Homogenization of Compositional Flow in Fractured Porous Media

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HOMOGENIZATION OF COMPOSITIONAL FLOW IN FRACTURED POROUS MEDIA*

TODD ARBOGAST† AND ZHANGXIN CHEN‡

Abstract. We derive a dual-porosity model of multidimensional, multicomponent, three-phase flow in naturally fractured porous media from the (formal) mathematical theory of homogenization. Special attention is paid to developing a general approach to incorporating gravitational forces and effects of mass transfer between phases. In particular, general equations for the interactions between matrix and fracture systems are obtained under homogenization by a careful scaling of these effects.

Key words. homogenization, dual-porosity, fractured porous medium, compositional flow

AMS(MOS) subject classifications. 35B27, 76S05, 76T05, 86A05

1. Introduction.

A naturally fractured porous medium has throughout its extent a system of interconnected fracture planes dividing the medium into a series of essentially disjoint blocks of porous rock, called the matrix. It has two main length scales of interest: the microscopic scale of the fracture thickness (about 10^{-4} m) and the macroscopic scale of the average distance between fracture planes, i.e., the size of the matrix blocks (about 1 m). Since the entire porous medium is about 10^2-10^3 m across, flow can be mathematically simulated only in some average sense. The concept of dual-porosity [9, 27, 21] has been used to model the flow of fluids on its various scales. In this concept, the fracture system is treated as a porous structure distinct from the usual porous structure of the matrix itself. The fracture system is highly permeable, but can store very little fluid, while the matrix has the opposite characteristics. When formulating a dual-porosity model, it is critical to relate fracture and matrix quantities, since they are defined on different scales.

The problem of modeling the simultaneous flow of multiple components with change of phase in naturally fractured porous media is considered herein. In this type of medium, various physical phenomena occur on disparate length scales, so it is difficult to properly average their effects. Gravitational forces pose special problems. Mass interchange between phases, which results in phase density (pressure) and phase saturation changes, significantly complicates the interaction between the matrix and fracture systems. The main purpose of this paper is to develop a general approach to incorporating especially gravitational forces and effects of mass interchange between phases in the dual-porosity concept.

Recently, the mathematical technique of two-scale homogenization [11, 23, 15] has been exploited to model single phase miscible and two phase, immiscible flow in naturally fractured porous media [4, 6, 7, 13]. The technique determines the proper form of the dual-porosity model, including explicit formula for relating microscopically defined fracture quantities to the macroscopic scale. The resulting macroscopic models have proven to be quite accurate [5, 3, 14].

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The two-scale homogenization technique averages the detailed microscopic equations of flow, and yields simpler, macroscopic equations of dual-porosity type. This is achieved by a careful scaling of the microscopic equations by the size of the matrix blocks ε, and then taking $\varepsilon \to 0$. However, the derivation of the three-phase model of compositional flow does not follow from the previously cited works, since mass transfer between phases has not here-to-for been treated. In this paper an approach based on chemical and mechanical equilibrium is introduced to derive the dynamical equations of the interactions between the fractures and the matrix blocks. This approach is related to that taken by one of the authors in [4]. It is a physically consistent derivation superior to that given in preliminary form by one of the authors and Douglas in [12].

The paper is organized as follows. In the next section we introduce some important notation. We also make some remarks on the scaling of the microscopic model that is needed to obtain a physically reasonable macroscopic model of the flow. In §3, the scaled microscopic equations of compositional flow in a naturally fractured porous medium are presented. In §4, the macroscopic model is stated. Formal homogenization from the microscopic model to the macroscopic one is carried out in §5.

We close this introduction with a remark on two-scale homogenization. It can often be made completely mathematically rigorous (in present case by means of "two-scale convergence"–see, e.g., [6, 1]). However, it is a common practice to use only the formal theory based on an assumed two-scale asymptotic expansion of the solution [23, 15]. This is done to simplify the homogenization and to gain intuition into the derivation of the macroscopic model. We use the formal theory, since our primary concern herein is to find the correct mathematical form of the microscopic and macroscopic models of the flow.

2. Geometry and Scaling Considerations. We idealize our naturally fractured porous medium by assuming that the fractures form three sets of parallel, equally-spaced planes (see Fig. 1) so that all matrix blocks are identical, and the medium has a periodic structure. The homogenization technique starts from the microscopic model, which consists of the known physical equations of flow on this medium defined on the microscopic scale. Let ε denote the homogenization parameter, which we interpret to be the diameter of the matrix blocks. For simplicity, $\varepsilon = 1$ refers to the physical medium. We embed this model in a family of similar models describing flow on a fractured porous medium with matrix blocks that are ε times the original size in any linear direction (see Fig. 2).

