Effective Pressure Loss Coefficients for Capillary Morphologies with Regular and Random Morphological Characteristics

Consistent research and development in porous medium morphology reveals that more and more realistic structures in the pore network image must be treated (see, for example, Mann and Yousef [44], etc). Inasmuch as each of the significant morphology structure elements can be randomly assigned, (Mann and Yousef, [44]; and other studies), workers have gradually developed a more sophisticated, randomized, network morphology, with up to 5 degrees of randomness; 1) pore surface roughness: 2) pore diameter; 3) pore length; 4) pore pathway between modes (for tortuosity); 5) pore cross-sectional shape.

In the work by Sahimi [45], diffusion controlled reaction and transport of species is being modeled as a network of branching pores, with no closed loops. It is called the wood approximation and does not allow the study of real pore networks. Another drawback to this kind of approach is a fixed pore length resulting because diffusion along the pore from one node to another has been approximated by a finite difference scheme, often based on constant internode spacing the pore length is fixed. These are very serious restrictions and have been noted elsewhere (Kheifets and Neimark, [12]).

Contemporary technology can measure, with certain confidence many of the pore‘s media characteristics, the total void fraction, the density of the solid phase, the relative pore size distribution for pores larger than 30 angstroms in diameter, and the equilibrium adsorption characteristics of the porous medium solid phase (Sircar and Rao, [46]). There is a problem of how to connect porous medium morphology characteristics that can and are being measured and to the transport equation, beign considered and their coefficients.

The method of effective medium approximation (EMA) is used in many previous works and shows excellent results, see Koplik [47]. Essential differences exist in our approach and the commonly used EMA approach where the actual problem pore network is replaced by a network with artificial uniform morphology (Sahimi, [45], Mojaradi and Sahimi, [48], Jerauld et al. [49], Koplik, [47], and etc.) and effective properties such as the effective diffusivity, D_{eff}, or the effective reactivity, R_{eff}. An important consideration, most often not dealt with, is determining which network morphology properties can be assigned externally, or from an effective properties point of view, which can be justified. Some of the network characteristics should be calculated to match the problem features and not assigned.

Another important point is that much of the previous research results are based on substitution of porous medium properties and functions using artificial network simulation capabilities without satisfying the initial equations. The concern is that the physical problem, which is simulated with the help of network modeling, must still be modeled on the basis of its initial physical and mathematical statements. The development of models of irregular and random networks of pores in the REV with consequent substitution of closed morpho-convective and morpho-diffusive terms into the transport equations is a part of current research. Numerical modeling and application of theoretical studies to this kind of closure approach is based on realities of medium morphologies.

It had been proven that the generalized momentum and scalar transport equations correctly involve additional terms which quantify the influence of the medium irregularity. Theoretical forms of these additional terms, derived from application of the closure methodology, were reviewed for both one- and two-dimensional cases in a porous medium morphology consisting of specified, stationary distributions of a polydisperse (including binary) system of straight, non-intersecting pores (Fig. 1). The differences among the modeling results, and their significance to the closure scheme, were increased by introducing specific kinds of nonregularity to the medium‘s morphology. In some cases, large deviations in the overall results were obtained by merely allowing small morphology nonregularities (Gratton et al., [50]). It was shown numerically that slight manipulations of this particular morphology descriptors can create large fluctuations in transport parameter values, signifying the potential for modeling errors if particular features of the morphology are neglected. Important physical behavior was extracted from the morphology model by illustrating how hydrodynamic flow regime considerations also significantly effect the transport parameter values.

Variants of the flow 1D creep transport equations for systems with impermeable interface can be obtained from the next forms of the equations (some details of derivation and similar equations can be found in Whitaker‘s, [9] work)

$$\begin{aligned} 0 &= -\nabla \langle p \rangle_f - \frac{1}{\Delta\Omega} \int\limits_{\partial S_w} p\vec{ds} + \mu \nabla \cdot \left(\nabla \langle m \rangle \widetilde{V} \right) \\ &\quad + \frac{\mu}{\Delta\Omega} \int\limits_{\partial S_w} \nabla V \cdot \vec{ds} + \langle m \rangle \varrho_f \vec{g}, \end{aligned} \tag{1}$$

or for constant porosity and with fluctuation integral term

$$\langle m \rangle \nabla \widetilde{p} = -\frac{1}{\Delta\Omega} \int\limits_{\partial S_w} \widehat{p}\vec{ds} + \mu \langle m \rangle \nabla^2 \widetilde{V} + \frac{\mu}{\Delta\Omega} \int\limits_{\partial S_w} \nabla \widehat{V} \cdot \vec{ds} + \langle m \rangle \varrho_f \vec{g}. \tag{2}$$

