \vec{d}s_m = \langle \rho_m \rangle_m \tag{159}$$

$$\nabla \times (\langle s_m \rangle \tilde{\mathbf{E}}_m) + \frac{1}{\Delta\Omega} \int_{\partial S_{ms}} \vec{d}s_m \times \mathbf{E}_m = -\frac{\partial}{\partial t} \langle \mu_m \mathbf{H}_m \rangle_1. \tag{160}$$

The phase averaged magnetic field equations are

$$\nabla \cdot (\langle s_m \rangle \tilde{\mu}_m \tilde{\mathbf{H}}_m) + \nabla \cdot [\langle s_m \rangle \{\hat{\mu}_m \hat{\mathbf{H}}_m\}_m] + \frac{1}{\Delta\Omega} \int_{\partial S_{ms}} (\mu_m \mathbf{H}_m) \cdot \vec{d}s_m = 0, \tag{161}$$

and

$$\nabla \times (\langle s_m \rangle \tilde{\mathbf{H}}_m) + \frac{1}{\Delta\Omega} \int_{\partial S_{ms}} \vec{d}s_m \times \mathbf{H}_m = \frac{\partial}{\partial t} \langle \varepsilon_m \mathbf{E}_m \rangle_m + [\langle s_m \rangle \tilde{\sigma}_m \tilde{\mathbf{E}}_m + \langle s_m \rangle \{\hat{\sigma}_m \hat{\mathbf{E}}_m\}_1]. \tag{162}$$

These equations and some of their variations, such as the electric field wave equations

$$\nabla^2 \mathbf{E}_m - \mu_m \sigma_m \frac{\partial \mathbf{E}_m}{\partial t} - \mu_m \varepsilon_m \frac{\partial^2 \mathbf{E}_m}{\partial t^2} = \nabla \left(\frac{\rho_m}{\varepsilon_m} \right), \tag{163}$$

which becomes

$$\begin{aligned} &\nabla^2 (\langle s_m \rangle \tilde{\mathbf{E}}_m) + \nabla \cdot \left[\frac{1}{\Delta\Omega} \int_{\partial S_{ms}} \mathbf{E}_m \vec{d}s_m \right] + \frac{1}{\Delta\Omega} \int_{\partial S_{ms}} \nabla \mathbf{E}_m \cdot \vec{d}s_m \\ &= \mu_m \sigma_m \frac{\partial \langle \mathbf{E} \rangle_m}{\partial t} + \mu_m \varepsilon_m \frac{\partial^2 \langle \mathbf{E} \rangle_m}{\partial t^2} + \frac{1}{\varepsilon_m} \nabla (\langle s_m \rangle \tilde{\rho}_m) + \frac{1}{\varepsilon_m \Delta\Omega} \int_{\partial S_{ms}} \rho_m \vec{d}s_m, \end{aligned} \tag{164}$$

are the basis for modeling of electric and magnetic fields at the microscale level in heterostructures.

The primary advantage of the VAT-based heterogenous media electrodynamics equations is the inclusion of terms reflecting phenomena on the interface surface ∂S_{ms} that can be used to precisely incorporate multiple morphological effects occuring at interfaces.

E. PHOTONIC CRYSTALS BAND-GAP PROBLEM: CONVENTIONAL DMM-DNM AND VAT TREATMENT

One of the possible applications of VAT electrodynamics is the formulation of models describing electromagnetic waves in a dielectric medium of materials considered to be photonic crystals [118, 116, 117, 119, 126, 120]. The problem of photonic band-gap in composite materials has received great attention since 1987 [118, 116] because of its exciting promises. The most interesting applications appear in the purposeful design of materials exhibiting selective, at least in some wave bands, propagation of electromagnetic energy [120].

Figotin and Kuchment [122] were the first who theoretically demonstrated the existence of band-gaps in certain morphologies. Unfortunately, this problem as presently formulated is based on the homogeneous Maxwell equations. The most common way to treat such problems has been to seek a solution by doing numerical experiments over more or less the exact morphology of interest, a method called detailed micromodeling (DMM), which is often done using direct numerical modeling (DNM) (for example, see [124]). As a result, questions arise about differences between DMM-DNM and heterogeneous media modeling (HMM), which is the modeling of an averaged medium to determine its properties. How the averaging for HMM is accomplished is often not clear or not done at all.

So, why cannot DMM be self-sufficient in the description of heterogeneous medium transport phenomena? The answers can be primarily understood by analyzing, among others [23], the following issues:

1. A basic principal mismatch occurs at the boundaries, causing boundary condition problems. This means that for DMM and for the bulk (averaged characteristics) material fields, the boundary conditions are principally different.
2. The DMM solution must be matched to a corresponding HMM to make it meaningful at the upper scales. This can only be done for regular morphologies. Discrete continuum gap closure or mismatching will occur with DMM-DNM, precluding generalization to the next or higher levels in the hierarchy.
3. The spatial scaling of heterogeneous problems with the chosen REV (for DMM) is needed to address large or small deviations in elements considered that are governed by different underlying physics. When spatial heterogeneities of the characteristics or morphology are evolving along the coordinates, DMM cannot be used.
4. Numerical experiments provided by DMM-DNM need to be translated to a form that implies that the overall spatially averaged bulk characteristics model random morphologies. It is not clear what kind of equations are to be used as the governing equations, nor what variables should be compared. In the case of the local porosity theory [128, 129], for example, the results of using real porous medium digitized images for morphological analysis to calculate the effective dielectric constant assumes that the HMM equations are applicable.
5. Interpretation of the results of DMM-DNM is always a problem. If results are presented for a heterogeneous continuum, then the previous point applies. If the results are being used as a solution for some *discrete* problem, then the question is how to relate that solution to the continuum problem of interest or even to a slightly different problem. If the results obtained are fit into a statistical model, then the phenomena are being subjected to a statistical averaging procedure that is in most cases only correct for independent events.
6. The most sought-after characteristics in heterogeneous media transport studies are the effective transport coefficients that can only be correctly evaluated from

$$-\langle \mathbf{j}\rangle = \sigma^*\nabla\langle\Phi\rangle = \sigma_2\nabla\langle\Phi\rangle + (\sigma_1-\sigma_2)\frac{1}{\Delta\Omega}\int_{\Delta\Omega_1}\nabla\Phi\,d\omega,$$

using the DMM-DNM exact solutions for a small fraction of the problems of interest. The issue is that problems of interest having inhomogeneous, nonlinear coefficients and, in many transient problems, two-field DMM-DNM exact solutions are not enough to find the effective coefficients.

Fractal methods are sometimes used to describe multiscale phenomena. The use of fractals is not relevant to most of the morphologies of interest and the fractal phenomenon description is generally too morphological, lacking many of the needed physical features. For example, descriptions of both phases, of the phase interchange, etc., are need to represent the physical phenomenon.

For the simplest case of a superlattice or multilayer medium there can be many difficulties. When the boundaries are not evenly located, crossing the regular boundary cells of the medium, then the problem must be solved again and again. If the coefficients are space dependent, because of the layers or grain boundaries, they will influence scattering. Grain boundaries are not perfect and are not just mathematical surfaces without thickness or physical properties. They cannot be treated as mathematical surfaces without any properties. Imperfections in the internal spacial structures must be treated as domain morphologies are not perfect at any spacial level.

The insufficiency of a homogeneous wave propagation description of a heterogeneous medium was addressed in [125] from a pure mathematical point of view by searching for another type of governing operator that could better explain the behavior of the frequency spectrum eigenmodes via "heuristic arguments." The general band-gap formulation should be treated using the HMM statements developed from the analysis of the VAT equations. A straightforward description of one of the band-gap problems is given next.

Representing electromagnetic field components with time-harmonic components,

$$\mathbf{E}(x, y, z)e^{i\omega t}, \quad \mathbf{H}(x, y, z)e^{i\omega t}, \quad \mathbf{i} = \sqrt{(-1)}, \tag{165}$$

The equations describing a dielectric medium becomes

$$\nabla\cdot(\varepsilon\mathbf{E}) = 0, \quad \nabla\cdot\mathbf{H} = 0, \quad \mu = 1 \tag{166}$$

$$\nabla\times\mathbf{E} = -\mathrm{i}\omega\mathbf{H}, \quad \nabla\times\mathbf{H} = \mathrm{i}\omega\bar{\varepsilon}\mathbf{E}, \tag{167}$$

where $\bar{\varepsilon}$ is the complex dielectric "constant" defined by $\bar{\varepsilon} = \varepsilon - \mathrm{i}(\sigma/\omega)$, and $\sigma = 0(\vec{\mathbf{x}})$, $\varepsilon = \varepsilon(\vec{\mathbf{x}})$, $\bar{\varepsilon} = \bar{\varepsilon}(\vec{\mathbf{x}}, \omega)$.

