Transport in Ordered and Disordered Porous Media III: Closure and Comparison Between Theory and Experiment

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Abstract. In this paper we examine the closure problem associated with the volume averaged form of the Stokes equations presented in Part II. For both ordered and disordered porous media, we make use of a spatially periodic model of a porous medium. Under these circumstances the closure problem, in terms of the *closure variables*, is independent of the weighting functions used in the spatial smoothing process. Comparison between theory and experiment suggests that the geometrical characteristics of the unit cell dominate the calculated value of the Darcy's law permeability tensor, whereas the periodic conditions required for the *local form* of the closure problem play only a minor role.

Key words: Darcy's law, closure problem, permeability tensor.

0. Nomenclature

Roman Letters

 $A_{\beta\sigma}$ interfacial area of the β - σ interface contained within the macroscopic region, m².

 $A_{\beta e}$ area of entrances and exits for the β -phase contained within the macroscopic system, m².

 $A_{\beta\sigma}$ interfacial area of the β - σ interface associated with the local closure problem, m^2 .

 A_p surface area of a particle, m^2 .

b vector used to represent the pressure deviation, m^{-1} .

 B^0 $\mathsf{B}+\mathsf{I}$, a second order tensor that maps $\langle \mathbf{v}_\beta \rangle_m^\beta$ onto \mathbf{v}_β .

B second-order tensor used to represent the velocity deviation.

 d_p $6V_p/A_p$, effective particle diameter, m.

d a vector related to the pressure, m.

D a second-order tensor related to the velocity, m².

g gravity vector, m/s².

l unit tensor.

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K traditional Darcy's law permeability tensor calculated on the basis of a spatially periodic model, m².

 K_m permeability tensor for the weighted average form of Darcy's law, m^2 .

L general characteristic length for volume averaged quantities, m.

 L_p characteristic length for the volume averaged pressure, m.

 L_{ε} characteristic length for the porosity, m.

 L_v characteristic length for the volume averaged velocity, m.

 ℓ_{β} characteristic length (pore scale) for the β -phase.

 ℓ_i i = 1, 2, 3 lattice vectors, m.

 $\tilde{m}(\mathbf{y})$ weighting function.

m(-y) $\tilde{m}(y)$, convolution product weighting function.

 $m_{\mathcal{V}}$ special convolution product weighting function associated with the traditional averaging volume.

 m_g general convolution product weighting function. m_V unit cell convolution product weighting function.

 $m_{\rm C}$ special convolution product weighting function for ordered media

which produces the cellular average. $\mathbf{n}_{\beta\sigma}$ unit normal vector pointing from the β -phase toward the σ -phase.

 p_{β} pressure in the β -phase, N/m².

 $\langle p_{\beta} \rangle_m$ superficial weighted average pressure, N/m².

 $\langle p_{\beta} \rangle_m^{\beta}$ intrinsic weighted average pressure, N/m².

 $\langle p_{\beta} \rangle^{\beta}$ traditional intrinsic volume averaged pressure, N/m².

 \tilde{p}_{β} $p_{\beta} - \gamma_{\beta} \langle p_{\beta} \rangle_{m}^{\beta}$, spatial deviation pressure, N/m².

 r_0 radius of a spherical averaging volume, m.

 r_m support of the convolution product weighting function.

r position vector, m.

 \mathbf{r}_{β} position vector locating points in the β -phase, m.

V averaging volume, m^3 .

 V_{β} volume of the β -phase contained in the averaging volume, m³.

 V_{cell} volume of a unit cell, m³.

 \mathbf{v}_{β} velocity vector in the β -phase, m/s.

 $\langle \mathbf{v}_{\beta} \rangle_m$ superficial weighted average velocity, m/s.

 $\langle \mathbf{v}_{\beta} \rangle_{m}^{\beta}$ intrinsic weighted average velocity, m/s.

 $\langle \mathbf{v}_{\beta} \rangle$ traditional superficial volume averaged velocity, m/s.

 $\tilde{\mathbf{v}}_{\beta}$ $\mathbf{v}_{\beta} - \gamma_{\beta} \langle \mathbf{v}_{\beta} \rangle_{m}^{\beta}$, spatial deviation velocity, m/s.

x position vector locating the centroid of the averaging volume or the convolution product weighting function, m.

y position vector relative to the centroid, m.

 \mathbf{y}_{β} position vector locating points in the β -phase relative to the centroid,

Greek Letters

 γ_{β} indicator function for the β -phase.

 $\delta_{\beta\sigma}$ Dirac distribution associated with the β - σ interface.

 ε_{β} V_{β}/\mathcal{V} , volume average porosity.

 $\varepsilon_{\beta m}$ $m * \gamma_{\beta}$, weighted average porosity.

 ρ_{β} mass density of the β -phase, kg/m³.

 μ_{β} viscosity of the β -phase, Ns/m².

1. Introduction

In Part I we introduced the physical process under consideration in terms of the following boundary value problem

$$\nabla \cdot \mathbf{v}_{\beta} = 0$$
, in the β -phase (1.1)

$$0 = -\nabla p_{\beta} + \rho_{\beta} \mathbf{g} + \mu_{\beta} \nabla^{2} \mathbf{v}_{\beta}, \quad \text{in the } \beta\text{-phase}$$
 (1.2)

B.C.1
$$\mathbf{v}_{\beta} = 0$$
, at $\mathcal{A}_{\beta\sigma}$ (1.3)

B.C.2
$$\mathbf{v}_{\beta} = \mathbf{f}(\mathbf{r}, t)$$
, at $A_{\beta e}$ (1.4)

The macroscopic system under consideration is illustrated in Figure 1, and in Equation 1.3 we have used $A_{\beta\sigma}$ to represent the area of the β - σ interface contained in the macroscopic region. The boundary condition at the β -phase entrances and exits of the macroscopic system is given by Equation (1.4) in which the function $\mathbf{f}(\mathbf{r},t)$ is generally unknown except for the fact that $\mathbf{f}(\mathbf{r},t)$ is on the order of $\langle \mathbf{v}_{\beta} \rangle_{m}^{\beta}$.