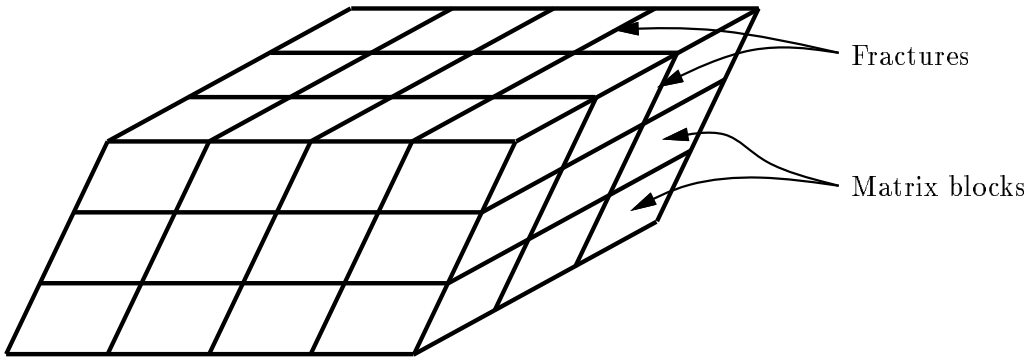

Fig. 1. The idealized periodic medium Ω.

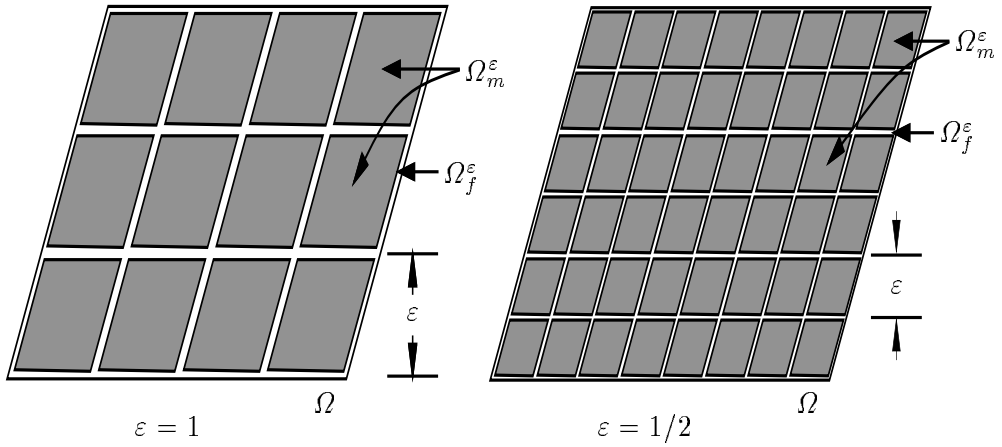

Fig. 2. The first two domains in our family of porous media (the fractures are exaggerated).

Let Ω denote the entire medium, and let Ω_f^ε and Ω_m^ε be the fracture and matrix part of the ε-medium, respectively. The fractures give each ε-medium a periodic structure. Each period is congruent to ε times the unit reference cell Q. The fracture part Q_f completely surrounds the matrix part Q_m (see Fig. 3). For simplicity, let the centroid of Q be the origin and let Q_f be connected. The matrix-fracture interface is indicated by $\partial\Omega_m$, and the outward unit normal vector to $\partial\Omega_m^\varepsilon$ or ∂Q_m is denoted by ν.

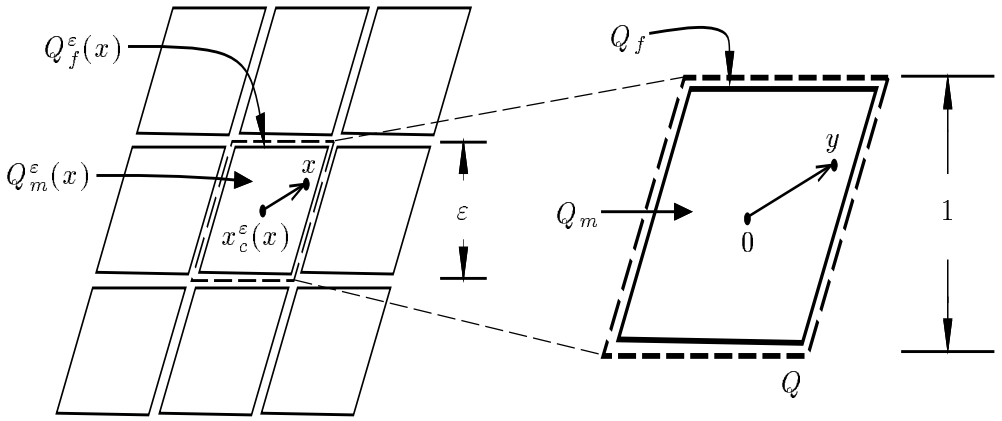

Fig. 3. The unit cell Q and its relation to a point $x = x_c^\varepsilon + \varepsilon y$ in the ε-medium Ω.

