0.0.1 EFFECTIVE DIFFUSIVE TRANSPORT COEFFICIENT MODELING

Determination effective transport coefficients for a heterogeneous (and porous) media has received considerable attention by researchers who are studying the transport through a porous media. Careful notation procedures are necessary when the turbulent thermal dispersivity is being studied. To evaluate experiment it is typical to use solution obtained by moment method or analytically. This was done by many researchers.

One of the methods of closure of mathematical models of diffusion processes in a heterogeneous media is the quasihomogeneous method. In this case, the transfer process is modeled as an ideal continuum with homogeneous effective transport characteristics instead of the real heterogeneous characteristics of a porous medium. This method of closure of the diffusive terms in the heat and mass diffusion equations results in certain limitations: (a) the two-phase medium components are without fluctuations of the type $\widehat{T}$, $\widehat{c}$ in each of the phases; and (b) the transfer coefficients being constant in each of the phases (Khoroshun, [68,69]) results in reducing them to additional algebraic equations. These equations relate the unknown averaged diffusion flows in each of the phases in the following form

$$\left\langle \vec{j} \right\rangle_f + \left\langle \vec{j} \right\rangle_s = -K^*_{c(ij)} \left\langle \nabla \overline{C} \right\rangle, \tag{1}$$

$$\left\langle \nabla \overline{C} \right\rangle = \nabla \left[\langle m \rangle \left\{ \overline{C} \right\}_f + (1 - \langle m \rangle) \left\{ \overline{C} \right\}_s \right] + \frac{1}{\Delta\Omega} \int\limits_{\partial S_w} \left(\bar{C}^{\ +} - \bar{C}^{\ -} \right) \vec{ds}, \tag{2}$$

$$\left(K^f_{c(ij)} \right)^{-1} \left\langle \vec{j} \right\rangle_f + \left(K^s_{c(ij)} \right)^{-1} \left\langle \vec{j} \right\rangle_s = -\left\langle \nabla \overline{C} \right\rangle. \tag{3}$$

Here, unlike the work of Khoroshun [68], Kudinov and Moyzes [70] and Hadley [71], $\overline{C}^+$ and $\overline{C}^-$ are the values of the concentrations (or temperatures) at both sides of the phase transition surface ∂S_w (they do not have to be equal), $K^f_{c(ij)}$, $K^s_{c(ij)}$ are the transfer coefficient tensors in each of the phases, and $K^*_{c(ij)}$ is the effective diffusion coefficient. Thus, at least in this case, the problem of closure has been reduced to finding $K^*_{c(ij)}$and integrals across the interface of the difference of the values of limits of admixture concentrations (or temperature) at both its sides. For temperature fields, the above relationships will be similar (neglecting the heat resistance of the interface boundary)

$$\left\langle \nabla \overline{T}\ \right\rangle_f + \left\langle \nabla \overline{T}\ \right\rangle_s = \left\langle \nabla \overline{T}\ \right\rangle, \ \ -K^f_{T,eff} \left\langle \nabla \overline{T}\ \right\rangle_f - K^s_{T,eff} \left\langle \nabla \overline{T}\ \right\rangle_s = -K^*_T \left\langle \nabla \overline{T}\ \right\rangle. \tag{4}$$

Applying the closure relation, for example

$$K^f_{T,eff} \left\langle \nabla \overline{T}\ \right\rangle_f = K^s_{T,eff} \left\langle \nabla \overline{T}\ \right\rangle_s, \tag{5}$$

yields the effective stagnant coefficient

$$K_T^* = \frac{2K_{T,eff}^f K_{T,eff}^s}{\left(K_{T,eff}^f + K_{T,eff}^s\right)}, \tag{6}$$

that represents the lower bound of the effective stagnant conductivity for a two-phase material from the known boundaries of Hashin-Shtrikman (see, for example, Beran [72], Kudinov and Moyzes [70]) for equal volume fraction of phases. Other closure equations for calculating the stagnant effective conductivity are found in work by Hadley [71], and by Kudinov and Moyzes [70]. The quasi-homogeneous approach has several defects:

a) the basis for the quasi-homogeneous equations is in question, b) the local fluctuation values, as well as inhomogeneity and dispersivity of the medium, are neglected, and c) the interdependence of the correlated coefficients and arbitrary adjustment to fit data significantly reduce the generality of the results.