In Part II we developed the weighted average form of Equations (1.1) and (1.2) in terms of the convolution product defined by

$$m * \psi = \int_{\mathbb{R}^3} m(\mathbf{x} - \mathbf{r}) \psi(\mathbf{r}) \, dV_r$$
 (1.5)

Here \mathbf{x} is a reference position vector and \mathbf{r} is a position vector that locates any point in \mathbb{R}^3 . In the traditional approach to volume averaging we think of \mathbf{x} as locating the centroid of the averaging volume shown in Figure 1, and this idea is expressed more precisely in Figure 2 where \mathbf{r}_{β} locates any point in the β -phase. In general, the quantity ψ in Equation (1.5) is a distribution given by

$$\psi = \begin{cases} \psi_{\beta}, & \text{in the } \beta\text{-phase} \\ \psi_{\sigma}, & \text{in the } \sigma\text{-phase} \end{cases}$$
 (1.6)

and in our analysis of Equations (1.1) and (1.2) we considered the velocity and the pressure to be *distributions* defined as

$$\mathbf{v}_{\beta} = \begin{cases} \mathbf{v}_{\beta}, & \text{in the } \beta\text{-phase} \\ 0, & \text{in the } \sigma\text{-phase} \end{cases}, \tag{1.7}$$

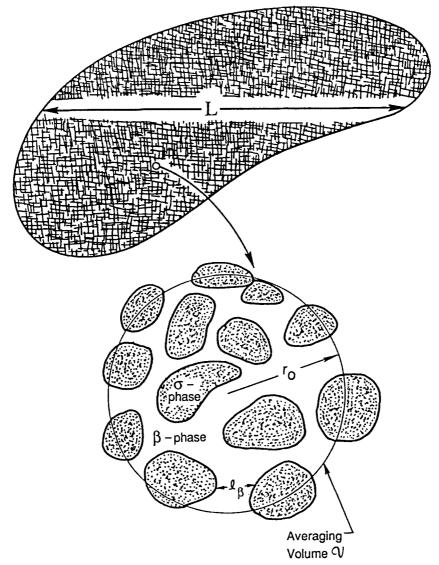


Fig. 1. Macroscopic region of a porous medium and an associated averaging volume.

$$p_{\beta} = \begin{cases} p_{\beta}, & \text{in the } \beta\text{-phase,} \\ 0, & \text{in the } \sigma\text{-phase.} \end{cases}$$
 (1.8)

According to Equation (1.5) the convolution product of v_{β} is given by

$$m * \mathbf{v}_{\beta} = \int_{\mathbb{R}^3} m(\mathbf{x} - \mathbf{r}) \mathbf{v}_{\beta}(\mathbf{r}) \, dV_r$$
 (1.9)

and we connect this to the more traditional nomenclature by writing

$$m * \mathbf{v}_{\beta} = \langle \mathbf{v}_{\beta} \rangle_{m}. \tag{1.10}$$

Here we think of $\langle \mathbf{v}_{\beta} \rangle_m$ as the *superficial weighted average velocity*, and if we take m to be the special weighting function given by

$$m(\mathbf{y}) = m_{\mathcal{V}}(\mathbf{y}) = \begin{cases} \frac{1}{\mathcal{V}}, & |\mathbf{y}| \leq r_0 \\ 0, & |\mathbf{y}| > r_0 \end{cases}$$
(1.11)

we see that Equation (1.9) reproduces the traditional superficial average velocity

$$m * \mathbf{v}_{\beta} = \frac{1}{\mathcal{V}} \int_{V_{\beta}} \mathbf{v}_{\beta} \, dV, \quad m = m_{\mathcal{V}}.$$
 (1.12)

The intrinsic average velocity and pressure are related to the superficial averages by

$$m * \mathbf{v}_{\beta} = \langle \mathbf{v}_{\beta} \rangle_{m} = \varepsilon_{\beta m} \langle \mathbf{v}_{\beta} \rangle_{m}^{\beta}, \tag{1.13a}$$

$$m * p_{\beta} = \langle p_{\beta} \rangle_m = \varepsilon_{\beta m} \langle p_{\beta} \rangle_m^{\beta}. \tag{1.13b}$$

Here $\varepsilon_{\beta m}$ is the weighted average porosity given by

$$\varepsilon_{\beta m} = m * \gamma_{\beta} \tag{1.14}$$

in which γ_{β} is the β -phase indicator function defined as

$$\gamma_{\beta}(\mathbf{y}) = \begin{cases} 1, & \mathbf{y} \text{ locates a point in the } \beta\text{-phase,} \\ 0, & \mathbf{y} \text{ locates a point in the } \sigma\text{-phase.} \end{cases}$$
 (1.15)

Here we have used y to represent the position vector relative to x as indicated by

$$\mathbf{r} = \mathbf{x} + \mathbf{y} \tag{1.16}$$

and illustrated in Figure 2 for the special case in which \mathbf{r} locates only points in the β -phase.

The spatially smoothed form of the continuity equation can be expressed in terms of the *superficial* average velocity

$$\nabla \cdot \langle \mathbf{v}_{\beta} \rangle_m = 0 \tag{1.17}$$

or in terms of the intrinsic average velocity

$$\nabla \cdot \langle \mathbf{v}_{\beta} \rangle_{m}^{\beta} = -\varepsilon_{\beta m}^{-1} \langle \mathbf{v}_{\beta} \rangle_{m}^{\beta} \cdot \nabla \varepsilon_{m}. \tag{1.18}$$

The intrinsic average form of the Stokes equations was developed in Part II where we found the following result.

$$0 = -\nabla \langle p_{\beta} \rangle_{m}^{\beta} + \rho_{\beta} \mathbf{g} + \mu_{\beta} \nabla^{2} \langle \mathbf{v}_{\beta} \rangle_{m}^{\beta} + \\ + \varepsilon_{\beta m}^{-1} \int_{\mathbb{R}^{3}} m(\mathbf{x} - \mathbf{r}) [\mathbf{n}_{\beta \sigma} \cdot (-|\tilde{p}_{\beta} + \mu_{\beta} \nabla \tilde{\mathbf{v}}_{\beta}) \delta_{\beta \sigma}] \, dV_{r}.$$

$$(1.19)$$

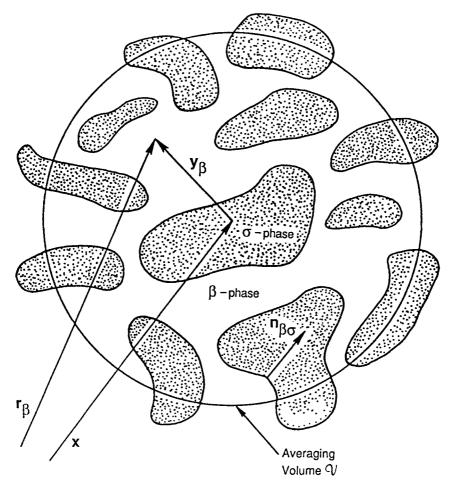


Fig. 2. Positions vectors in a fluid-solid system.