In general, x will denote a position in Ω, while y will indicate a position in Q as measured from its centroid. Thus, x is a variable on the macroscopic scale, while y is a microscopic variable. The period at a point x will be represented by $Q^\varepsilon(x)$ with its centroid at $x_c^\varepsilon(x)$. As shown in Fig. 3, we define y by $x = x_c^\varepsilon + \varepsilon y$.

The success of our homogenization depends heavily on the fact that the family of scaled microscopic models we consider below satisfies the following four properties:

(P1) The correct microscopic model of Darcy flow is obtained if $\varepsilon = 1$;

(P2) Within the ε-medium, if any matrix block Q_m^ε is expanded to unit size Q_m, the transformed equations reflect Darcy's law;

(P3) If the fracture system is in chemical and mechanical equilibrium near a matrix block, that block's boundary conditions reflect this equilibrium;

(P4) If the entire system is in chemical and mechanical equilibrium in the vicinity of a matrix block, there must be agreement between the total mass of each phase in the matrix block as calculated from the perspective of the matrix and fracture systems (or, equivalently, from the scaled and unscaled versions of the governing equations).

As remarked in [4], property (P1) assumes that we stay above the Darcy scale, so that Darcy's law governs the system as $\varepsilon = 1$. This is well-known to be the correct physical description of the matrix flow. It is also correct for the fracture flow by the results of Witherspoon *et al.* [28]. Property (P2) is necessary to describe the physics of the flow for $\varepsilon < 1$; that is, flow in the ε-medium "looks like" flow in the *original* system ($\varepsilon = 1$). Property (P3) says that the matrix recognizes when the fracture system is in chemical and mechanical equilibrium. We need to scale the governing equations to obtain (P2); thus, property (P4) is introduced to ensure that our scaling does not introduce changes in the total mass of any phase.

Since the point in this paper is to understand the flow in the interior of the porous medium, we ignore outer boundary conditions on $\partial\Omega$ in the following sections; likewise, we ignore external sources/sinks. We also neglect to specify the initial conditions.

3. The Scaled Microscopic Model. In this section we state the microscopic equations of multiphase flow with mass interchange between phases. See [10, 8, 19, 2, 25, 26] for general references on this subject. The fluid phases will be gas, oil, and water, and they will be referred to by the subscripts g, o, and w. (A straightforward generalization holds for more than three phases.) We consider the general case of N chemical species, or components, each of which may exist in the three phases. Let $c_{i\alpha}$ denote the mass fraction of the ith component in the α-phase, and denote by p_α phase pressure, $\rho_\alpha(c_{1\alpha}, \cdots, c_{N\alpha}; p_\alpha)$ density, $\mu_\alpha(c_{1\alpha}, \cdots, c_{N\alpha})$ viscosity, s_α saturation, and v_α volumetric flow rate, $\alpha = g, o, w$ and $i = 1, \cdots, N$. Denote by $k_{r,\alpha}(s_g, s_o, s_w)$ the relative permeability to flow for the α-phase, and by $D_{i\alpha}(v_\alpha)$ the diffusion coefficient of component i in the α-phase. We assume that only molecular diffusion occurs in the fractures, so the microscopic fracture diffusion coefficients are of the form $D^*_{i\alpha,f}$. The capillary pressure between phases α and β is defined by

$$p_{c\alpha\beta}(s_g, s_o, s_w) = p_\alpha - p_\beta.$$

Finally, let $J_{i\alpha}$ denote the diffusive flux of the ith component in the α-phase such that

$$\sum_{i=1}^{N} J_{i\alpha} = 0, \quad \alpha = g, o, w.$$

For medium and fluid properties, we use subscript f for fracture quantities and m for matrix quantities. Let g be the gravitational, downward-pointing, constant vector, and let e_j denote the standard unit vector in the jth Cartesian direction, with e_3 pointing in the direction of gravity. Denote by ϕ^*_f and k^*_f the fracture porosity and absolute permeability defined on the microscopic, fracture thickness scale. Then $\phi^*_f \approx 1$ and k^*_f is very large (often this is assumed to be approximately the fracture thickness squared divided by 12 [28]). The corresponding matrix quantities are denoted by ϕ_m and k_m. For simplicity of exposition, we assume that the entire medium is incompressible, i.e., ϕ^*_f and ϕ_m do not vary with pressure.

We are now ready to state the microscopic model, which represents the Darcy law, diffusion and dispersion, equations for the conservation of mass imposed over the entire medium on the microscopic scale of the fracture thickness (with porosity and permeability discontinuous across the interface $\partial\Omega_m^\varepsilon$), capillary pressure, and equations for phase equilibria. The microscopic model is stated in three parts: the equations in the fractures, the equations in the matrix, and the matrix-fracture interface conditions.