Taking the curl of the both sides of the vector equations,

$$\nabla\times\left(\frac{1}{\bar{\varepsilon}}\nabla\times\mathbf{H}\right) = \nabla\times(\mathrm{i}\omega\mathbf{E}), \quad \nabla\times(\nabla\times\mathbf{E}) = \nabla\times(-\mathrm{i}\omega\mathbf{H}), \tag{168}$$

yields

$$\nabla\times\left(\frac{1}{\bar{\varepsilon}}\nabla\times\mathbf{H}\right) = \mathrm{i}\omega(-\mathrm{i}\omega\mathbf{H}) = \omega^2\mathbf{H} \tag{169}$$

$$\nabla\times(\nabla\times\mathbf{E}) = -\mathrm{i}\omega(\mathrm{i}\bar{\varepsilon}\omega\mathbf{E}) = \bar{\varepsilon}\omega^2\mathbf{E}. \tag{170}$$

This is the set of equations usually used when problems of photonic band-gap materials are under investigation; see the study by Figotin and Kuchment [123], p. 1564. These equations can be transformed to

$$-\Delta\mathbf{E}_3(\vec{\mathbf{x}}) = \omega^2\bar{\varepsilon}(\vec{\mathbf{x}})\mathbf{E}_3(\vec{\mathbf{x}}) \tag{171}$$

for *E*-polarized fields and

$$-\nabla\cdot\left(\frac{1}{\bar{\varepsilon}(\vec{\mathbf{x}})}\nabla\mathbf{H}_3(\vec{\mathbf{x}})\right) = \omega^2\mathbf{H}_3(\vec{\mathbf{x}}) \tag{172}$$

for *H*-polarized fields.

The further treatment by Figotin and Kuchment [123] reduces the mathematics to two equations,

$$-\nabla\cdot\left(\frac{1}{\bar{\varepsilon}(\vec{\mathbf{x}})}\nabla f_p(\vec{\mathbf{x}})\right) = \lambda f_p(\vec{\mathbf{x}}) \tag{173}$$

$$-\frac{1}{\bar{\varepsilon}(\vec{\mathbf{x}})}\Delta f_p(\vec{\mathbf{x}}) = \lambda f_p(\vec{\mathbf{x}}), \tag{174}$$

where f_p is the $\mathbf{H}_3$ or $\mathbf{E}_3$ polarization determined components of electric or magnetic fields.

These equations state the eigenvalue problem characterizing the spectrum of electromagnetic wave propagation in a dielectric two-phase medium, which is supposed to describe the photonic materials band-gap problem of EM propagation (see equations on p. 1568 in Figotin and Kuchment [123]) There are no spatial morphological terms or functions involved in the description, just the permittivity, which is supposed to be a space-dependent function with changes at the interface boundary.

When these equations are phase averaged to represent the macroscale characteristics of wave propagation in a two-phase dielectric medium, the equations become

$$\begin{aligned}\nabla\cdot(\tilde{\gamma}_1\nabla(\langle m_1\rangle\tilde{f}_{p1})) + \nabla\cdot\left[\tilde{\gamma}_1\frac{1}{\Delta\Omega}\int_{\partial S_{12}} f_{p1}\vec{d}s_1\right]& \\ + \nabla\cdot(\langle\hat{\gamma}^1\nabla\hat{f}_{p1}\rangle_1) + \frac{1}{\Delta\Omega}\int_{\partial S_{12}}\gamma_1\nabla f_{p1}\cdot\vec{d}s_1 &= -\lambda\langle m_1\rangle\widetilde{f_{p1}}\end{aligned} \tag{175}$$

$$\gamma(\vec{\mathbf{x}}) = \frac{1}{\bar{\varepsilon}}$$

$$\begin{aligned}\nabla^2(\langle m_1\rangle\tilde{f}_{p1}) + \nabla\cdot\left[\frac{1}{\Delta\Omega}\int_{\partial S_{12}} f_{p1}\vec{d}s_1\right] + \frac{1}{\Delta\Omega}\int_{\partial S_{12}}\nabla f_{p1}\cdot\vec{d}s_1& \\ = -\lambda[\langle m_1\rangle\tilde{\varepsilon}_1\tilde{f}_{p1} + \langle m_1\rangle\{\hat{\varepsilon}_1\widehat{f_{p1}}\}_1].&\end{aligned} \tag{176}$$

The three additional terms appear along with the porosity (or volume fraction) function $\langle m_1\rangle$ as a factor on the right-hand side of each of the equations. When the dielectric permittivity function is homogeneous in each of the two phases, then the VAT photonic band-gap equations can be reduced to one equation in each phase and written in a simpler form,

$$\nabla^2(\langle m_1\rangle\tilde{f}_{p1}) + \nabla\cdot\left[\frac{1}{\Delta\Omega}\int_{\partial S_{12}} f_{p1}\vec{d}s_1\right] + \frac{1}{\Delta\Omega}\int_{\partial S_{12}}\nabla f_{p1}\cdot\vec{d}s_1 = -\lambda\bar{\varepsilon}_1\langle m_1\rangle\widetilde{f_{p1}} \tag{177}$$

and

$$\nabla^2(\langle m_2\rangle\tilde{f}_{p1})+\nabla\cdot\left[\frac{1}{\Delta\Omega}\int_{\partial S_{12}}f_{p1}\vec{d}s_2\right]+\frac{1}{\Delta\Omega}\int_{\partial S_{12}}\nabla f_{p1}\cdot\vec{d}s_2=-\lambda\bar{\varepsilon}_2\langle m_2\rangle\tilde{f}_{p1}. \tag{178}$$

The equations are almost the same as equations for heat or charge conductance in a heterogeneous medium. The similarity of the equations means that the analysis of the simplest band-gap problem should also be very similar.

Using DMM-DNM, Pereverzev and Ufimtsev [121] found that exact micromodel solutions among others features can have "medium... internal generation" that might be well characterized by the impact of the additional terms in the VAT Maxwell equations in both phases and in the combined electric field and effective coefficient equations; see Sections V and VIII. The exact closure and direct numerical modeling derived by Travkin and Kushch [33, 34] demonstrated how important and influential the additional VAT morphoterms can be (Section I). These terms do not explicitly appear in either the microscale basic mathematical statements or in microscale field solutions. The terms appear and become very important when averaged bulk characteristics are being modeled and calculated.

V. Radiative Heat Transport in Porous and Heterogeneous Media

Radiation transport problems in porous (and heterogeneous) media, including work by Tien [130], Siegel and Howell [131], Hendricks and Howell [132], Kumar *et al.* [133], Singh and Kaviany [134], Tien and Drolen [135], and Lee *et al.* [139], are primarily based on governing equations resulting from the assumption of a homogeneous medium. This implicitly implies that specific problem features due to heterogeneities can be decribed using different methods for evaluation of the interim transport coefficients, as, for example, done by Al-Nimr and Arpaci [136], Kumar and Tien [137], Lee [138], Lee *et al.* [139], and Dombrovsky [140]. Although this kind of approach is legitimate, it presents no fundamental understanding of the processes because the governing equations suffer from the initial assumption that strictly describes only homogeneous media. Further, it is difficult to represent hierarchical physical systems behavior with such models as will be touched on later.

Review papers like that of Reiss [141] describe the progress in the field of dispersed media radiative transfer. The few works on heterogeneous radiative or electromagnetic transport (see Dombrovsky [140], Adzerikho *et al.* [142], van de Hulst [143], Bohren and Huffman [144], Lorrain and Corson [145], Lindell *et al.* [146], and Lakhtakia *et al.* [147]) approach the study of transport in disperse media with the emphasis on known scattering techniques and their improvements.

The area of neutron transport and radiative transport in heterogeneous medium being developed by Pomraning [148–151] and Malvagi and Pomraning [152] treats linear transport in a two-phase (two materials) medium with stochastic coefficients. This approach is the same as that which has been used to treat thermal and electrical conductivity in heterogeneous media, and to this point it has not been brought to a high enough level to include variable properties, their nonlinearities, and cross-field (electrical and thermal or magnetic) phenomena.

Research by Lee *et al.* [139] on attenuation of electromagnetic and radiation fields in fibrous media has shown a high extinction rate for infrared radiation. The problem is treated as a scattering problem for a single two-layer cylinder by Farone and Querfeld [153], Samaddar [154], and Bohren and Huffman [144]. The process of radiative heat transport in porous media is very similar to propagation of electromagnetic waves in porous media and will also be evaluated. These two very close fields seem not to have been considered as a coherent area. Complicated problems of propagation of electromagnetic waves through the fiber gratings have been primarily the subject of electrodynamics. The most notable work in this area is that of Pereverzev and Ufimtsev [121], Figotin and Kuchment [122, 125], Figotin and Godin [124], Botten *et al.* [155], and McPhedran *et al.* [156, 157]. No effort seems to have been made to translate results obtained for polarized electromagnetic radiation to the area of heat radiative transfer.

Detailed micromodeling (DMM) of electromagnetic wave scattering has been based on single particles or specific arrangements of particulate media. Direct numerical modeling (DNM) of the problem seems enables one to do a full analysis of the fields involved. As already discussed, the analysis of the results of a DNM is limited in the performance of a scaling analysis, which is the goal in most situations. Performing DNM without a proper scaling theory is like performing experiments, often very challenging and expensive; without proper data analysis, it yields a certain amount of detailed field results, but not the needed bulk or mean media physical characteristics.