The spatial deviations, \tilde{p}_{β} and $\tilde{\mathbf{v}}_{\beta}$, were defined in Part II by the decompositions

$$p_{\beta} = \gamma_{\beta} \langle p_{\beta} \rangle_{m}^{\beta} + \tilde{p}_{\beta}, \tag{1.20a}$$

$$\mathbf{v}_{\beta} = \gamma_{\beta} \langle \mathbf{v}_{\beta} \rangle_{m}^{\beta} + \tilde{\mathbf{v}}_{\beta} \tag{1.20b}$$

thus both \tilde{p}_{β} and $\tilde{\mathbf{v}}_{\beta}$ are zero in the σ -phase on the basis of Equations (1.7) and (1.8) along with the definition of the indicator function given by Equation (1.15).

In the derivation of Equations (1.18) and (1.19) we imposed the following three general conditions on the weighting function, m

$$H1. \quad m \in \mathbb{C}^{\infty}, \tag{1.21}$$

H2.
$$m$$
 has a compact support over \mathbb{R}^3 , (1.22)

H3. m satisfies the normalization condition

$$\int_{\mathbb{R}^3} m(\mathbf{x} - \mathbf{r}) \, \mathrm{d}V_r = 1. \tag{1.23}$$

The normalization condition is very convenient, but it is not a necessary condition for the derivation of Equations (1.18) and (1.19). For *disordered porous media* we also restricted the weighting function by

H4.
$$r_m \gg \ell_\beta$$
 (1.24a)

$$r_m^2 \ll L_\varepsilon L_p,\tag{1.24b}$$

$$r_m^2 \ll L_\varepsilon L_v \tag{1.24c}$$

in which r_m is the support for m and the large length-scales are estimated according to

$$\nabla \varepsilon_{\beta m} = 0 \left(\frac{\Delta \varepsilon_{\beta m}}{L_{\varepsilon}} \right), \tag{1.25}$$

$$\nabla\nabla\langle p_{\beta}\rangle_{m}^{\beta} = 0 \left[\frac{\Delta(\nabla\langle p_{\beta}\rangle_{m}^{\beta})}{L_{p}} \right], \tag{1.26}$$

$$\nabla\nabla\nabla\langle\mathbf{v}_{\beta}\rangle_{m}^{\beta} = 0 \left[\frac{\Delta(\nabla\nabla\langle\mathbf{v}_{\beta}\rangle_{m}^{\beta})}{L_{v}} \right]. \tag{1.27}$$

In addition to the conditions imposed on m by Equations (1.24) for disordered porous media, we also made use of our *definition* of a disordered porous media given by

$$\nabla[m * (\gamma_{\beta} \mathbf{y})] \ll 1. \tag{1.28}$$

One should remember that this constraint cannot be satisfied at the interface between a porous medium and an impermeable solid.

For *ordered porous media* we restricted the weighting function by Equations (1.21) through (1.23) and by H5 which can be described as

H5.
$$m = m_q * m_V * m_V$$
 (1.29)

in which m_g is any weighting function satisfying Equations (1.21) through (1.23) and m_V is defined by

$$m_V(\mathbf{y}) = \begin{cases} \frac{1}{V_{\text{cell}}}, & \mathbf{y} \in V_{\text{cell}}, \\ 0, & \mathbf{y} \notin V_{\text{cell}}. \end{cases}$$
(1.30)

The convolution product, $m_V * m_V$, provides the weighting function that, when used in Equation (1.5), produces the *cellular average*. The reason for introducing m_g in H5 is that $m_V * m_V$ is only C^0 and since m_g satisfies H1 we know that $m_g * m_V * m_V$ will also satisfy H1. From a practical point of view, the role of m_g is to simply remove the corners in $m_C = m_V * m_V$ as illustrated in Figure 6b of Part II.

2. Closure

In order to develop a closed form of Equation (1.19) we need to represent \tilde{p}_{β} and $\tilde{\mathbf{v}}_{\beta}$ in terms of spatially smoothed quantities. To accomplish this we will derive the governing differential equations for \tilde{p}_{β} and $\tilde{\mathbf{v}}_{\beta}$ on the basis of the *point* equations given by Equations (1.1) and (1.2) and the spatially smoothed equations represented by Equations (1.18) and (1.19). It is important to note that the point equations are only valid in the β -phase whereas the spatially smoothed equations are valid everywhere. In our development of the closure problem we will be entirely restricted to the β -phase, thus in order to develop the continuity equation for $\tilde{\mathbf{v}}_{\beta}$ we consider Equations (1.1), (1.18), and (1.20b) expressed as

$$\nabla \cdot \mathbf{v}_{\beta} = 0$$
, in the β -phase, (2.1)

$$\nabla \cdot \langle \mathbf{v}_{\beta} \rangle_{m}^{\beta} = -\varepsilon_{\beta m}^{-1} \langle \mathbf{v}_{\beta} \rangle_{m}^{\beta} \cdot \nabla \varepsilon_{\beta m}, \quad \text{in the } \beta\text{-phase}, \tag{2.2}$$

$$\mathbf{v}_{\beta} = \langle \mathbf{v}_{\beta} \rangle_{m}^{\beta} + \tilde{\mathbf{v}}_{\beta}, \quad \text{in the } \beta\text{-phase.}$$
 (2.3)