Finding effective parameters for heterogeneous medium using a perturbation expansion to derive the higher-order exact bounds of a composite‘s properties has many difficulties. Torquato‘s approach (see, for example, Torquato et al., [38], Miller and Torquato, [39], etc.) is an application of the perturbation expansion method to a composite medium using advanced statistical information about medium morphology based on the n-point probability functions. The difficulty in this approach is in the determination of the n-point morphological characteristics that should be considered. Torquato [73] provided a comparison of his predictions with experimental data of Turner [74] for a medium (composite) with periodic and randomly located spherical inclusions. Excellent agreement was obtained for regular morphology. However, for a composite with a random disperse phase spatial distribution, the calculated values were not in good agreement with the experimental data of Turner. The two first terms of the perturbation expansion and 3-point probability distribution functions were used in the simulation.

Rather comprehensive analysis of the same problem is presented by Sangani and Yao [75] where the random microstructure of the composite was approximated by a spatially periodic array with a unit cell containing N (16) arbitrary placed inclusions. In other words, the spatial model consists N periodic lattices of inclusions. Their mutual position is generated in a special way so that the radial distribution function is in a good agreement with solution of the Percus-Yevick equation. This solution was used then to obtain the Pade approximations and higher-order bounds of the effective conductivity, Milton‘s numbers as well as the sixth and eighth-order bounds. It was shown, that this approach gives better agreement with the Turner‘s [74] data than Torquato‘s formulae because more morphological (essentially stochastic) information was involved into consideration and the rigorous solution of the boundary-value problem

Effective coefficients, usually thought to be the universal solution to most heterogeneous media problems, are not easily described when applying mathematical model like the VAT. The “heterogeneous“ terms in the momentum equation yields, by the overall representation of diffusive and "diffusion-like" terms

$$K_{m,eff}\frac{\partial\widetilde{\overline{U}}}{\partial x}=\left(\langle m\rangle\left(\widetilde{K}_{m}+\nu\right)\frac{\partial\widetilde{\overline{U}}}{\partial x}+\left\langle\widehat{K}_{m}\frac{\partial\,\widehat{\overline{u}}}{\partial x}\right\rangle_{f}+\left\langle-\widehat{\overline{u}}\,\widehat{\overline{u}}\right\rangle_{f}.\right). \tag{7}$$

Here the variables of velocity and viscosity coefficient are taken in a form suitable for both laminar and turbulent flow regimes. From this expression the thought effective coefficient $K_{m,eff}$is not seen to be a constant value, but rather a complex nonlinear function explicitly dependent on other functions and variables. The additional friction and drag resistance terms in equation still need to be closed in some way.

For problems with a constant bulk viscosity coefficient (K_m= constant) the second term in this relation vanishes and the whole problem essentially assumes the role of evaluating the influence on the momentum due to dispersion by irregularities of the porous medium. Diffusion-dispersion effects realized through the second derivative terms and relaxation terms in the fluid phase mass transport equation can be expressed,

$$K_{c,eff}\frac{\partial\widetilde{\overline{C_f}}}{\partial x}=\left(\langle m\rangle\left(\widetilde{K}_{C}+D_f\right)\frac{\partial\widetilde{\overline{C}}_f}{\partial x}+\left\langle\widehat{K}_{C}\frac{\partial\,\widehat{\overline{C}}_f}{\partial x}\right\rangle_{f}+\right)$$

$$+\langle m\rangle\left\{-\widehat{\overline{c}}_f\,\widehat{\overline{u}}\right\}_f+\frac{\left(\widetilde{K}_{C}+D_f\right)}{\Delta\Omega}\int\limits_{\partial S_w}\widehat{\overline{c}}_f\vec{ds}, \tag{8}$$

where the first and last terms resemble the effective thermal conductivity coefficient for each phase, using constant coefficients, see Nozad et al. [42]. Interpretation of this equation as one that to be the equation for effective coefficient calculation meaning simply by adding the one more equation to the whatever problem was stated at the beginning.

Considering the effective coefficient problem as the cornerstone issue in the heterogeneous media transport, one needs to accommodate the reasoning that the absolute majority of problem stated and studies include the following assumptions: 1) a composite is a two-phase media consisting of a continuous matrix phase and embedded inclusions of disperse phase; 2) phase materials are homogeneous and isotropic, their properties are temperature-independent; 3) disperse phase consists of the equally sized spherical particles, uniformly distributed within a matrix phase. As a result, the composite is assumed to be macroscopically isotropic; 4) interfaces have the conditions of conventional boundary transport laws, for example, perfect thermal contact is supposed to be maintained; 5) the external (heat) flux is supposed to be time-independent and macroscopically uniform, etc.

At this time it can be concluded that the two-phase heat conductivity effective coefficient problem for the periodic morphologies is practically resolved

(at least in the scientific sense), whereas, for disordered, random morphologies of composites it is far from the resolved even when the above assumptions are appropriate.