In the fractures, for $i = 1, \cdots, N$, $\alpha = g, o, w$, and $x \in \Omega_f^\varepsilon$,

$$v_{\alpha,f}^\varepsilon = -\frac{k_f^* k_{r,\alpha,f}^\varepsilon}{\mu_{\alpha,f}^\varepsilon}\left(\nabla p_{\alpha,f}^\varepsilon - \rho_{\alpha,f}^\varepsilon g\right), \tag{3.1a}$$

$$J_{i\alpha,f}^\varepsilon = -\rho_{\alpha,f}^\varepsilon D_{i\alpha,f}^* \nabla c_{i\alpha,f}^\varepsilon, \tag{3.1b}$$

$$\phi_f^* \frac{\partial}{\partial t}\sum_{\beta=g}^{w}(c_{i\beta,f}^\varepsilon \rho_{\beta,f}^\varepsilon s_{\beta,f}^\varepsilon) + \nabla\cdot\sum_{\beta=g}^{w}(c_{i\beta,f}^\varepsilon \rho_{\beta,f}^\varepsilon v_{\beta,f}^\varepsilon + J_{i\beta,f}^\varepsilon) = 0, \tag{3.1c}$$

$$p_{cgo,f}(s_{g,f}^\varepsilon, s_{o,f}^\varepsilon, s_{w,f}^\varepsilon) = p_{g,f}^\varepsilon - p_{o,f}^\varepsilon, \tag{3.1d}$$

$$p_{cow,f}(s_{g,f}^\varepsilon, s_{o,f}^\varepsilon, s_{w,f}^\varepsilon) = p_{o,f}^\varepsilon - p_{w,f}^\varepsilon, \tag{3.1e}$$

$$\sum_{\beta=g}^{w} s_{\beta,f}^\varepsilon = 1, \tag{3.1f}$$

$$\sum_{j=1}^{N} c_{j\alpha,f}^\varepsilon = 1. \tag{3.1g}$$

(When a given function, such as $k_{r,\alpha}$, μ_α, or ρ_α, has a superscript ε, it refers to the argument(s).)

It should be noted that there are more dependent variables than there are equations. To close the system, we assume that thermodynamic equilibrium exists between the fluid phases, and that this equilibrium is expressed in a set of N constraints requiring that the phase fugacities $f_{i\alpha}$ are equal for each component. Namely, we use the following relations to calculate the mole fractions $\chi_{i\alpha}$: for $i = 1, \cdots, N$, $\alpha = g, o, w$, and $x \in \Omega_f^\varepsilon$,

$$f_{i,g}(\chi_{1g,f}^\varepsilon, \cdots, \chi_{Ng,f}^\varepsilon; p_{g,f}^\varepsilon) = f_{i,o}(\chi_{1o,f}^\varepsilon, \cdots, \chi_{No,f}^\varepsilon; p_{o,f}^\varepsilon), \tag{3.1h}$$

$$f_{i,g}(\chi_{1g,f}^\varepsilon, \cdots, \chi_{Ng,f}^\varepsilon; p_{g,f}^\varepsilon) = f_{i,w}(\chi_{1w,f}^\varepsilon, \cdots, \chi_{Nw,f}^\varepsilon; p_{w,f}^\varepsilon), \tag{3.1i}$$

$$c_{i\alpha,f}^\varepsilon = w_i \chi_{i\alpha,f}^\varepsilon / \sum_{j=1}^{N}(w_j \chi_{j\alpha,f}^\varepsilon), \tag{3.1j}$$

where w_i is the molecular weight of the ith-component (we have assumed constant temperature). It can be seen that there are as many relations as there are dependent variables: $9 + 9N$. The system (3.1) is solvable if proper expressions for the fugacities are given [19, 22]. The $6 + 3N$ primary unknowns are $\chi_{i\alpha,f}^\varepsilon$, $s_{\alpha,f}^\varepsilon$, and $p_{\alpha,f}^\varepsilon$; alternatively, since

$$\chi_{i\alpha,f}^\varepsilon = \frac{c_{i\alpha,f}^\varepsilon}{w_i} \Big/ \sum_{j=1}^{N}\frac{c_{j\alpha,f}^\varepsilon}{w_j},$$

we may choose $c_{i\alpha,f}^\varepsilon$ as primary unknowns in place of $\chi_{i\alpha,f}^\varepsilon$.

We remark that the phase fugacities can be obtained from, for example, the Peng-Robinson equation of state [20]. A simpler example is to take

$$\chi^\varepsilon_{ig,f} = \kappa_{igo,f}(p^\varepsilon_{g,f}, p^\varepsilon_{o,f})\chi^\varepsilon_{io,f},$$
$$\chi^\varepsilon_{ig,f} = \kappa_{igw,f}(p^\varepsilon_{g,f}, p^\varepsilon_{w,f})\chi^\varepsilon_{iw,f},$$

where $\kappa_{igo,f}$ and $\kappa_{igw,f}$ are the phase equilibrium constants.