Most recent work on radiative transport is based on linearized radiative transfer equations for porous media. We first review this work to set the stage for the development that follows. This radiative transport related work extends our results in the theoretical advancement of fluid mechanics, heat transport, and electrodynamics in heterogeneous media (Travkin *et al.* [19]; Catton and Travkin [28, 158]; Travkin and Catton [20, 159–163]; Travkin *et al.* [114, 115]) and provides a means for formulation of radiative transport problem in porous media using the heterogeneous VAT approach and electrodynamics language. Based on our previous work, a theoretical description of radiative transport in porous media is developed along with the Maxwell equations for a heterogeneous medium.

1. *Linear Radiative Transfer Equations in Porous Media*

The equation for radiative transport in a homogeneous medium can be written in the general form

$$\frac{1}{c}\frac{\partial I_\nu}{\partial t} + \nabla\cdot(\Omega I_\nu) + [\kappa_a(\mathbf{r}) + \kappa_s(\mathbf{r})]I_\nu = \kappa_a(\mathbf{r})I_{\nu b}(T) + \frac{1}{4\pi}\kappa_s(\mathbf{r})\int_{4\pi} p(\Omega'\cdot\Omega)I_\nu(\mathbf{r}, \Omega')d\Omega' \qquad (179)$$

$$I_\nu = I_\nu(\mathbf{r}, \Omega, t),$$

with $\kappa_a(r)$ the absorption and $\kappa_s(r)$ scattering coefficients, and for steady state, using the identity

$$\nabla\cdot(\Omega I_\nu) = \Omega\cdot\nabla I_\nu,$$

in the form

$$\Omega\cdot\nabla I_\nu + [\kappa_a(\mathbf{r}) + \kappa_s(\mathbf{r})]I_\nu = \kappa_a(\mathbf{r})I_{\nu b}(T) + \frac{1}{4\pi}\kappa_s(\mathbf{r})\int_{4\pi} p(\Omega'\cdot\Omega)I_\nu(\mathbf{r}, \Omega')\,d\Omega'. \qquad (180)$$

In terms of a spectral source function $S_\nu(s)$, the equation can be written in a particularly simple form,

$$\frac{1}{\beta_\nu}\Omega\cdot\nabla I_\nu + I_\nu = S_\nu(s), \qquad (181)$$

where the extinction coefficient (total cross section—Pomraning [150, 151] is

$$\beta_\nu = \kappa_a(\mathbf{r}) + \kappa_s(\mathbf{r}).$$

Linear particle (neutron, for example) transport in heterogeneous medium is assumed by Malvagi and Pomraning [152] and Pomraning [151] to be decribed by

$$\Omega\cdot\nabla\psi + \beta(\mathbf{r})\psi = S(\mathbf{r}, \Omega) + \frac{1}{4\pi}\int_{4\pi}\kappa_s(\mathbf{r}, \Omega'\cdot\Omega)\psi(\mathbf{r}, \Omega')\,d\Omega', \qquad (182)$$

where the quantities $\beta(\mathbf{r})$, $\kappa_s(\mathbf{r})$, and $S(\mathbf{r}, \Omega)$ are taken to be two-states discrete random variables. By assuming this, one needs to treat the porous (heterogeneous) medium as a binary medium that has two magnitudes for each of the random variables, and a particle encounters alternating segments of medium with those magnitudes while traversing the medium. When β, κ_s, and S are assumed to be random variables, Eq. (182) is treated as an ensemble-averaged equation (see Malvagi and Pomraning [152] and Pomraning and Su [164])

$$\Omega\cdot\nabla(p_i\{\psi_i\}) + p_i\{\beta_i\}\{\psi_i\} = p_i\{S_i\} + \frac{\{\kappa_{si}\}}{4\pi}p_i\varphi_i + \frac{p_j\tilde{\psi}_j^{se}}{\lambda_j} - \frac{p_i\tilde{\psi}_i^{se}}{\lambda_i}, \quad i=1, 2,\ j\neq i \qquad (183)$$

$$\varphi = \int_{4\pi}\psi(\mathbf{r}, \Omega')d\Omega',$$

where $\{\psi_i\}$ is the conditional ensemble averaged function ψ at some point $\mathbf{r}$ that is in phase i, and $\tilde{\psi}_j^{se}$ and $\tilde{\psi}_i^{se}$ are the interface ensemble-averaged fluxes. The solution to this equation is also supposed to be ensemble-averaged. The overall averaging over the both phases is given by

$$\langle\psi(\mathbf{r}, \Omega)\rangle = p_1\{\psi_1\} + p_2\{\psi_2\}, \qquad (184)$$

where p_1 and p_2 are the probabilities of point $\mathbf{r}$ being in medium $i = 1$ or 2, and $\{\psi_i\}$ is the conditional ensemble averaged value of ψ, when $\mathbf{r}$ is in medium i.

Ensemble averaging in this representation is obtained by averaging of medium features, including coefficients, along a straight line the Ω direction—or by nonlocal 1D line averaging in terms of the physical fields considered. Most of this kind of work is related to the Markovian statistics by alternating along the line of two phases of the medium (Pomraning [148, 151]).

The ensemble averaging procedure suggested in (183) signifies that the two last terms in the averaged equation reflect the finite correlation length (interconnection) in a single nonlinear term $\beta(\mathbf{r})\psi$. This kind of averaging results in very simple closure statements derived using hierarchical volume averaging theory procedures, as shown later. A major problem in using ensemble averaging techniques is that the processes and phenomena going at each separate site within separate elements of the heterogeneous medium cannot be resolved completely with the purely statistical approach of ensemble averaging.

To make an ensemble averaging method workable, researchers always need to formulate the final problem or solution in terms of spacially specific statements or in terms of the original spatial volume averaging theory (VAT). Examples of this are numerous; see the review by Buyevich and Theofanous [165].

2. *Nonlocal Volume Averaged Radiative Transfer Equations*

The basis for the development in this field will be the volume averaging theory. We will present some aspects of VAT that are now becoming well understood and have seen substantial progress in thermal physics and in fluid mechanics. The need for a method that enables one to develop general, physically based models of a group of physical objects (for example, molecules, atoms, crystals, phases) that can be substantiated by data (statistical or analytical) is clear. In modern physics it is usually accomplished using statistical data and theoretical methods. One of the major drawbacks of this widely used approach is that it does not give a researcher the capability to relate the spatial and morphological parameters of a group of objects to the phenomena of interest when it is described at the upper level of the hierarchy. Often the equations obtained by these methods differ from one another even when describing the same physical phenomena.

The drawbacks of existing methods do not arise when the VAT mathematical approach is used. At the present time, there is an extensive literature and many books on linear, homogeneous, and layered system electromagnetic and acoustic wave propagation (Adzerikho *et al.* [142]; Bohren and Huffman [144]; Dombrovsky [140]; Lindell *et al.* [146]; Lakhtakia *et al.* [147]; Lorrain and Corson [145]; Siegel and Howell [131]; van de Hulst [143]). It is surprising that these phenomena are often described by almost identical mathematical statements and governing equations for both heterogeneous and homogeneous media.

Major developments in the use of VAT, showing the potential for application to eletrophysical and acoustics phenomena in heterogeneous media, are found in Travkin and Catton [21], Travkin *et al.* [159, 114, 115], and with experimental applications to ferromagnetism in Ryvkina *et al.* [160, 162] and Ponomarenko *et al.* [161].

It has been demonstrated during the past 20 years of VAT-based modeling in the thermal physics and fluid mechanics area (see Slattery [6]; Whitaker [10]; Kaviany [7]; Gray *et al.* [8]) that the potential of the approach is enormous. Substantial success has also been achieved in analyzing the more narrow phenomena of electromagnetic wave propagation in porous media.

We consider here radiative transfer in porous media using a hierarchical approach to describe physical phenomena in a heterogeneous medium. The physical features of lowest scale of the medium are considered and their averaged characteristics are obtained using special mathematical instruments for describing hierarchical processes, namely VAT. At the next higher level of the hierarchy, physical phenomena have the physical medium pointwise characteristics resulting from averaged lower scale characteristics.

The same kind of operators and averaging theorems used in preceding sections are applied to the following development, involving the **rot** operator, in which averaging will result because of the following averaging theorems:

$$\langle \nabla \times \mathbf{f} \rangle_1 = \nabla \times \langle \mathbf{f} \rangle_1 + \frac{1}{\Delta\Omega} \int_{\partial S_{12}} \vec{d}s_1 \times \mathbf{f} \tag{185}$$

$$\{\nabla \times \mathbf{f}\}_1 = \nabla \times \{\mathbf{f}\}_1 + \frac{1}{\Delta\Omega} \int_{\partial S_{12}} \vec{d}s_1 \times \hat{\mathbf{f}}. \tag{186}$$

Rigorous application to linear and nonlinear electrodynamics and electrostatic problems is described in Travkin *et al.* [114, 115].