If we subtract Equation (2.2) from Equation (2.1) and make use of Equation (2.3) we obtain

$$\nabla \cdot \tilde{\mathbf{v}}_{\beta} = \varepsilon_{\beta m}^{-1} \langle \mathbf{v}_{\beta} \rangle_{m}^{\beta} \cdot \nabla \varepsilon_{\beta m}, \quad \text{in the } \beta\text{-phase.}$$
 (2.4)

The term on the right hand side of this result can be thought of as a *source* for the $\tilde{\mathbf{v}}_{\beta}$ -field, and we need to decide if this represents an important contribution to the $\tilde{\mathbf{v}}_{\beta}$ -field. From the no-slip condition we know that $\tilde{\mathbf{v}}_{\beta}$ is the same order of magnitude as $\langle \mathbf{v}_{\beta} \rangle_m^{\beta}$, thus the order of magnitude estimates associated with Equation (2.4) are given by

$$\frac{\partial \tilde{v}_{\beta x}}{\partial x} + \frac{\partial \tilde{v}_{\beta y}}{\partial y} + \frac{\partial \tilde{v}_{\beta z}}{\partial z} = \varepsilon_{\beta m}^{-1} \langle \mathbf{v}_{\beta} \rangle_{m}^{\beta} \cdot \nabla \varepsilon_{\beta m}
\downarrow \qquad \downarrow \qquad \downarrow \qquad \downarrow
\frac{\langle \mathbf{v}_{\beta} \rangle_{m}^{\beta}}{\ell_{x}} \quad \frac{\langle \mathbf{v}_{\beta} \rangle_{m}^{\beta}}{\ell_{y}} \quad \frac{\langle \mathbf{v}_{\beta} \rangle_{m}^{\beta}}{\ell_{z}} \quad \frac{\langle \mathbf{v}_{\beta} \rangle_{m}^{\beta}}{\ell_{z}}.$$
(2.5)

The three length scales, ℓ_x , ℓ_y , and ℓ_z , are all on the order of ℓ_β which is much, much less than L_ε since the latter is constrained by

$$L_{\varepsilon} = \infty$$
, ordered media, (2.6)

$$L_{\varepsilon} \gg \ell_{\beta}$$
, disordered media. (2.7)

The second of these inequalities is required by Equation (1.24a), while the first results from the fact that an ordered porous medium is necessarily homogeneous. Given Equation (2.6) and (2.7), we see that the source on the right hand side of

Equation (2.5) will have a negligible influence on the $\tilde{\mathbf{v}}_{\beta}$ -field and we can express the continuity equation for $\tilde{\mathbf{v}}_{\beta}$ as

$$\nabla \cdot \tilde{\mathbf{v}}_{\beta} = 0$$
, in the β -phase. (2.8)

In order to develop the momentum equation for the spatial deviations, we follow the same procedure and subtract Equation (1.19) from Equation (1.1) and impose Equation (1.20) to obtain

$$0 = -\nabla \tilde{p}_{\beta} + \mu_{\beta} \nabla^{2} \tilde{\mathbf{v}}_{\beta} - \\ -\varepsilon_{\beta m}^{-1} \int_{\mathbb{R}^{3}} m(\mathbf{x} - \mathbf{r}) [\mathbf{n}_{\beta \sigma} \cdot (-\mathsf{I} \tilde{p}_{\beta} + \mu_{\beta} \nabla \tilde{\mathbf{v}}_{\beta}) \delta_{\beta \sigma}] \, dV_{r},$$
in the β -phase. (2.9)

On the basis of Equations (1.3) and (1.4), we can express the boundary conditions for $\tilde{\mathbf{v}}_{\beta}$ as

B.C.1
$$\tilde{\mathbf{v}}_{\beta} = -\langle \mathbf{v}_{\beta} \rangle_{m}^{\beta}$$
, at $\mathcal{A}_{\beta\sigma}$, (2.10)

B.C.2
$$\tilde{\mathbf{v}}_{\beta} = \mathsf{G} \cdot \langle \mathbf{v}_{\beta} \rangle_{m}^{\beta}$$
, at $\mathcal{A}_{\beta \epsilon}$ (2.11)

in which we have assumed that Equation (1.4) could be represented as

B.C.2
$$\mathbf{v}_{\beta} = \mathbf{A} \cdot \langle \mathbf{v}_{\beta} \rangle_{m}^{\beta}$$
, at $\mathcal{A}_{\beta e}$. (2.12)

Here A is a tensor of order one, and this requires that G be given by

$$G = A - I$$
, at $A_{\beta e}$. (2.13)

We know that G is order one; however, the details of this function, like those of $f(\mathbf{r}, t)$ in Equation (1.4), are generally unknown.

The boundary value problem given by Equations (2.8) through (2.11) is referred to as the closure problem and it must be solved to determine \tilde{p}_{β} and $\tilde{\mathbf{v}}_{\beta}$. In that boundary value problem there are only two nonhomogeneous terms, $\langle \mathbf{v}_{\beta} \rangle_m^{\beta}$ in the boundary condition imposed at $\mathcal{A}_{\beta\sigma}$ and $\mathbf{G} \cdot \langle \mathbf{v}_{\beta} \rangle_m^{\beta}$ in the boundary condition imposed at the entrances and exits of the β -phase contained in the macroscopic region illustrated in Figure 1. The form of the closure problem suggests that \tilde{p}_{β} and $\tilde{\mathbf{v}}_{\beta}$ are linear functions of $\langle \mathbf{v}_{\beta} \rangle_m^{\beta}$, and to explore this idea we propose the representations

$$\tilde{\mathbf{v}}_{\beta} = \mathsf{B} \cdot \langle \mathbf{v}_{\beta} \rangle_{m}^{\beta} + \psi, \tag{2.14}$$

$$\tilde{p}_{\beta} = \mu_{\beta} \mathbf{b} \cdot \langle \mathbf{v}_{\beta} \rangle_{m}^{\beta} + \mu_{\beta} \xi. \tag{2.15}$$