We turn now to the matrix flow on the ε-medium Ω^ε_m. The equations are the same, except for the introduction of some scaling factors ε in (3.2a)-(3.2c) below. For $i = 1, \cdots, N$, $\alpha = g, o, w$, and $x \in \Omega^\varepsilon_m$,

$$v^\varepsilon_{\alpha,m} = -\frac{k_m k^\varepsilon_{r,\alpha,m}}{\mu^\varepsilon_{\alpha,m}} \left(\varepsilon\nabla p^\varepsilon_{\alpha,m} - \rho^\varepsilon_{\alpha,m} g\right), \tag{3.2a}$$

$$J^\varepsilon_{i\alpha,m} = -\varepsilon\rho^\varepsilon_{\alpha,m} D^\varepsilon_{i\alpha,m}\nabla c^\varepsilon_{i\alpha,m}, \tag{3.2b}$$

$$\phi_m \frac{\partial}{\partial t}\sum_{\beta=g}^{w}(c^\varepsilon_{i\beta,m}\rho^\varepsilon_{\beta,m}s^\varepsilon_{\beta,m}) + \varepsilon\nabla\cdot\sum_{\beta=g}^{w}(c^\varepsilon_{i\beta,m}\rho^\varepsilon_{\beta,m}v^\varepsilon_{\beta,m} + J^\varepsilon_{i\beta,m}) = 0, \tag{3.2c}$$

$$p_{cgo,m}(s^\varepsilon_{g,m}, s^\varepsilon_{o,m}, s^\varepsilon_{w,m}) = p^\varepsilon_{g,m} - p^\varepsilon_{o,m}, \tag{3.2d}$$

$$p_{cow,m}(s^\varepsilon_{g,m}, s^\varepsilon_{o,m}, s^\varepsilon_{w,m}) = p^\varepsilon_{o,m} - p^\varepsilon_{w,m}, \tag{3.2e}$$

$$\sum_{\beta=g}^{w} s^\varepsilon_{\beta,m} = 1, \tag{3.2f}$$

$$\sum_{j=1}^{N} c^\varepsilon_{j\alpha,m} = 1, \tag{3.2g}$$

$$f_{i,g}(\chi^\varepsilon_{1g,m}, \cdots, \chi^\varepsilon_{Ng,m}; p^\varepsilon_{g,m}) = f_{i,o}(\chi^\varepsilon_{1o,m}, \cdots, \chi^\varepsilon_{No,m}; p^\varepsilon_{o,m}), \tag{3.2h}$$

$$f_{i,g}(\chi^\varepsilon_{1g,m}, \cdots, \chi^\varepsilon_{Ng,m}; p^\varepsilon_{g,m}) = f_{i,w}(\chi^\varepsilon_{1w,m}, \cdots, \chi^\varepsilon_{Nw,m}; p^\varepsilon_{w,m}), \tag{3.2i}$$

$$c^\varepsilon_{i\alpha,m} = w_i\chi^\varepsilon_{i\alpha,m} / \sum_{j=1}^{N}(w_j\chi^\varepsilon_{j\alpha,m}). \tag{3.2j}$$

To satisfy (P3), we need to treat pressure gradient effects on the same footing as gravitational effects. This is easily done if we introduce the equilibrium pressure distribution $\psi_\alpha : [0,1]^N \times \mathbb{R} \to \mathbb{R}$ by

$$\begin{cases} \partial\psi_\alpha/\partial x_3 = \rho_\alpha(\xi_1, \cdots, \xi_N; \psi_\alpha(\xi_1, \cdots, \xi_N; x_3))g, \\ \psi_\alpha(\xi_1, \cdots, \xi_N; 0) = p_{0,\alpha}, \end{cases}$$

for some reference pressure $p_{0,\alpha}$ at $x_3 = 0$ (as was done in [4]). If we assume that $\xi_1, \cdots, \xi_N$ are fixed and that $\partial\rho_\alpha/\partial p_\alpha \geq 0$, this is solvable by the monotonicity; that is, $\psi_\alpha(\xi_1, \cdots, \xi_N; x_3)$ satisfies

$$\int_{p_{0,\alpha}}^{\psi_\alpha(\xi_1,\cdots,\xi_N;x_3)} \frac{d\pi}{\rho_\alpha(\xi_1, \cdots, \xi_N; \pi)} = x_3 g.$$

The inverse of ψ_α is denoted by $\psi_\alpha^{-1}(\xi_1, \cdots, \xi_N; \cdot)$, again for $\xi_1, \cdots, \xi_N$ fixed. Since $\rho_\alpha = \rho_\alpha(c_{1\alpha}, \cdots, c_{N\alpha}; p_\alpha)$, $\psi_\alpha^{-1}(c_{1\alpha}, \cdots, c_{N\alpha}; p_\alpha)$ is the pseudo-potential [17] plus x_3 under the condition that concentrations are constant.