The phase averaging the equation for linear local thermal equilibrium radiative transfer,

$$\Omega \cdot \nabla I_\nu + \beta_\nu(\mathbf{r}) I_\nu = \kappa_a(\mathbf{r}) I_{\nu b}(T) + \frac{1}{4\pi} \kappa_s(\mathbf{r}) \int_{4\pi} p(\Omega' \cdot \Omega) I_\nu(\mathbf{r}, \Omega')\, d\Omega', \tag{187}$$

in phase 1 yields the VAT radiative equation (VARE)

$$\Omega \cdot \left[\nabla \langle I_{\nu 1} \rangle_1 + \frac{1}{\Delta\Omega} \int_{\partial S_{12}} I_{\nu 1} \vec{d}s_1 \right] + \langle \tilde{\beta}_{\nu 1} \tilde{I}_{\nu 1} \rangle_1$$

$$= \langle \kappa_{a1}(\mathbf{r}) I_{\nu b1}(T) \rangle_1 + \frac{\kappa_{s1}}{4\pi} \langle \varphi_1 \rangle_1 - \langle \hat{\beta}_{\nu 1} \hat{I}_{\nu 1} \rangle_1, \quad i = 1 \tag{188}$$

$$\varphi = \int_{4\pi} p(\Omega' \cdot \Omega) I_\nu(\mathbf{r}, \Omega')\, d\Omega',$$

when it is assumed that κ_{si} is a constant, as done by Malvagi and Pomraning [152], Pomraning and Su [164], and others.

The additional terms appearing in the VARE in some instances are similar, but in others they have a different interpretation in the ensemble averaged equation (183). For example, the term

$$-\langle \hat{\beta}_{\nu 1} \hat{I}_{\nu 1} \rangle_1 \tag{189}$$

in (188) is the result of fluctuations correlation inside of medium 1 in the REV, but it is described by

$$\frac{p_j \tilde{\psi}_j^{se}}{\lambda_j} - \frac{p_i \tilde{\psi}_i^{se}}{\lambda_i} \tag{190}$$

in Malvagi and Pomraning [152], as it is an exchange of energy term between the two phases across the interface surface area ∂S_{12}. Because ensemble averaging methodologies in Malvagi and Pomraning [152] do not treat nonlinear terms very well and incorrectly average differential operators such as ∇, terms do not appear in equation (183) that reflect the interface flux exchange. In VARE, Eq. (188), the interface exchange term naturally appears as a result of averaging the ∇ operator,

$$\Omega\cdot\left(\frac{1}{\Delta\Omega}\int_{\partial S_{12}} I_{\nu 1}\vec{d}s_1\right). \tag{191}$$

When the coefficients in the radiative transfer equation are dependent functions, more linearized terms are observed in the corresponding VARE,

$$\begin{aligned}\Omega\cdot\nabla\langle I_{\nu 1}\rangle_1 + \langle\tilde{\beta}_{\nu 1}\tilde{I}_{\nu 1}\rangle_1 \\ = \langle\tilde{\kappa}_{a1}\tilde{I}_{\nu b1}(T)\rangle_1 + \langle\hat{\kappa}_{a1}\hat{I}_{\nu b1}\rangle_1 + \frac{1}{4\pi}\left(\langle\tilde{\kappa}_{s1}\tilde{\varphi}_1\rangle_1 + \langle\hat{\kappa}_{s1}\hat{\varphi}_1\rangle_1\right) \\ - \Omega\cdot\left(\frac{1}{\Delta\Omega}\int_{\partial S_{12}} I_{\nu 1}\vec{d}s_1\right) - \langle\hat{\beta}_{\nu 1}\hat{I}_{\nu 1}\rangle_1, \quad i = 1,\end{aligned} \tag{192}$$

while continuing to treat the emissivity as via the Planck's function. This equation should be accompanied by the VAT heat transfer equations in both porous medium phases (see, for example, Travkin and Catton [21]).

The heat transport within solid phase 2, combining conductive and possible radiative transfer, is described by

$$\begin{aligned}\langle s_2\rangle(\rho c_p)_2\frac{\partial\tilde{T}_2}{\partial t} = k_2\nabla^2(\langle s_2\rangle\tilde{T}_2) + k_2\nabla\cdot\left[\frac{1}{\Delta\Omega}\int_{\partial S_{12}} T_2\vec{d}s_2\right] \\ + \frac{k_2}{\Delta\Omega}\int_{\partial S_{12}}\nabla T_2\cdot\vec{d}s_2 + \nabla\cdot\langle\mathbf{q}^r\rangle_2 + \frac{1}{\Delta\Omega}\int_{\partial S_{12}}\mathbf{q}^r\cdot\vec{d}s_2.\end{aligned} \tag{193}$$

The third and fifth terms on the r.h.s. model the heat exchange rate between the phases. In an optically thick medium, for example, the radiation flux term written in terms of the total blackbody radiation intensity is

$$\nabla\cdot\langle\mathbf{q}^r\rangle_2 = \nabla\cdot\left\langle -\frac{4}{3\beta}\nabla(I_b)\right\rangle_2 = \nabla\cdot\left\langle -\frac{4}{3\beta}\nabla\left(\frac{n^2\sigma T^4}{\pi}\right)\right\rangle_2, \tag{194}$$

where β is the total extinction coefficient. An energy equation similar to Eq. (193) needs to be written for the fluid-filled volume, phase 1 of the porous medium. The radiation flux term would be much more complex because of the spectral characteristics of radiation in a fluid.

Closure is needed for the second, third, and fifth terms in Eq. (193) on the r.h.s. For convective heat exchange, the last term can be written

$$\frac{k_2}{\Delta\Omega}\int_{\partial S_{12}}\frac{\partial T}{\partial x_i}\cdot\vec{d}s_2 = \tilde{\alpha}_{21}S_{12}(\{T\}_1 - \{T\}_2) \tag{195}$$

by noting that

$$\begin{aligned}\frac{1}{\Delta\Omega}\int_{\partial S_{12}} k_2\frac{\partial T}{\partial x_i}\cdot\vec{d}s_2 = -\frac{1}{\Delta\Omega}\int_{\partial S_{12}} k_2\frac{\partial T}{\partial \mathbf{n}_1}\,ds\cdot\mathbf{n}_1 \\ = \frac{1}{\Delta\Omega}\int_{\partial S_{12}}\mathbf{q}_1\cdot\vec{d}s_1 = \bar{\alpha}_{21}S_{12}(\{T\}_1 - \{T\}_2).\end{aligned} \tag{196}$$

This type of closure procedure is appropriate for description of fluid–solid media heat exchange and has been considered by many as an analog for solid–solid heat exchange. A more strict and precise integration of the heat flux over the interfce surface, using the IVth kind of boundary conditions, gives the exact closure for the term in the governing equations for the neighboring phase. This would be an adequate solution for the portion of heat exchange by conduction to and from the fluid phase, a conjugate problem.

The radiative energy exchange across the interface surface is difficult to formulate because of its spectral characteristics and the boundary conditions that must be satisfied. When the fluid phase is assumed to be optically thin, an approximate closure expression results,

$$\begin{aligned}\frac{1}{\Delta\Omega}\int_{\partial S_{12}}\mathbf{q}^r\cdot\vec{d}s_2 = \frac{1}{\Delta\Omega}\int_{\partial S_{12}}\left(\frac{\sigma(T_{12}^4 - T_{21}^4)}{\left(\dfrac{1}{\varepsilon_{12}} + \dfrac{1}{\varepsilon_{21}} - 1\right)}\right)\cdot\vec{d}s_2 \\ \cong \left(\frac{\sigma((\tilde{T}_{12}^s)^4 - (\tilde{T}_{21}^s)^4)S_{12}}{\left(\dfrac{1}{\varepsilon_{12}} + \dfrac{1}{\varepsilon_{21}} - 1\right)}\right),\end{aligned} \tag{197}$$

using an interpretation of the averaged surface temperatures on opposite sides of the interface developed by Malvagi and Pomraning [152]. Another approximation is justifiable for an optically thick fluid phase. It uses the specific blackbody surface radiation intensity $I_{b21} = n^2\sigma T_{21}^4$ to close the integral energy exchange term as follows:

$$\frac{1}{\Delta\Omega}\int_{\partial S_{12}}\mathbf{q}^r\cdot\vec{d}s_2 \cong \frac{1}{\Delta\Omega}\int_{\partial S_{12}}(n^2\sigma T_{21}^4)\vec{d}s_2 \cong \varepsilon_{21}^r\sigma(\tilde{T}_{21}^s)^4 S_{12}. \tag{198}$$

Here, ε_{21}^r is the total radiative hemispherical emissivity from phase 2 to phase 1 in the REV.

The closure of Eqs. (183) is accomplished by assuming equality (Malvagi and Pomraning [152]; Pomraning and Su [164]) between the interface surface and ensemble (1D in this case) averaged functions,

$$\tilde{\psi}_j^{se} = \{\psi_i\}, \tag{199}$$

as was done in heat and mass transfer porous medium problems; see, for example, Crapiste *et al.* [41].