When the vector field **b** and the tensor field B are specified by the following boundary value problem

$$\nabla \cdot \mathsf{B} = 0, \tag{2.16a}$$

$$-\nabla \mathbf{b} + \nabla^2 \mathbf{B} = \varepsilon_{\beta m}^{-1} \int_{\mathbb{R}^3} m(\mathbf{x} - \mathbf{r}) [\mathbf{n}_{\beta \sigma} \cdot (-\mathbf{l}\mathbf{b} + \nabla \mathbf{B}) \delta_{\beta \sigma}] \, dV_r, \qquad (2.16b)$$

B.C.1
$$B = -I$$
, at $A_{\beta\sigma}$, (2.16c)

B.C.2 B = G, at
$$A_{\beta e}$$
 (2.16d)

one can follow the analysis of Whitaker (1986) to prove that ψ and ξ make negligible contributions to $\tilde{\mathbf{v}}_{\beta}$ and \tilde{p}_{β} . Under these circumstances our representations simplify to

$$\tilde{\mathbf{v}}_{\beta} = \mathsf{B} \cdot \langle \mathbf{v}_{\beta} \rangle_{m}^{\beta},\tag{2.17}$$

$$\tilde{p}_{\beta} = \mu_{\beta} \mathbf{b} \cdot \langle \mathbf{v}_{\beta} \rangle_{m}^{\beta}. \tag{2.18}$$

These representations led to Equation (2.67) in Part II and thus provided the form of Darcy's law given by Equation (2.68). This can be seen by substituting Equations (2.17) and (2.18) into the convolution product in Equation (1.19), and then removing $\langle \mathbf{v}_{\beta} \rangle_m^{\beta}$ from the integral on the basis of the type of analysis given by Equations (2.41) through (2.48) of Part II. This allows us to express Equation (1.19) as

$$0 = -\nabla \langle p_{\beta} \rangle_{m}^{\beta} + \rho_{\beta} \mathbf{g} + \mu_{\beta} \nabla^{2} \langle \mathbf{v}_{\beta} \rangle_{m}^{\beta} + + \mu_{\beta} \left\{ \varepsilon_{\beta m}^{-1} \int_{\mathbb{R}^{3}} m(\mathbf{x} - \mathbf{r}) [\mathbf{n}_{\beta \sigma} \cdot (-\mathsf{I}\mathbf{b} + \nabla \mathsf{B}) \delta_{\beta \sigma}] \, dV_{r} \right\} \cdot \langle \mathbf{v}_{\beta} \rangle_{m}^{\beta}$$
(2.19)

and if the last term is represented in terms of the superficial velocity we obtain

$$0 = -\nabla \langle p_{\beta} \rangle_{m}^{\beta} + \rho_{\beta} \mathbf{g} + \mu_{\beta} \nabla^{2} \langle \mathbf{v}_{\beta} \rangle_{m}^{\beta} + + \mu_{\beta} \left\{ \varepsilon_{\beta m}^{-2} \int_{\mathbb{R}^{3}} m(\mathbf{x} - \mathbf{r}) [\mathbf{n}_{\beta \sigma} \cdot (-\mathbf{l} \mathbf{b} + \nabla \mathbf{B}) \delta_{\beta \sigma}] \, dV_{r} \right\} \cdot \langle \mathbf{v}_{\beta} \rangle_{m}.$$
(2.20)

We now define the inverse of the permeability tensor by

$$\mathsf{K}_{m}^{-1} = -\left\{\varepsilon_{\beta m}^{-2} \int_{\mathbb{R}^{3}} m(\mathbf{x} - \mathbf{r}) [\mathbf{n}_{\beta \sigma} \cdot (-\mathsf{I}\mathbf{b} + \nabla \mathsf{B}) \delta_{\beta \sigma}] \, \mathrm{d}V_{r}\right\}$$
(2.21)

so that Equation (2.19) takes the form

$$\langle \mathbf{v}_{\beta} \rangle_{m} = -\frac{1}{\mu_{\beta}} \mathsf{K}_{m} \cdot (\nabla \langle p_{\beta} \rangle_{m}^{\beta} - \rho_{\beta} \mathbf{g}) + \mathsf{K}_{m} \cdot \nabla^{2} \langle \mathbf{v}_{\beta} \rangle_{m}^{\beta}. \tag{2.22}$$

Here we should remind the reader that the Brinkman correction is only non-negligible when $(1 - \varepsilon_{\beta m}) \ll 1$ and that Equation (2.22) cannot be considered valid in the neighborhood of an impermeable solid surface under any circumstances. In the neighborhood of a homogeneous fluid, we consider Equation (2.22) to be valid only if $(1 - \varepsilon_{\beta m}) \ll 1$.

2.1. LOCAL CLOSURE PROBLEM

It should be clear that we have no intention of solving for the closure variables, **b** and B, over the entire macroscopic region as suggested by Equations (2.16). Instead we make use of the idea that the boundary condition imposed at $A_{\beta e}$ will have little influence on the **b** and B-fields except in a thin layer at the boundary of the macroscopic region illustrated in Figure 1. This motivates us to seek a solution in some *representative region* such as the one illustrated in Figure 3. In this region, the local version of Equations (2.16) is given by

$$\nabla \cdot \mathsf{B} = 0, \tag{2.23a}$$

$$-\nabla \mathbf{b} + \nabla^2 \mathbf{B} = \frac{1}{V_{\beta}} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot (-\mathsf{I}\mathbf{b} + \nabla \mathsf{B}) \, \mathrm{d}A, \tag{2.23b}$$

B.C.1
$$B = -I$$
, at $A_{\beta\sigma}$, (2.23c)