Variable porosity presence will resume in an equation

$$\begin{aligned} \langle m \rangle \nabla \widetilde{p} &= -\frac{1}{\Delta\Omega} \int\limits_{\partial S_w} \widehat{p}\vec{ds} + \mu \langle m \rangle \nabla^2 \widetilde{V} + \mu \nabla \cdot \left(\widetilde{V} \nabla \langle m \rangle \right) + \\ &\quad + \frac{\mu}{\Delta\Omega} \int\limits_{\partial S_w} \nabla \widehat{V} \cdot \vec{ds} + \langle m \rangle \varrho_f \vec{g}. \end{aligned} \tag{3}$$

or second version when $\langle m \rangle \neq$const and interface is impermeable

$$\langle m \rangle \nabla \widetilde{p} = -\frac{1}{\Delta\Omega} \int\limits_{\partial S_w} \widehat{p}\vec{ds} + \mu \nabla^2 \left(\langle m \rangle \widetilde{V} \right) - \mu \nabla \widetilde{V} \cdot (\nabla \langle m \rangle) +$$

$$+\frac{\mu}{\Delta\Omega}\int\limits_{\partial S_w}\nabla\widehat{V}\cdot\overrightarrow{ds}+\langle m\rangle\,\varrho_f\,\overrightarrow{g}. \tag{4}$$

Using more common notations, these equations are written

$$\nu\frac{\partial}{\partial x}\left(\frac{\partial\langle m\rangle\,\widetilde{U}}{\partial x}\right)+\frac{\nu}{\Delta\Omega}\int\limits_{\partial S_w}\frac{\partial U}{\partial x_i}\cdot\overrightarrow{ds}-\frac{1}{\varrho_f\Delta\Omega}\int\limits_{\partial S_w}p\overrightarrow{ds}+$$

$$+\langle m\rangle\,\overrightarrow{g}=\frac{1}{\varrho_f}\frac{\partial}{\partial x}\left(\langle m\rangle\,\widetilde{p}\right), \tag{5}$$

or with fluctuation terms ($\langle m\rangle$ =const)

$$\frac{\nu}{\Delta\Omega}\int\limits_{\partial S_w}\frac{\partial\widehat{U}}{\partial x_i}\cdot\overrightarrow{ds}+\nu\,\langle m\rangle\,\frac{\partial}{\partial x}\left(\frac{\partial\widetilde{U}}{\partial x}\right)-\frac{1}{\varrho_f\Delta\Omega}\int\limits_{\partial S_w}\widehat{p}\overrightarrow{ds}+\langle m\rangle\,\overrightarrow{g}=\frac{\langle m\rangle}{\varrho_f}\frac{\partial}{\partial x}\left(\widetilde{p}\right). \tag{6}$$

These two equations can be simplified for well defined morphologies such as, for example, straight pore morphology to a form more useful for comparisons with the published results of different workers.Droping the gravitation force term for simplicity and expressing interface stress term through the full velocity variable one can get

$$-\frac{\partial}{\partial x}\left\{p\right\}_f=\frac{1}{\langle m\rangle\,\Delta\Omega}\int\limits_{\partial S_w}\widehat{p}\overrightarrow{ds}-\frac{\mu}{\langle m\rangle\,\Delta\Omega}\int\limits_{\partial S_w}\nabla V\cdot\overrightarrow{ds}. \tag{7}$$

Which differentiates from the equation (3.1) found in the work by Ma and Ruth [6]

$$-\frac{\partial}{\partial x}\left\{p\right\}_f=\frac{1}{\langle m\rangle\,\Delta\Omega}\int\limits_{\partial S_w}p\overrightarrow{ds}-\frac{\mu}{\langle m\rangle\,\Delta\Omega}\int\limits_{\partial S_w}\frac{\partial U}{\partial x_i}\cdot\overrightarrow{ds}\;=$$

$$=-\frac{\widetilde{p}}{\langle m\rangle}\left(\nabla\langle m\rangle\right)+\frac{1}{\langle m\rangle\,\Delta\Omega}\int\limits_{\partial S_w}\widehat{p}\overrightarrow{ds}-\frac{\mu}{\langle m\rangle\,\Delta\Omega}\int\limits_{\partial S_w}\frac{\partial U}{\partial x_i}\cdot\overrightarrow{ds}, \tag{8}$$

by one term - the first term on the right hand side of Ma and Ruth [6] equation. The latter equation is the equation developed by Ma and Ruth for morphology of straight periodically contracted pores (tubes). This equation is correct only for constant porosity $<$ m $>$ and that condition fortunately is satisfied.