3. *Radiation Transport in Heterogeneous Media Using Harmonic Field Equations*

Representing the electromagnetic field components with time-harmonic components results in

$$\nabla\cdot(\varepsilon_d\mathbf{E}) = \rho, \quad \nabla\cdot(\mu_m\mathbf{H}) = 0 \tag{200}$$

$$\nabla\times\mathbf{E} = -\mathbf{i}\omega\mu_m\mathbf{H}, \quad \nabla\times\mathbf{H} = \mathbf{i}\omega\bar{\varepsilon}_d\mathbf{E}. \tag{201}$$

Here, as outlined earlier, $\bar{\varepsilon}_d$ is the complex dielectric function $\bar{\varepsilon}_d = \varepsilon_d - \mathbf{i}(\sigma_e/\omega)$, and $\varepsilon_d = \varepsilon_d(\vec{\mathbf{x}})$, $\sigma_e = \sigma_e(\vec{\mathbf{x}})$, $\mu_m = \mu_m(\vec{\mathbf{x}}, \omega)$, $\bar{\varepsilon}_d = \bar{\varepsilon}_d(\vec{\mathbf{x}}, \omega)$. In many contemporary applications the spatial dependency of these functions is neglected. Electrophysical coefficients often need to be treated as nonlinear. For example, the dielectric function can depend on $\mathbf{E}$ and $\varepsilon_d = \varepsilon_d(\vec{\mathbf{x}}, \mathbf{E})$. The wave formulation of the Maxwell equations with constant phase coefficients for the magnetic field is

$$\nabla^2\mathbf{H} - \mu_m\sigma_e\frac{\partial\mathbf{H}}{\partial t} - \mu_m\varepsilon_d\frac{\partial^2\mathbf{H}}{\partial t^2} = 0, \tag{202}$$

whereas the electric field wave equation is almost the same,

$$\nabla^2\mathbf{E} - \mu_m\sigma_e\frac{\partial\mathbf{E}}{\partial t} - \mu_m\varepsilon_d\frac{\partial^2\mathbf{E}}{\partial t^2} = \nabla\left(\frac{\rho}{\varepsilon}\right). \tag{203}$$

Another form of the equation for $\mathbf{E}$ appears in Cartesian coordinates when electromagnetic fields are time-harmonic functions:

$$\nabla^2\mathbf{E} + k^2\mathbf{E} = 0, \tag{204}$$

Here, the inhomogeneous function $k^2 = \omega^2\mu_m\varepsilon_d$ is the wave number squared. This equation is often applicable to linear acoustics phenomena. This category of equations can be transformed to a form legitimate for application to heterogeneous media problems.

The time-harmonic forms of equations for **rot** of electromagnetic fields are

$$\nabla\times(\langle m_1\rangle\tilde{\mathbf{E}}_1) + \frac{1}{\Delta\Omega}\int_{\partial S_{12}}\vec{d}s_1\times\mathbf{E}_1 = -\mathbf{i}\omega[\langle m_1\rangle\tilde{\mu}_{m1}\tilde{\mathbf{H}}_1 + \langle m_1\rangle\{\hat{\mu}_{m1}\hat{\mathbf{H}}_1\}_1] \tag{205}$$

$$\nabla\times(\langle m_1\rangle\tilde{\mathbf{H}}_1) + \frac{1}{\Delta\Omega}\int_{\partial S_{12}}\vec{d}s_1\times\mathbf{H}_1 = \mathbf{i}\omega[\langle m_1\rangle\tilde{\bar{\varepsilon}}_{d1}\tilde{\mathbf{E}}_1 + \langle m_1\rangle\{\hat{\bar{\varepsilon}}_{d1}\hat{\mathbf{E}}_1]. \tag{206}$$

The magnetic field wave form equation with constant coefficients, when averaged over phase 1, transforms to

$$\nabla^2(\langle m_1\rangle\tilde{\mathbf{H}}_1) + \nabla\cdot\left[\frac{1}{\Delta\Omega}\int_{\partial S_{12}}\mathbf{H}_1\vec{d}s_1\right] + \frac{1}{\Delta\Omega}\int_{\partial S_{12}}\nabla\mathbf{H}_1\cdot\vec{d}s_1 = \mu_m\sigma_e\frac{\partial\langle\mathbf{H}\rangle_1}{\partial t} + \mu_m\varepsilon_d\frac{\partial^2\langle\mathbf{H}\rangle_1}{\partial t^2}, \tag{207}$$

and the electric field wave equation (203) becomes

$$\nabla^2(\langle m_1\rangle\tilde{\mathbf{E}}_1) + \nabla\cdot\left[\frac{1}{\Delta\Omega}\int_{\partial S_{12}}\mathbf{E}_1\vec{d}s_1\right] + \frac{1}{\Delta\Omega}\int_{\partial S_{12}}\nabla\mathbf{E}^1\cdot\vec{d}s_1 = \mu_m\sigma_e\frac{\partial\langle\mathbf{E}\rangle_1}{\partial t} + \mu_m\varepsilon_d\frac{\partial^2\langle\mathbf{E}\rangle_1}{\partial t^2} + \frac{1}{\varepsilon_d}\nabla(\langle m_1\rangle\tilde{\rho}_1) + \frac{1}{\varepsilon_d\Delta\Omega}\int_{\partial S_{12}}\rho_1\vec{d}s_1. \tag{208}$$

An analogous form of the averaged equation is obtained for the time-harmonic electrical field:

$$\nabla^2(\langle m_1\rangle\tilde{\mathbf{E}}_1) + \nabla\cdot\left[\frac{1}{\Delta\Omega}\int_{\partial S_{12}}\mathbf{E}_1\vec{d}s_1\right] + \frac{1}{\Delta\Omega}\int_{\partial S_{12}}\nabla\mathbf{E}_1\cdot\vec{d}s_1 + \langle m_1\rangle k^2\tilde{\mathbf{E}}_1 = 0. \tag{209}$$

It is the naturally appearing feature of the heterogeneous medium electrodynamics equations as the terms reflecting phenomena on the interface surface ∂S_{12}, and that fact is to be used to incorporate morphologically precise polarization phenomena as well as tunneling into heterogeneous electrodynamics, as is being done in fluid mechanics and heat transport (Travkin and Catton [21]; Catton and Travkin [28]).

Using the orthogonal locally calculated directional fields $\tilde{E}_{l1}$ and $\tilde{E}_{r1}$ of averaged electrical field $\tilde{\mathbf{E}}_1$, one can seek the Stokes parameters I, Q, U, and V,

$$I = \langle\tilde{E}_{l1}\tilde{E}^*_{l1}\rangle_t + \langle\tilde{E}_{r1}\tilde{E}^*_{r1}\rangle_t \tag{210}$$

$$Q = \langle\tilde{E}_{l1}\tilde{E}^*_{l1}\rangle_t - \langle\tilde{E}_{r1}\tilde{E}^*_{r1}\rangle_t \tag{211}$$

$$U = \mathrm{Re}[\langle 2\tilde{E}_{l1}\tilde{E}^*_{r1}\rangle_t] \tag{212}$$

$$V = \mathrm{Im}[\langle 2\tilde{E}_{l1}\tilde{E}^*_{r1}\rangle_t], \tag{213}$$

which characterize the intensity of polarized radiation in a porous medium.

We will not here construct the general forms of equations for effective coefficients, as this will be done in a succeeding section for the case of temperature fields; still, the same questions of multiple versions, applicability of current methods, and variance in interpretation are the present agenda.

VAT-based models were developed recently while addressing the problems of modeling of electrodynamic properties of a liquid-impregnated porous ferrite medium (Ponomarenko *et al.* [161]), coupled electrostatic-diffusion processes in composites (Travkin *et al.* [159]), and to analyze heat conductivity experimental data in high-T_c superconductors (Travkin and Catton [166]). Powders of ferrites with NFMR frequency in the microwave range were used as the porous magnetic medium in Ponomarenko *et al.* [161]. The search for tunable levels of reflection and absorption of electromagnetic waves was conducted using a few morphologies that were arbitrarily chosen. Thus, the need for closer consideration of experiment and models presenting the data using VAT heterogeneous description tools for both became obvious.

VI. Flow Resistance Experiments and VAT-Based Data Reduction in Porous Media

It is well known that existing measurements of transport coefficients in porous (and heterogeneous) media must be used with care. As long as a complete description of an experiment is provided and the data analysis is carried out using correct mathematical formulations (models), the relationship between the experiment and its analysis is maintained in a comsistent, general, and useful way. Unfortunately, this is not always the case, because heuristic equations and models are often the basis for coefficient matching and model tuning when heterogeneous medium experimental data is reduced to correlations.

The various approaches, and even disarray, in the field can be contributed to a lack of understanding of the general theoretical basis for transport phenomena in porous and heterogeneous media. As long as the correlations used for momentum transport comparison are generated from empirical Darcy and Reynolds–Forchheimer expressions, or effective heat and electrical conductivity and permittivity derived from homogeneous models, problems in heterogeneous media experimental validation and comparison will persist.

Modeling based on volume averaging theory will be shown to provide a basis for consistency to experimental procedures and to data reduction processes by a series of analyses and examples. Many of the common correlations, and their weaknesses, are examined using a unified scaling procedure that allows them to be compared to one another. For example, momentum resistance and internal heat transfer dependencies are analyzed and compared. VAT-based analysis is shown to reveal the influence of morphological characteristics of the medium; to suggest scaling parameters that allow a wide variety of different porous medium morphologies to be normalized, often eliminating the need for further experimental efforts; and to clarify the relationships between differing experimental configurations. The origin, and insufficiency, of electrical conductivity and momentum transport "cross-correlation" approaches based on analogies using mathematical models without examining the physical foundation of the phenomena will be described and explained.