Periodicity:
$$\mathbf{b}(\mathbf{r} + \ell_i) = \mathbf{b}(\mathbf{r}), \ \mathsf{B}(\mathbf{r} + \ell_i) = \mathsf{B}(\mathbf{r}), \ i = 1, 2, 3 \ (2.23d)$$

in which the Dirichlet condition expressed by Equation (2.16d) has been replaced by the periodic conditions represented by Equation (2.23d). Here we see that in order to develop a *local* closure problem we have been forced to use a spatially periodic model of a porous medium with the lattice vectors given by ℓ_i , i=1,2,3. Equations (2.23) are entirely consistent with *ordered media* while they represent an approximation for *disordered media*. In going from Equations (2.16) to Equations (2.23), we have simplified the integral in Equation (2.16b), and we need to explain this simplification. Since the local closure problem is based on an ordered porous medium, we impose H5 to express the convolution product as

$$\int_{\mathbb{R}^{3}} m(\mathbf{x} - \mathbf{r}) [\mathbf{n}_{\beta\sigma} \cdot (-\mathsf{I}\mathbf{b} + \nabla\mathsf{B})\delta_{\beta\sigma}] \, dV_{r}$$

$$= m_{g} * m_{V} * m_{V} * [\mathbf{n}_{\beta\sigma} \cdot (-\mathsf{I}\mathbf{b} + \nabla\mathsf{B})\delta_{\beta\sigma}].$$
(2.24)

In terms of the local problem given by Equations (2.23) we have

$$m_V * [\mathbf{n}_{\beta\sigma} \cdot (-\mathsf{I}\mathbf{b} + \nabla \mathsf{B})\delta_{\beta\sigma}] = \text{constant}$$
 (2.25)

and since m_g and m_V satisfy H3, we conclude that

$$m_g * m_V * (constant) = constant$$
 (2.26)

Under these circumstances Equation (2.24) simplifies to

$$\int_{\mathbb{R}^{3}} m(\mathbf{x} - \mathbf{r}) [\mathbf{n}_{\beta\sigma} \cdot (-\mathsf{I}\mathbf{b} + \nabla\mathsf{B})\delta_{\beta\sigma}] \, dV_{r}$$

$$= \frac{1}{V_{\text{cell}}} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot (-\mathsf{I}\mathbf{b} + \nabla\mathsf{B}) \, dA, \qquad (2.27a)$$

Periodicity:
$$\mathbf{b}(\mathbf{r} + \ell_i) = \mathbf{b}(\mathbf{r});$$

 $\mathbf{B}(\mathbf{r} + \ell_i) = \mathbf{B}(\mathbf{r}), \quad i = 1, 2, 3$ (2.27b)

thus indicating that the weighting function has no influence on the permeability tensor when a spatially periodic model is used to complete the closure. Under these circumstances we replace Equation (2.21) with

$$\varepsilon_{\beta} \mathsf{K}^{-1} = \frac{1}{V_{\beta}} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot (-\mathsf{Ib} + \nabla \mathsf{B}) \, \mathrm{d}A$$
 (2.28)

and express our local closure problem in the form

$$\nabla \cdot \mathsf{B} = 0, \tag{2.29a}$$

$$-\nabla \mathbf{b} + \nabla^2 \mathbf{B} = \varepsilon_\beta \, \mathbf{K}^{-1},\tag{2.29b}$$

$$B = -I, \quad \text{at } A_{\beta\sigma}, \tag{2.29c}$$

Periodicity:
$$\mathbf{b}(\mathbf{r} + \ell_i) = \mathbf{b}(\mathbf{r}),$$

 $\mathbf{B}(\mathbf{r} + \ell_i) = \mathbf{B}(\mathbf{r}), \quad i = 1, 2, 3.$ (2.29d)

In this representation of the local closure problem it is understood that V_{β} represents the volume of the β -phase contained within a unit cell and that $A_{\beta\sigma}$ represents the interfacial area associated with a unit cell. The representative region shown in Figure 3 is an illustration of a complex unit cell, while several simple unit cells are shown in Figure 3 of Part I.

One of the characteristics of this closure problem is that **b** is determined only to within an *arbitrary constant* and a second characteristic is that the **b** and B-fields can be determined by Equations (2.29) *only if* the parameter K⁻¹ is known. Clearly this form of the local closure problem cannot be used to determine the permeability tensor K.

2.2. AVERAGE OF A DEVIATION

In one of the early studies of closure problems, Carbonell and Whitaker (Sec. 2, 1984) showed that the average of spatial deviations could be expressed as

$$\langle \tilde{\mathbf{v}}_{\beta} \rangle_{m}^{\beta} = -\langle \mathbf{y}_{\beta} \rangle_{m}^{\beta} \cdot \nabla \langle \mathbf{v}_{\beta} \rangle_{m}^{\beta} - \frac{1}{2} \langle \mathbf{y}_{\beta} \mathbf{y}_{\beta} \rangle_{m}^{\beta} : \nabla \nabla \langle \mathbf{v}_{\beta} \rangle_{m}^{\beta} - \dots,$$

$$(2.30)$$

$$\langle \tilde{\mathbf{p}}_{\beta} \rangle_{m}^{\beta} = -\langle \mathbf{y}_{\beta} \rangle_{m}^{\beta} \cdot \nabla \langle \mathbf{p}_{\beta} \rangle_{m}^{\beta} - \frac{1}{2} \langle \mathbf{y}_{\beta} \mathbf{y}_{\beta} \rangle_{m}^{\beta} : \nabla \nabla \langle \mathbf{p}_{\beta} \rangle_{m}^{\beta} -$$

$$= -2.31$$

One can use these results to support the inequalities

$$\langle \tilde{\mathbf{v}}_{\beta} \rangle_m^{\beta} \ll \tilde{\mathbf{v}}_{\beta},$$
 (2.32)

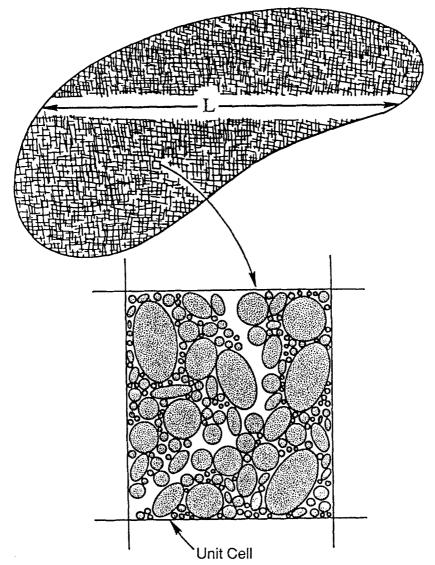


Fig. 3. Representative region of a porous medium.