The intrinsic averaging process used in this work for the momentum equation is inappropriate for vector quantity equations (equation (2.3) given by Ma and Ruth, [6]). One of the problems arises from the boundary conditions for vector quantities, velocity in this case. The correctly averaged momentum equation for periodically contracted straight pore morphology has the form 7. Despite the almost correct 1D momentum equation form derived by Ma and Ruth [6], closure of the additional integral terms was not achieved. The authors found a way to represent the integral terms as outstanding constant values. Meanwhile, the closure of these terms can be obtained following the procedures described by Travkin and Catton [4], where the skin friction term treated as, for example, for a laminar boundary layer

$$\frac{\mu}{\Delta\Omega}\int\limits_{\partial S_{wL}}\frac{\partial U}{\partial x_i}\cdot\overrightarrow{ds} = \frac{\varrho_f}{\varrho_f\Delta\Omega}\int\limits_{\partial S_w}\tau_{wL}\cdot\overrightarrow{ds} =$$

$$= -\frac{1}{2}c_{fL}(\overrightarrow{x})S_{wL}(\overrightarrow{x})\left[\varrho_f\widetilde{U}^2(\overrightarrow{x})\right], \tag{9}$$

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

where τ_{wL} is the wall laminar shear stress, S_{wL} is the laminar part of the specific surface in the REV, c_{fL} is the mean skin friction coefficient in the REV laminar region. The form drag integral term is approximated by

$$\frac{1}{\Delta\Omega}\int\limits_{\partial S_w}p\overrightarrow{ds} = \frac{1}{2}c_{dp}(\overrightarrow{x})S_{wp}(\overrightarrow{x})\left[\varrho_f\widetilde{U}^2(\overrightarrow{x})\right]. \tag{10}$$

where c_{dp} is the mean form resistance coefficient in the REV, S_{wp} is the ratio of the cross flow projected area of obstacles to the representative elementary volume $\Delta\Omega$. One should to note that these are well established ideas used in the different areas of fluid mechanics. Here they are applied to a separate elementary subarea on the interface surface ∂S_w with the consecutive averaging over the ∂S_w. Substituting these expressions into equation 7 yields

$$-\frac{\partial}{\partial x}\{p\}_f = \frac{1}{\langle m\rangle\Delta\Omega}\int\limits_{\partial S_w}\widehat{p}\overrightarrow{ds} - \frac{\mu}{\langle m\rangle\Delta\Omega}\int\limits_{\partial S_w}\nabla V\cdot\overrightarrow{ds} =$$

$$= \frac{1}{2}c_{dp}\frac{S_{wp}}{\langle m\rangle}\left[\varrho_f\widetilde{U}^2\right] + \frac{\widetilde{p}}{\langle m\rangle}(\nabla\langle m\rangle) + \frac{1}{2}c_{fL}\frac{S_{wL}}{\langle m\rangle}\left[\varrho_f\widetilde{U}^2\right]. \tag{11}$$

Finally this equation yields the form for a constant bulk pressure loss for a constant porosity media that is quite applicable to many nondemanding problems, as well as being appropriate for comparison with existing experimental data on drag resistance in porous media:

$$-\frac{\partial}{\partial x}\{p\}_f = (c_{fL}\ S_{wL} + c_{dp}S_{wp})\frac{\varrho_f\widetilde{U}^2}{2\langle m\rangle}. \tag{12}$$

It is clear that the morphology which comprise directly a drag resistance experimental data has obvious relieve for final evaluation. Hsu and Cheng [32] given an approach for closure of the resistance integral terms in dilute spherical particle suspensions which is based on a solution for a single particle in a cell. The expression for drag coefficient c_d they derived is

$$F = c_d \left(d_p^2 \right) \frac{\left[\varrho_f \widetilde{U}^2 \right]}{2},$$

which is very close to what is usually assumed for globular morphologies

$$F = c_d \left(\pi R_p^2 \right) \frac{\left[\varrho_f \widetilde{U}^2 \right]}{2}.$$

The authors managed to determine the constant coefficients in the drag force relation and obtain Ergun expression with two integral resistance terms in the averaged momentum Navier-Stokes equation.

The simplicity of the equation 12 is achieved mainly because of the simplicity of straight pore morphology. The integral drag resistance terms in the creep or Stokes flow transport equations can be closed whenever theoretical or experimental values of the drag resistance are available.

There presently are only a few studies of large Reynolds number flows where constant coefficient Navier-Stokes equations could be applied (see, for example, Jaiswall et al., [51], LeClair and Hamielec, [52]). It is unfortunate that when Jaiswall et al. [51] were describing the variances between their results and similar ones obtained by LeClair and Hamielec [52] they did not recognize that the morphologies of the media were different.