1. *Experimental Assessment of Flow Resistance in Porous Medium*

A one-term flow resistance model for porous medium experimental data analysis often used is

$$-\frac{d\tilde{\bar{p}}}{dx} = f\left(\frac{S_w}{\langle m\rangle}\right)\frac{\rho_f \tilde{\bar{u}}^2}{2}, \tag{214}$$

where f is some coefficient of hydraulic resistance. On the other hand, most two-term models used for flow resistance experimental data reduction have first-order and second-order velocity terms, the Darcy–Forchheimer flow resistance models. These models were obtained primarily for direct comparison with established empirical and semiempirical Darcy and Darcy–Forchheimer type flow resistance data. Thus, the momentum equation for laminar as well as the high (turbulent) flow regime often used is the model by Ergun [167],

$$-\frac{d\tilde{\bar{p}}}{dx} = \frac{\mu}{k_D}\langle m\rangle\,\tilde{u} + \rho_f A\langle m\rangle^2\tilde{\bar{u}}^2. \tag{215}$$

Similarly, the model given by Vafai and Kim [168] for the middle part of a porous layer is

$$-\frac{d\tilde{\bar{p}}}{dx} = \frac{\mu}{k_D}\langle m\rangle\tilde{\bar{u}} + \rho_f\langle m\rangle^3\,\frac{F}{k_D^{1/2}}\,\tilde{\bar{u}}^2, \tag{216}$$

and the Poulikakos and Renken [169] equation for the turbulent regime is

$$-\frac{d\tilde{\bar{p}}}{dx} = \frac{\mu}{k_D}\,\tilde{u} + \rho_f A\tilde{\bar{u}}^2. \tag{217}$$

Analysis of a simple idealized morphology where solutions are known will show that the Darcy and Darcy–Forchheimer or Ergun type model correlations are not matched consistently for any regime. Further, they are also without theoretical foundation. Thus, problems arise when studies to improve the description of transport use combined models for flow resistance and momentum transport in a porous medium because the analysis does not start with the correct theoretical basis. Further, which of the three equations just listed should one use?

A model of ideal parallel tube morphology yields the following Darcy friction coefficient (see, for example, Schlichting [170]):

$$f_D = \frac{8\tau_w}{(\rho_f \tilde{\bar{U}}^2)}, \quad \tau_w = \frac{d_h \Delta p}{4L}, \quad u_*^2 = \frac{\tau_w}{\rho_f} = \frac{f_D \tilde{\bar{U}}^2}{8} \tag{218}$$

$$\frac{\Delta p}{L} = -\frac{d\tilde{\bar{p}}}{dx} = \frac{4}{d_h}\rho_f u_*^2 = \frac{f_D}{d_h}\frac{\rho_f \tilde{\bar{U}}^2}{2}. \tag{219}$$

The morphology function $S_w/\langle m\rangle$ for a straight equal-diameter tube morphology is

$$S_w = \frac{\partial S_w}{\Delta\Omega} = \frac{2\pi R}{p\Delta y}, \quad \langle m\rangle = \frac{\pi R^2}{p\Delta y}, \quad \frac{S_w}{\langle m\rangle} = \frac{4}{d_h} \tag{220}$$

and an exact expression for the Darcy friction factor is

$$\frac{\Delta p}{L} = f_D \frac{\rho_f}{d_h}\frac{\tilde{\bar{U}}^2}{2}, \quad f_D = \frac{2d_h}{\rho_f \tilde{\bar{U}}^2}\frac{\Delta p}{L}. \tag{221}$$

The Fanning friction factor for this specific morphology is (using (220))

$$\frac{\Delta p}{L} = \frac{f_D}{4}\left(\frac{4}{d_h}\right)\frac{\rho_f \tilde{\bar{U}}^2}{2} = \left(\frac{f_D}{4}\right)\left(\frac{S_w}{\langle m\rangle}\right)\frac{\rho_f \tilde{\bar{U}}^2}{2} \tag{222}$$

$$f_f = \frac{d_h}{2\rho_f \tilde{\bar{U}}^2}\frac{\Delta p}{L}, \tag{223}$$

and a relationship to the Darcy friction coefficient is (Travkin and Catton [16, 20])

$$f_f = \frac{f_D}{4}. \tag{224}$$

The friction coefficient c_d for smooth tubes often calculated using the Nikuradze and Blasius formulas [170] is the same as the Fanning friction factor.

A model representing a porous medium with slit morphology was treated in conformity with the definition

$$\tau_w = \frac{\Delta p}{L} h = c_f' \frac{\rho_f \tilde{\bar{U}}^2}{2}, \quad c_f' = \frac{2\tau_w}{\rho_f \tilde{\bar{U}}^2} = \frac{2u_*^2}{\tilde{\bar{U}}^2} = \frac{2h}{\rho_f \tilde{\bar{U}}^2}\frac{\Delta p}{L}, \quad u_*^2 = \frac{h}{\rho_f}\frac{\Delta p}{L}. \tag{225}$$

The morphology ratio $S_w/\langle m\rangle$ for a porous medium morphology model of straight equal slits is found as follows:

$$S_w = \frac{(2L\Delta y)}{(pL\Delta y)} = \frac{2}{p}, \quad \langle m\rangle = \frac{(HL\Delta y)}{(pL\Delta y)} = \frac{H}{p} \tag{226}$$

$$\frac{S_w}{\langle m\rangle} = \frac{2}{H} = \frac{1}{h}, \quad d_h = 4h, \tag{227}$$

yielding the Fanning friction factor,

$$-\frac{d\tilde{\bar{p}}}{dx} = \frac{\Delta p}{L} = f_f\left(\frac{1}{h}\right)\left(\frac{\rho_f \tilde{\bar{U}}^2}{2}\right) = f_f\left(\frac{S_w}{\langle m\rangle}\right)\left(\frac{\rho_f \tilde{\bar{U}}^2}{2}\right) \tag{228}$$

$$f_f = \frac{H}{\rho_f \tilde{\bar{U}}^2}\frac{\Delta p}{L} \tag{229}$$

As one can easily see, these flow resistance models are written with the second power of bulk velocity variable. The convergency of the VAT-based flow resistance transport models to these classical constructions was demonstrated on several occasions by Travkin and Catton [16, 20, 21, 23] and Travkin *et al.* [25].

Exact flow resistance results obtained on the basis of VAT governing equations by Travkin and Catton [16, 26, 23] for the random pore diameter distribution for almost the same morphology as was used by Achdou and Avellaneda [171] demonstrated the wide departure from the Darcy-law-based treatments. That was shown even for the morphology where a single pore exists with diameter different from the all others. Meanwhile, by consistently using the VAT-based procedures (Travkin and Catton [23]), one can easily develop the needed variable, nonlinear permeability coefficient for Darcy dependency,

$$k_{dc} = \left[c_d\left(\frac{S_w}{\langle m\rangle^2}\right)\left(\frac{\tilde{\bar{U}}}{2\nu}\right)\right]^{-1}, \tag{230}$$

where $c_d = f_f$ is derived for this particular morphology using exact analytical (in the laminar regime) or well-established correlations for the Fanning friction factor in tubes.

2. *Momentum Resistance in 1D Membrane and Porous Layer Transport*

The steady-state VAT-based governing equations for laminar transport in porous media (Travkin and Catton [21]) are

$$\langle m\rangle\tilde{U}\,\frac{\partial\tilde{U}}{\partial x}+\frac{\partial}{\partial x}\,\langle\hat{u}\hat{u}\rangle_f+\frac{1}{\rho_f}\frac{\partial}{\partial x}\,(\langle m\rangle\{p\}_f)$$

$$=-\frac{1}{\rho_f\Delta\Omega}\int_{\partial S_w}p\vec{d}s+\nu\,\frac{\partial}{\partial x}\left(\frac{\partial\langle m\rangle\tilde{U}}{\partial x}\right)+\frac{\nu}{\Delta\Omega}\int_{\partial S_w}\frac{\partial U}{\partial x_i}\cdot\vec{d}s \qquad (231)$$

and

$$c_{pf}\rho_f\langle m\rangle\tilde{U}\,\frac{\partial\tilde{T}_f}{\partial x}=k_f\,\frac{\partial}{\partial x}\left[\frac{\partial\langle m\rangle\tilde{T}_f}{\partial x}\right]+c_{pf}\rho_f\,\frac{\partial}{\partial x}\,(\langle m\rangle\{-\hat{T}_f\hat{u}\}_f)$$

$$+\frac{\partial}{\partial x}\left[\frac{k_f}{\Delta\Omega}\int_{\partial S_w}T_f\vec{d}s\right]+\frac{1}{\Delta\Omega}\int_{\partial S_w}k_f\,\frac{\partial T_f}{\partial x_i}\cdot\vec{d}s \qquad (232)$$

$$\frac{\partial}{\partial x}\left(\frac{\partial\langle s\rangle\{T_s\}_s}{\partial x}\right)+\frac{\partial}{\partial x}\left[\frac{1}{\Delta\Omega}\int_{\partial S_w}T_s\vec{d}s_1\right]+\frac{1}{\Delta\Omega}\int_{\partial S_w}\frac{\partial T_s}{\partial x_i}\cdot\vec{d}s_1=0. \qquad (233)$$