$$\langle \tilde{p}_{\beta} \rangle_m^{\beta} \ll \tilde{p}_{\beta} \tag{2.33}$$

and the mathematical consequence of these physical conditions is generally accepted as

$$\langle \tilde{\mathbf{v}}_{\beta} \rangle_m^{\beta} = 0, \tag{2.34}$$

$$\langle \tilde{p}_{\beta} \rangle_m^{\beta} = 0. \tag{2.35}$$

In terms of the representations of $\tilde{\mathbf{v}}_{\beta}$ and \tilde{p}_{β} given by Equations (2.17) and (2.18) and used in Equations (2.29), we express these results as

$$\langle \mathbf{b} \rangle^{\beta} = 0, \tag{2.36}$$

$$\langle \mathsf{B} \rangle^{\beta} = 0. \tag{2.37}$$

The first of these actually plays no role in the determination of K since any arbitrary constant associated with **b** has no influence in the calculation indicated by Equation (2.28). On the other hand, Equation (2.37) is essential to the determination of the permeability tensor.

2.3. SOLUTION OF THE CLOSURE PROBLEM

In order to develop a convenient computation method for the determination of K, we first define a new tensor B⁰ according to

$$B^0 = B + I \tag{2.38}$$

This allows us to express the local closure problem as

$$\nabla \cdot \mathbf{B}^0 = 0 \tag{2.39a}$$

$$-\nabla \mathbf{b} + \nabla^2 \mathsf{B}^0 = \varepsilon_\beta \; \mathsf{K}^{-1} \tag{2.39b}$$

B.C.1
$$B^0 = 0$$
, at $A_{\beta\sigma}$, (2.39c)

Periodicity:
$$\mathbf{b}(\mathbf{r} + \ell_i) = \mathbf{b}(\mathbf{r}),$$

 $\mathbf{B}^0(\mathbf{r} + \ell_i) = \mathbf{B}^0(\mathbf{r}), \quad i = 1, 2, 3,$ (2.39d)

Average:
$$\langle \mathbf{b} \rangle^{\beta} = 0$$
, (2.39e)

Average:
$$\langle B^0 \rangle^{\beta} = I$$
. (2.39f)

In order to obtain the final form of this result, we define a new vector field and a new tensor field by

$$\mathbf{d} = -\varepsilon_{\beta}^{-1} \mathbf{b} \cdot \mathsf{K}, \qquad \mathsf{D} = -\varepsilon_{\beta}^{-1} \mathsf{B}^{0} \cdot \mathsf{K}$$
 (2.40)

so that Equations (2.39) take the form

$$\nabla \cdot \mathsf{D} = 0, \tag{2.41a}$$

$$-\nabla \mathbf{d} + \nabla^2 \mathbf{D} = \mathbf{I},\tag{2.41b}$$

$$D = 0, \quad \text{at } A_{\beta\sigma}, \tag{2.41c}$$

Periodicity:
$$\mathbf{d}(\mathbf{r} + \ell_i) = \mathbf{d}(\mathbf{r}),$$

 $\mathsf{D}(\mathbf{r} + \ell_i) = \mathsf{D}(\mathbf{r}), \quad i = 1, 2, 3,$ (2.41d)

Average:
$$\langle \mathbf{d} \rangle^{\beta} = 0$$
 (2.41e)

Average:
$$\langle \mathsf{D} \rangle^{\beta} = -\varepsilon_{\beta}^{-1} \mathsf{K}$$
. (2.41f)

In this form one determines \mathbf{d} and D by classical means on the basis of Equations (2.41a) through (2.41d). The arbitrary constant associated with the vector \mathbf{d} can be removed by Equation (2.41e) if one so desires, and the Darcy's law permeability tensor is determined by the all-important average condition given by Equation (2.41f). The result given by Equations (2.41) was presented previously by Barrère et al. (1992); however, the development was less direct than we have presented here.

We are now ready to return to Darcy's law as given by Equation (2.22) and note that it was derived for either ordered or disordered porous media. However, our theoretical prediction of the permeability tensor is based on a spatially periodic model for which the convolution product given by Equation (2.21) collapses to the simple integral over a unit cell as indicated by Equation (2.28). If the geometry of the unit cell used with Equations (2.41) accurately captures the porous medium under consideration, one would hope that K, as determined by Equation (2.28), would be essentially equal to K_m , as determined by Equation (2.21). The idea here is that the D-field will be dominated by Equations (2.41a) through (2.41c), and only slightly influenced by the weak periodicity conditions given by Equations (2.41d).

2.4. CELLULAR AVERAGE

In Part I we remarked that the cellular average appeared to be the correct average to be used for the pressure field for flow in spatially periodic porous media. In Part II we proved that the correct form of the intrinsic average pressure is

$$\langle p_{\beta} \rangle_{m}^{\beta} = \varepsilon_{\beta m}^{-1}(m * p_{\beta}) \tag{2.42}$$

in which the weighting function is given by

$$m = m_g * m_V * m_V. (2.43)$$

Here m_g is any weighting function that satisfies H1, H2, and H3 and m_V is given by Equation (1.30). Under these circumstances $\varepsilon_{\beta m}$ can be replaced by ε_{β} and Equation (2.42) takes the form

$$\langle p_{\beta} \rangle_m^{\beta} = \varepsilon_{\beta}^{-1} (m_g * m_V * m_V * p_{\beta}). \tag{2.44}$$

It is of some interest to consider the special case in which the pressure is given by

$$p_{\beta} = \mathbf{h}_{\beta} \cdot \mathbf{r}_{\beta} + f_{\beta} + \mathbf{C}_{\beta} \tag{2.45}$$

where h_{β} is a constant vector, f_{β} is a periodic function, and C_{β} is a constant. For this special case we can follow the development given by Equations (2.30) through (2.40) in Part II to prove that the average of p_{β} is given by the cellular average

$$\langle p_{\beta} \rangle_{m}^{\beta} = \varepsilon_{\beta}^{-1} (m_{V} * m_{V} * p_{\beta}) \tag{2.46}$$

The details available in Part II can also be used to show that

$$\nabla \langle p_{\beta} \rangle_{m}^{\beta} = \mathbf{h}_{\beta}, \quad m = m_{V} * m_{V} \tag{2.47}$$

This result is consistent with our study of fluid statics presented in Sec. 1 of Part I, and Barrère (1990) has confirmed it for Stokes flow in periodic arrays of cylinders. After having calculated the velocity and pressure fields for a large array of cylinders, Barrère calculated both $m_V * p_\beta$ and $m_V * m_V * p_\beta$. His illustrative results (Barrère, Figures 3.9 and 3.10, 1990) are shown in Figure 4 where it is clear that the cellular average provides the desired spatial smoothing.