We define now the continuity equations on the matrix-fracture interface $\partial\Omega_m^\varepsilon$. An explanation of the form of these equations will follow. For $i = 1, \cdots, N$, $\alpha = g, o, w$, and $x \in \partial\Omega_m^\varepsilon$,

$$\sum_{\beta=g}^{w} (c_{i\beta,f}^\varepsilon \rho_{\beta,f}^\varepsilon v_{\beta,f}^\varepsilon + J_{i\beta,f}^\varepsilon) \cdot \nu = \sum_{\beta=g}^{w} \varepsilon (c_{i\beta,m}^\varepsilon \rho_{\beta,m}^\varepsilon v_{\beta,m}^\varepsilon + J_{i\beta,m}^\varepsilon) \cdot \nu, \tag{3.3a}$$

$$c_{i\alpha,m}^\varepsilon = c_{i\alpha,f}^\varepsilon, \tag{3.3b}$$

$$p_{\alpha,m}^\varepsilon = \psi_\alpha(c_{1\alpha,m}^\varepsilon, \cdots, c_{N\alpha,m}^\varepsilon; \psi_\alpha^{-1}(c_{1\alpha,f}^\varepsilon, \cdots, c_{N\alpha,f}^\varepsilon; p_{\alpha,f}^\varepsilon) - Z_{\mathrm{ref},\alpha}^\varepsilon + (\varepsilon^{-1} - 1)(x_3 - x_{c,3}^\varepsilon)). \tag{3.3c}$$

We also need to define the pressure distribution reference value $Z_{\mathrm{ref},\alpha}^\varepsilon$ on each matrix block $Q_m^\varepsilon(x)$. Any reasonable definition results in the macroscopic model presented later; therefore, let us simply define $Z_{\mathrm{ref},\alpha}^\varepsilon$ on $Q_m^\varepsilon(x)$ such that, for $i = 1, \cdots, N$ and $\alpha = g, o, w$,

$$\overline{c}_{i\alpha}^\varepsilon = \frac{1}{|\partial Q_m^\varepsilon|} \int_{\partial Q_m^\varepsilon(x)} c_{i\alpha,f}^\varepsilon(X,t)\, d\sigma(X), \tag{3.4a}$$

$$\overline{Z}_\alpha^\varepsilon = \frac{1}{|\partial Q_m^\varepsilon|} \int_{\partial Q_m^\varepsilon(x)} \left[\psi_\alpha^{-1}(\overline{c}_{1\alpha}^\varepsilon, \cdots, \overline{c}_{N\alpha}^\varepsilon; p_{\alpha,f}^\varepsilon(X,t)) - X_3\right] d\sigma(X), \tag{3.4b}$$

$$\begin{aligned} \int_{Q_m^\varepsilon(x)} \phi_m \rho_\alpha(\overline{c}_{1\alpha}^\varepsilon, \cdots, \overline{c}_{N\alpha}^\varepsilon; \psi_\alpha(\overline{c}_{1\alpha}^\varepsilon, \cdots, \overline{c}_{N\alpha}^\varepsilon; x_{c,3}^\varepsilon + \overline{Z}_\alpha^\varepsilon - Z_{\mathrm{ref},\alpha}^\varepsilon \\ + \varepsilon^{-1}(X_3 - x_{c,3}^\varepsilon)))\, dX \\ = \int_{Q_m^\varepsilon(x)} \phi_m \rho_\alpha(\overline{c}_{1\alpha}^\varepsilon, \cdots, \overline{c}_{N\alpha}^\varepsilon; \psi_\alpha(\overline{c}_{1\alpha}^\varepsilon, \cdots, \overline{c}_{N\alpha}^\varepsilon; \overline{Z}_\alpha^\varepsilon + X_3))\, dX, \end{aligned} \tag{3.4c}$$

where $|\cdot|$ indicates the volume or area of the given domain.

We close this section with three remarks. Firstly, in (3.1b) and (3.2b), we have adopted an extension of the single-phase Fick's law to multiphase flow for the diffusive fluxes $J_{i\alpha}$. While the precise constitutive relations for these quantities in the case of multiphase flow remain unknown at this time, from a practical point of view these expressions have been in widespread use [10, 18, 24].

Secondly, our four properties are reflected in the microscopic model. If $\varepsilon = 1$, Darcy flow is imposed over the medium in the standard way. Furthermore, $Z_{\mathrm{ref},\alpha}^\varepsilon = 0$ in this case, so that we have the usual interface conditions; that is, (3.3a), (3.3b), and (3.3c) enforce continuity of the mass flux, concentrations, and pressures across $\partial\Omega_m^\varepsilon$, respectively. Thus (P1) holds.

The matrix equations have been scaled so that (P2) is satisfied. This can be easily seen by means of a dimensional argument [4, 13] (it will be seen later in §5, as well).