The momentum equation for turbulent flow of an incompressible fluid in porous media based on K-theory can be written in the form (Gratton *et al.* [26], Travkin and Catton [20])

$$\langle m\rangle\left(\frac{\partial\bar{\tilde{U}}}{\partial t}+\bar{\tilde{U}}\,\frac{\partial\bar{\tilde{U}}}{\partial x}\right)=\frac{1}{\Delta\Omega}\int_{\partial S_w}(K_m+\nu)\,\frac{\partial\bar{U}}{\partial x_i}\cdot\vec{d}s+\frac{\partial}{\partial x}\left[\langle m\rangle(\tilde{K}_m+\nu)\,\frac{\partial\bar{\tilde{U}}}{\partial x}\right]$$

$$+\frac{\partial}{\partial x}\left[\langle m\rangle\left\{\hat{K}_m\,\frac{\partial\hat{\bar{u}}}{\partial x}\right\}_f\right]+\frac{\partial}{\partial x}\,(\langle m\rangle\{-\hat{\bar{u}}\hat{\bar{u}}\}_f)$$

$$-\left[\frac{1}{\rho_f\Delta\Omega}\int_{\partial S_w}\bar{p}\vec{d}s\right]-\frac{1}{\rho_f}\frac{\partial}{\partial x}\,(\langle m\rangle\bar{\tilde{p}}). \qquad (234)$$

By comparing these equations with conventional mathematical models and experimental correlations, one can easily see the differences.

The one-dimensional momentum equation for a homogeneous, regular porous medium is

$$-\frac{\partial}{\partial x}\,\{p\}_f=\frac{1}{\langle m\rangle\Delta\Omega}\int_{\partial S_w}\hat{p}\vec{d}s-\frac{\mu}{\langle m\rangle\Delta\Omega}\int_{\partial S_w}\nabla V\cdot\vec{d}s. \qquad (235)$$

Closure of the flow resistance terms in the simplified VAT equation can be obtained following procedures developed by Travkin and Catton [16, 17]. The skin friction term is

$$\frac{\mu}{\Delta\Omega}\int_{\partial S_{wL}}\frac{\partial U}{\partial x_i}\cdot\vec{d}s=\frac{\rho_f}{\rho_f\Delta\Omega}\int_{\partial S_w}\tau_{wL}\cdot\vec{d}s=-\frac{1}{2}\,c_{fL}(\bar{x})S_{wL}(\vec{x})[\rho_f\tilde{U}^2(\bar{x})], \qquad (236)$$

with

$$\tau_{wL}=\mu\,\frac{\partial U}{\partial x_i},\quad u_{*rk}=\tfrac{1}{2}c_{fL}\tilde{U}^2(\vec{x}),$$

and closure of the form drag resistance integral term using a form drag coefficient, c_{dp}, is

$$\frac{1}{\Delta\Omega}\int_{\partial S_w}p\vec{d}s=\frac{1}{2}\,c_{dp}S_{wp}(\vec{x})[\rho_f\tilde{U}^2(\vec{x})]. \qquad (237)$$

For these equations, the specific surface has two parts. The first part, S_{wL}, is

$$S_{wL}(\vec{x})=\frac{1}{\Delta\Omega}\int_{\partial S_{wL}}ds,\quad\left(\frac{1}{m}\right), \qquad (238)$$

where ∂S_{wL} is the laminar subregion of the interface surface element ∂S_w, and

$$S_{wp}(\vec{x})=\frac{1}{\Delta\Omega}\int_{\partial S_{wp}}ds=\frac{S_\perp}{\Delta\Omega},\quad\left(\frac{1}{m}\right), \qquad (239)$$

where ∂S_{wp} is the cross flow projected area of the surface of the solid phase inside the REV. Substitution into the one-dimensional momentum equation yields

$$-\frac{\partial}{\partial x}\,\{p\}_f=(c_{fL}(x)S_{wL}(x)+c_{dp}S_{wp}(x))\,\frac{\rho_f\tilde{U}^2(x)}{2\langle m\rangle}+\frac{\tilde{p}}{\langle m\rangle}\,(\nabla\langle m\rangle). \qquad (240)$$

When the porosity is constant, the flow is laminar and $S_{wL}=S_w$, the equation becomes

$$-\frac{d\tilde{p}}{dx}=\left(c_f+c_{dp}\,\frac{S_{wp}}{S_w}\right)\left(\frac{S_w}{\langle m\rangle}\right)\frac{\rho_f\tilde{U}^2}{2}=c_d(\bar{\tilde{U}},M_\Omega)\left(\frac{S_w}{\langle m\rangle}\right)\frac{\rho_f\tilde{U}^2}{2}, \qquad (241)$$

where c_f is the friction factor and c_{dp} the form drag, S_{wp} is the cross flow form drag specific surface, and M_Ω is a set of porous medium morphological parameters or descriptive functions (see Travkin and Catton [16, 20]). The drag terms can be combined for simplicity into a single total drag coefficient to model the flow resistance terms in the general simplified momentum VAT equation

$$c_d\,(\bar{\tilde{U}},M_\Omega)=\left(c_f+c_{dp}\,\frac{S_{wp}}{S_w}\right). \qquad (242)$$

Correlations for drag resistance can be evaluated for a homogeneous porous medium from experimental relationships for pressure drop. For example, the equation often used for packed beds is

$$-\frac{d\tilde{\tilde{p}}}{dx} = f_f\left(\frac{S_w}{\langle m\rangle}\right)\frac{\rho_f\tilde{\tilde{U}}^2}{2}. \tag{243}$$

The complete VAT version of this equation is

$$\frac{\partial}{\partial x}(\langle m\rangle\tilde{p}) + \frac{1}{\Delta\Omega}\int_{\partial S_w} p\vec{d}s + \rho_f u_{*rk}^2 S_w(x) = -\langle m\rangle\rho_f\tilde{U}\frac{\partial\tilde{U}}{\partial x} + \mu\frac{\partial}{\partial x}\left[\frac{\partial\langle m\rangle\tilde{U}}{\partial x}\right] + \frac{\partial}{\partial x}[\rho_f\langle m\rangle\{-\hat{u}\hat{u}\}_f]. \tag{244}$$

If the porosity function is constant (a frequent assumption), the left-hand side of Eq. (244) reduces to

$$-\frac{d\tilde{p}}{dx} - f_f\left(\frac{S_w}{\langle m\rangle}\right)\frac{\rho_f\tilde{U}^2}{2}. \tag{245}$$

Setting Eq. (245) equal to zero recovers equation (243). As a result, data correlation using Eq. (243) incorporates the right-hand side of Eq. (244) implicitly into the correlation. Friction factor data presented in this way detracts from objectivity. The correlation can be written to reflect all the right-hand terms from Eq. (244),

$$-\frac{d(\langle m\rangle\tilde{p})}{dx} = \left(c_f + c_{dp}\frac{S_{wp}}{S_w} + F_1 + F_2 + F_3\right)(S_w(x))\frac{\rho_f\tilde{U}^2}{2}, \tag{246}$$

where $F_1, \ldots, F_3$ are deduced from the following relationship:

$$(F_1 + F_2 + F_3)\left(S_w(x)\frac{\rho_f\tilde{U}^2}{2}\right) = \langle m\rangle\rho_f\tilde{U}\frac{\partial\tilde{U}}{\partial x} + \rho_f\frac{\partial}{\partial x}[\langle m\rangle\{\hat{u}\hat{u}\}_f] - \mu\frac{\partial}{\partial x}\left[\frac{\partial\langle m\rangle\tilde{U}}{\partial x}\right]. \tag{247}$$

In the middle part of a porous medium sample, one can assume that the porosity and flow regime are constant and steady state and then neglect all terms on the right-hand side of (244). In reality, a large number of experiments are being carried out under conditions where input–output zones are present and can add significantly to the value of the friction coefficient because of the input–output pressure losses. If one wants to separate the effects of input–output pressure loss from the viscous friction and drag resistance components inside the porous medium, then taking into account the terms shown in Eq. (247) is essential. There are correlations that reflect a dependence on sample thickness as a result of this oversight. An even more complex situation arises when the flow and temperature inside the medium are transient, such as one might find in a regenerator, and very inhomogeneous in space because of sharp gradients. The inhomogeneity in space and time precludes neglecting the four right-hand terms in Eq. (244).