While the results given in Sec. 1 of Part I, and those presented here, clearly indicate the necessity of using the cellular average to spatially smooth the pressure field in ordered porous media, the situation concerning the velocity is quite different. A reasonable representation for the velocity would be

$$\mathbf{v}_{\beta} = \mathbf{H} \cdot \mathbf{r}_{\beta} + \mathbf{f}_{\beta} + \mathbf{C}_{\beta} \tag{2.48}$$

in which H_{β} is a constant tensor, \mathbf{f}_{β} is a spatially periodic vector, and \mathbf{C}_{β} is a constant vector. The development presented in Part II (see Equations (2.30) through (2.40)) can be used to immediately demonstrate that

$$m * \mathbf{v}_{\beta} = m_V * m_V * (\mathsf{H}_{\beta} \cdot \mathbf{r}_{\beta}) + m_V * \mathbf{f}_{\beta} + m_V * \mathbf{C}_{\beta}. \tag{2.49}$$

The tensor H_{β} is obviously associated with $\nabla \langle \mathbf{v}_{\beta} \rangle_m$ and in general the following inequality will be valid

$$m_V * m_V * (\mathsf{H}_\beta \cdot \mathbf{r}_\beta) \ll m_V * \mathbf{f}_\beta + m_V * \mathbf{C}_\beta.$$
 (2.50)

Under these circumstances we obtain

$$m * \mathbf{v}_{\beta} = m_{V} * \mathbf{v}_{\beta}. \tag{2.51}$$

This means that the superficial velocity given by Equation (1.3) in Part I, with \mathcal{V} being the volume of a unit cell, represents the correct velocity to be used with Darcy's law for flow in ordered porous media. It is important to note that the velocity represents a special case in terms of transport in porous media, when the no-slip condition is valid. The no-slip condition suppresses the generation of significant values of $\nabla \langle \mathbf{v}_{\beta} \rangle_m$, as indicated by the inequality presented by Equation (2.50). Because of this, the cellular average velocity will be equal to the volume average velocity, i.e.

$$m_V * m_V * \mathbf{v}_\beta = m_V * \mathbf{v}_\beta \tag{2.52}$$

for most practical problems of flow in spatially periodic porous media. However, this will not be the case for the pressure, the temperature, or the concentration.

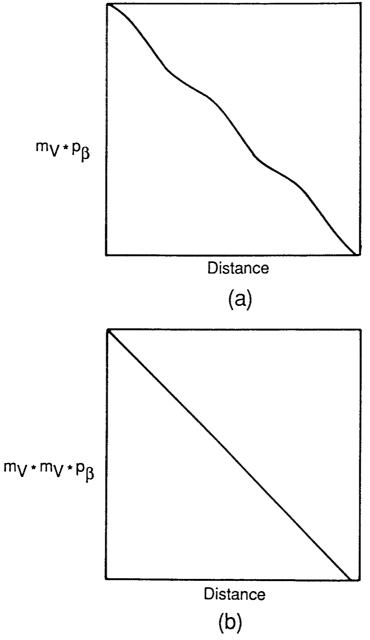


Fig. 4. Volume averaged and cellular averaged pressures for flow in spatially periodic porous media.

2.5. COMPARISON WITH EXPERIMENT

The closure problem specified by Equations (2.41) has been compared with experimental results by Barrère *et al.* (1992) and their comparison is illustrated in Figure

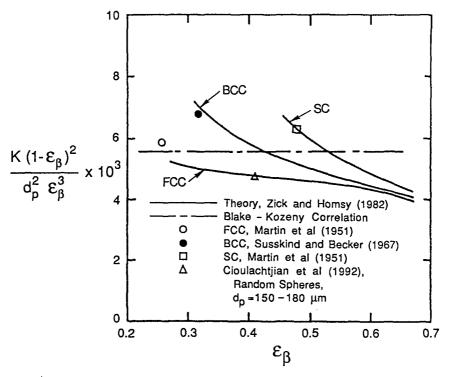


Fig. 5. Comparison between theory and experiment.

- 5. The agreement with three-dimensional spatially periodic media is excellent and the agreement with the Blake-Kozeny correlation and the results of Cioulachtjian *et al.* (1992) for disordered media are very attractive. In thinking about the possibility of using spatially periodic models to predict effective transport coefficients for disordered media, one must remember two things:
 - (1) A spatially periodic porous medium is described by a unit cell and a set of lattice vectors
 - (2) A unit cell is described by the geometry within the unit cell.

The *lattice vectors* are used to specify the *weak* periodicity conditions given by Equations (2.21), while the geometry within the unit cell is used to specify the *strong* boundary condition given by Equation (2.41c). For the spatially periodic porous medium illustrated in Figure 3 of Part I, the periodicity conditions may influence the final calculated value of K. For the unit cell illustrated in Figure 3 of this paper, it seems likely that the governing equations and the no-slip condition given by Equations (2.41a) through (2.41c) will dominate the D-field and therefore the value of K. Recent solutions of Equations (2.41) by Anguy and Bernard (1992) have been carried out for extremely complex unit cells and when more calculations of this type are completed we will be able to assess the importance of the periodicity conditions.

3. Conclusions

In this paper we have developed the closed form of the Stokes equations for both ordered and disordered porous media. This leads to Darcy's law with the Brinkman correction and a closure problem that can be used to determine the generalized permeability tensor, K_m . In order to develop a local version of the closure problem, we have made use of the spatially periodic model of a porous medium. This can be used to determine theoretically the permeability tensor K. With the use of robust unit cells, we expect that K will closely resemble K_m for disordered porous media.

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