If the fracture system is in chemical and mechanical equilibrium near a block, then $c_{i\alpha,f}^\varepsilon$ is constant and

$$p_{\alpha,f}^\varepsilon = \psi_\alpha(c_{1\alpha,f}^\varepsilon, \cdots, c_{N\alpha,f}^\varepsilon; x_3 + x_{\mathrm{ref},3})$$

for some constant reference depth $x_{\mathrm{ref},3}$. Then (3.3b) implies that the matrix fracture interface is in chemical equilibrium, and (3.3c) implies that there

$$p_{\alpha,m}^\varepsilon = \psi_\alpha(c_{1\alpha,m}^\varepsilon, \cdots, c_{N\alpha,m}^\varepsilon; x_{c,3}^\varepsilon + x_{\mathrm{ref},3} - Z_{\mathrm{ref},\alpha}^\varepsilon + \varepsilon^{-1}(x_3 - x_{c,3}^\varepsilon)).$$

This is a scaled mechanical equilibrium; when expanded to unit size, we have actual mechanical equilibrium on the interface. Thus (P3) holds. Moreover, in this case, (3.4) tells us that for $x \in \partial\Omega_m^\varepsilon$,

$$\begin{aligned} \overline{c}_{i\alpha}^\varepsilon &= c_{i\alpha,f}^\varepsilon = c_{i\alpha,m}^\varepsilon = \text{constant}, \\ \overline{Z}_\alpha^\varepsilon &= x_{\mathbf{ref},3}. \end{aligned}$$

Hence, (3.4c) is simply

$$\int_{Q_m^\varepsilon(x)} \phi_m \rho_\alpha(c_{1\alpha,m}^\varepsilon, \cdots, c_{N\alpha,m}^\varepsilon; p_{\alpha,m}^\varepsilon)\, dX = \int_{Q_m^\varepsilon(x)} \phi_m \rho_\alpha(c_{1\alpha,f}^\varepsilon, \cdots, c_{N\alpha,f}^\varepsilon; p_{\alpha,f}^\varepsilon)\, dX.$$

This says that if the entire system were in chemical and mechanical equilibrium, then the amount of mass in the matrix block $Q_m^\varepsilon(x)$ from the perspective of the matrix and fracture systems agree, giving (P4).

Finally, we make a remark on the solvability of (3.4c). Let

$$\begin{aligned} Z_{1,\alpha} &= \max_{X \in Q_m^\varepsilon(x)} (\varepsilon^{-1} - 1)(X_3 - x_{c,3}), \\ Z_{2,\alpha} &= \min_{X \in Q_m^\varepsilon(x)} (\varepsilon^{-1} - 1)(X_3 - x_{c,3}). \end{aligned}$$

By the monotonicity assumption on the densities (i.e., $\partial\rho_\alpha/\partial p_\alpha \geq 0$), there is a unique $Z_{\mathbf{ref},\alpha}^\varepsilon$ between $Z_{1,\alpha}$ and $Z_{2,\alpha}$ solving (3.4c), unless the α-phase fluid is incompressible (then set $Z_{\mathbf{ref},\alpha}^\varepsilon = 0$, since its value is immaterial).

4. The Macroscopic Model. Define the auxiliary functions $\omega_j(y), j = 1, 2, 3$, as Q_f-periodic solutions to the problems

$$\nabla_y^2 \omega_j = 0, \qquad y \in Q_f, \tag{4.1a}$$

$$\nabla_y \omega_j \cdot \nu = -e_j \cdot \nu, \qquad y \in \partial Q_m, \tag{4.1b}$$

and a tensor $\mathcal{A}$ whose (j, ℓ) component is $\partial\omega_\ell/\partial y_j$. For a function or tensor φ, define a local average as

$$\overline{\varphi} = \frac{1}{|Q|} \int_{Q_f} \varphi(y)\, dy.$$

Let

$$\phi_f = \frac{|Q_f|}{|Q|} \phi_f^*, \tag{4.2a}$$

$$k_f = \left[\frac{|Q_f|}{|Q|} I + \overline{\mathcal{A}} \right] k_f^*, \tag{4.2b}$$

$$D_{i\alpha,f} = \left[\frac{|Q_f|}{|Q|} I + \overline{\mathcal{A}} \right] D_{i\alpha,f}^*, \tag{4.2c}$$

where I is the identity tensor. We call ϕ_f, k_f, and $D_{i\alpha,f}$, respectively, the macroscopic fracture system porosity, the macroscopic permeability, and the macroscopic diffusion coefficient of component i in the α-phase. These are the effective macroscopic parameters derived by homogenization in the next section and defined in terms of the physically measurable microscopic quantities.