The inhomogeneous terms on the right-hand side of (247) may be analyzed by scaling. Some of these terms are easily interpreted. For example, the first term on the right-hand side is the convective term

$$\left(S_w(x)\frac{\rho_f\tilde{\tilde{U}}^2}{2}\right)F_1 = \langle m\rangle\rho_f\tilde{\tilde{U}}\frac{\partial\tilde{\tilde{U}}}{\partial x}, \tag{248}$$

and its importance can be strongly dependent on the thickness of the porous specimen. This is why many studies report an obvious correlation with specimen thickness. The remaining terms are the "morphoconvective" term

$$\left(S_w(x)\frac{\rho_f\tilde{\tilde{U}}^2}{2}\right)F_2 = \frac{\partial}{\partial x}(\rho_f\langle m\rangle\{\hat{\hat{u}}\hat{\hat{u}}\}_f) \tag{249}$$

and the momentum diffusion term

$$\left(S_w(x)\frac{\rho_f\tilde{\tilde{U}}^2}{2}\right)F_3 = -\mu\frac{\partial}{\partial x}\left[\frac{\partial\langle m\rangle\tilde{\tilde{U}}}{\partial x}\right]. \tag{250}$$

The complete momentum equation written in a proper form for experimental data reduction is

$$-\frac{d(\langle m\rangle\tilde{p})}{dx} = \left(c_f + c_{dp}\frac{S_{wp}}{S_w} + F_1 + F_2 + F_3\right)(S_w(x))\frac{\rho_f\tilde{U}^2}{2} = (c_d + R_M)(S_w(x))\frac{\rho_f\tilde{U}^2}{2}, \tag{251}$$

where

$$c_d = c_f + c_{dp}\frac{S_{wp}}{S_w} \tag{252}$$

and

$$R_M = F_1 + F_2 + F_3. \tag{253}$$

The features of an experiment needed to treat terms such as F_1, F_2, F_3 are discussed later.

The momentum resistance coefficient for a heterogeneous porous medium can be written in the form

$$f_{por} = c_d + R_M. \tag{254}$$

This is the variable usually determined in most of porous medium flow resistance experiments. Nevertheless, if this correlation value taken from an experiment is later substituted into a modeling equation (with variable porosity) of the form

$$\langle m\rangle\tilde{U}\,\frac{\partial\tilde{U}}{\partial x}=-\frac{1}{\rho_f}\frac{\partial}{\partial x}\left(\langle m\rangle\{p\}_f\right)+\nu\frac{\partial}{\partial x}\left(\frac{\partial\langle m\rangle\tilde{U}}{\partial x}\right)-c_D(x)\,\frac{S_w(x)}{\langle m\rangle}\,\frac{\rho_f\tilde{U}^2}{2} \tag{255}$$

or

$$\langle m\rangle\tilde{U}\,\frac{\partial\tilde{U}}{\partial x}=-\frac{1}{\rho_f}\frac{\partial}{\partial x}\left(\langle m\rangle\{p\}_f\right)+\nu\frac{\partial}{\partial x}\left(\frac{\partial\langle m\rangle\tilde{U}}{\partial x}\right)-\frac{\mu}{k_D}\langle m\rangle\tilde{U}-\rho_f\langle m\rangle^3\,\frac{F}{k_D^{1/2}}\,\tilde{U}^2, \tag{256}$$

as is done by many, then the fluctuation term $\partial[\langle m\rangle\{-\hat{u}\hat{u}\}_f]/\partial x$ is neglected and the equation

$$2\langle m\rangle\tilde{U}\,\frac{\partial\tilde{U}}{\partial x}=-\frac{1}{\rho_f}\frac{\partial}{\partial x}\left(\langle m\rangle\{p\}_f\right)+2\nu\frac{\partial}{\partial x}\left(\frac{\partial\langle m\rangle\tilde{U}}{\partial x}\right)-\frac{1}{\rho_f\Delta\Omega}\int_{\partial S_2}p\vec{d}s+\frac{\nu}{\Delta\Omega}\int_{\partial S_w}\frac{\partial U}{\partial x_i}\cdot\vec{d}s+\frac{\partial}{\partial x}\left[\langle m\rangle\{-\hat{u}\hat{u}\}_f\right] \tag{257}$$

is being used as the problem's model instead of

$$\langle m\rangle\tilde{U}\,\frac{\partial\tilde{U}}{\partial x}=-\frac{1}{\rho_f}\frac{\partial}{\partial x}\left(\langle m\rangle\{p\}_f\right)+\nu\frac{\partial}{\partial x}\left(\frac{\partial\langle m\rangle\tilde{U}}{\partial x}\right)-\frac{1}{\rho_f\Delta\Omega}\int_{\partial S_w}p\vec{d}s+\frac{\nu}{\Delta\Omega}\int_{\partial S_w}\frac{\partial U}{\partial x_i}\cdot\vec{d}s+\frac{\partial}{\partial x}\left[\langle m\rangle\{-\hat{u}\hat{u}\}_f\right] \tag{258}$$

because the model used the coefficient $c_D(x)$ determined from

$$\begin{aligned}c_D(x)\,\frac{S_w(x)}{\langle m(x)\rangle}\,\frac{\rho_f\tilde{U}^2}{2}&=\left(c_d(x)+R_M(x)\right)\frac{S_w(x)}{\langle m(x)\rangle}\,\frac{\rho_f\tilde{U}^2}{2}\\&=\left(c_f+c_{dp}\frac{S_{wp}}{S_w}+F_1+F_2+F_3\right)\frac{S_w(x)}{\langle m(x)\rangle}\,\frac{\rho_f\tilde{U}^2}{2}\\&=\frac{1}{\rho_f\Delta\Omega}\int_{\partial S_w}p\vec{d}s-\frac{\nu}{\Delta\Omega}\int_{\partial S_w}\frac{\partial U}{\partial x_i}\cdot\vec{d}s-\frac{\partial}{\partial x}\left[\langle m\rangle\{-\hat{u}\hat{u}\}_f\right]\\&\quad-\nu\frac{\partial}{\partial x}\left(\frac{\partial\langle m\rangle\tilde{U}}{\partial x}\right)+\langle m\rangle\tilde{U}\,\frac{\partial\tilde{U}}{\partial x},\end{aligned} \tag{259}$$

instead of using the coefficient $c_d(x)$ determined from

$$\begin{aligned}c_d(x)\,\frac{S_w(x)}{\langle m(x)\rangle}\,\frac{\rho_f\tilde{U}^2}{2}&=\left(c_f+c_{dp}\frac{S_{wp}}{S_w}+F_2\right)\frac{S_w(x)}{\langle m(x)\rangle}\,\frac{\rho_f\tilde{U}^2}{2}\\&=\frac{1}{\rho_f\Delta\Omega}\int_{\partial S_w}p\vec{d}s-\frac{\nu}{\Delta\Omega}\int_{\partial S_w}\frac{\partial U}{\partial x_i}\cdot\vec{d}s+\frac{\partial}{\partial x}\left[\langle m\rangle\{\hat{u}\hat{u}\}_f\right].\end{aligned} \tag{260}$$

The terms needed for experimental data reduction model should include all five active terms,

$$\begin{aligned}-\frac{d(\langle m\rangle\tilde{p})}{dx}&=\left(c_f+c_{dp}\frac{S_{wp}}{S_w}+F_1+F_2+F_3\right)(S_w(x))\,\frac{\rho_f\tilde{U}^2}{2}\\&=(c_d+R_M)(S_w(x))\,\frac{\rho_f\tilde{U}^2}{2},\end{aligned} \tag{261}$$

with

$$f_{por}=c_d+R_M. \tag{262}$$

The general 1D VAT laminar regime constant viscosity momentum equation has six terms,

$$\begin{aligned}&\langle m\rangle\bar{U}\,\frac{\partial\tilde{U}}{\partial x}+\frac{\partial}{\partial x}\langle\hat{u}\hat{u}\rangle_f+\frac{1}{\rho_f}\frac{\partial}{\partial x}\left(\langle m\rangle\{p\}_f\right)\\&\quad=-\frac{1}{\rho_f\Delta\Omega}\int_{\partial S_w}p\vec{d}s+\nu\frac{\partial}{\partial x}\left(\frac{\partial\langle m\rangle\tilde{U}}{\partial x}\right)+\frac{\nu}{\Delta\Omega}\int_{\partial S_w}\frac{\partial U}{\partial x_i}\cdot\vec{d}s.\end{aligned} \tag{263}$$

For simplicity, Eq. (263) is written in the following shorthand notation:

$$UC_1+UMC_1+UP_1=-UMP_1+UD_1+UMF_1. \tag{264}$$

The two right-hand integral terms reflect the morphology-induced flow resistance of the medium. Three flow resistance models are needed to properly tie everything together.

a. Flow Resistance Model 1 The first flow resistance model is for the internal frictional and form drag resistance:

$$\begin{aligned}-\mathbf{c}_{d1}(\tilde{\bar{U}},M_\Omega,\mathbf{x})\left(\frac{S_w(x)\tilde{U}^2(x)}{2}\right)&=\left(-c_{dp}S_{wp}(x)-c_{fL}(x)S_{wL}(x)\right)\frac{\tilde{U}^2(x)}{2}\\&=-\frac{1}{\rho_f\Delta\Omega}\int_{\partial S_w}p\vec{d}s+\frac{\nu}{\Delta\Omega}\int_{\partial S_w}\frac{\partial U}{\partial x_i}\cdot\vec{d}s.\end{aligned} \tag{265}$$