Homogenization ($\varepsilon \to 0$) of the microscopic model leads to the following macroscopic model. The fracture system is defined on Ω. The matrix system is defined on $\Omega \times Q_m$; that is, at each point $x \in \Omega$, there is a matrix block Q_m (albeit "infinitely small"). In the fracture system, we have the usual equations except for the introduction of $q^0_{m,i}$ in (4.3c) and defined in (4.3k). For $i = 1, \cdots, N$, $\alpha = g, o, w$, and $x \in \Omega$,

$$v_{\alpha,f} = -\frac{k_f k^0_{r,\alpha,f}}{\mu^0_{\alpha,f}} \left(\nabla_x p^0_{\alpha,f} - \rho^0_{\alpha,f} g\right), \tag{4.3a}$$

$$J_{i\alpha,f} = -\rho^0_{\alpha,f} D_{i\alpha,f} \nabla_x c^0_{i\alpha,f}, \tag{4.3b}$$

$$\phi_f \frac{\partial}{\partial t} \sum_{\beta=g}^{w} (c^0_{i\beta,f} \rho^0_{\beta,f} s^0_{\beta,f}) + \nabla_x \cdot \sum_{\beta=g}^{w} (c^0_{i\beta,f} \rho^0_{\beta,f} v_{\beta,f} + J_{i\beta,f}) = q_{m,i}, \tag{4.3c}$$

$$p_{cgo,f}(s^0_{g,f}, s^0_{o,f}, s^0_{w,f}) = p^0_{g,f} - p^0_{o,f}, \tag{4.3d}$$

$$p_{cow,f}(s^0_{g,f}, s^0_{o,f}, s^0_{w,f}) = p^0_{o,f} - p^0_{w,f}, \tag{4.3e}$$

$$\sum_{\beta=g}^{w} s^0_{\beta,f} = 1, \tag{4.3f}$$

$$\sum_{j=1}^{N} c^0_{j\alpha,f} = 1, \tag{4.3g}$$

$$f_{i,g}(\chi^0_{1g,f}, \cdots, \chi^0_{Ng,f}; p^0_{g,f}) = f_{i,o}(\chi^0_{1o,f}, \cdots, \chi^0_{No,f}; p^0_{o,f}), \tag{4.3h}$$

$$f_{i,g}(\chi^0_{1g,f}, \cdots, \chi^0_{Ng,f}; p^0_{g,f}) = f_{i,w}(\chi^0_{1w,f}, \cdots, \chi^0_{Nw,f}; p^0_{w,f}), \tag{4.3i}$$

$$c^0_{i\alpha,f} = w_i \chi^0_{i\alpha,f} / \sum_{j=1}^{N} (w_j \chi^0_{j\alpha,f}), \tag{4.3j}$$

$$q_{m,i} = -\frac{1}{|Q|} \int_{Q_m} \phi_m \frac{\partial}{\partial t} \sum_{\beta=g}^{w} (c^0_{i\beta,m} \rho^0_{\beta,m} s^0_{\beta,m})\, dy. \tag{4.3k}$$

In the matrix system, for $i = 1, \cdots, N$, $\alpha = g, o, w$, and $(x, y) \in \Omega \times Q_m$,

$$v^0_{\alpha,m} = -\frac{k_m k^0_{r,\alpha,m}}{\mu^0_{\alpha,m}} \left(\nabla_y p^0_{\alpha,m} - \rho^0_{\alpha,m} g\right), \tag{4.4a}$$

$$J^0_{i\alpha,m} = -\rho^0_{\alpha,m} D^0_{i\alpha,m} \nabla_y c^0_{i\alpha,m}, \tag{4.4b}$$

$$\phi_m \frac{\partial}{\partial t} \sum_{\beta=g}^{w} (c^0_{i\beta,m} \rho^0_{\beta,m} s^0_{\beta,m}) + \nabla_y \cdot \sum_{\beta=g}^{w} (c^0_{i\beta,m} \rho^0_{\beta,m} v^0_{\beta,m} + J^0_{i\beta,m}) = 0, \tag{4.4c}$$

$$p_{cgo,m}(s^0_{g,m}, s^0_{o,m}, s^0_{w,m}) = p^0_{g,m} - p^0_{o,m}, \tag{4.4d}$$

$$p_{cow,m}(s^0_{g,m}, s^0_{o,m}, s^0_{w,m}) = p^0_{o,m} - p^0_{w,m}, \tag{4.4e}$$

$$\sum_{\beta=g}^{w} s^0_{\beta,m} = 1, \tag{4.4f}$$

$$\sum_{j=1}^{N} c^0_{j\alpha,m} = 1, \tag{4.4g}$$

$$f_{i,g}(\chi^0_{1g,m}, \cdots, \chi^0_{Ng,m}; p^0_{g,m}) = f_{i,o}(\chi^0_{1o,m}, \cdots, \chi^0_{No,m}; p^0_{o,m}), \tag{4.4h}$$

$$f_{i,g}(\chi^0_{1g,m},\cdots,\chi^0_{Ng,m};p^0_{g,m}) = f_{i,w}(\chi^0_{1w,m},\cdots,\chi^0_{Nw,m};p^0_{w,m}), \tag{4.4i}$$

$$c^0_{i\alpha,m} = w_i\chi^0_{i\alpha,m}/\sum_{j=1}^{N}(w_j\chi^0_{j\alpha,m}). \tag{4.4j}$$

The matrix boundary conditions are defined as follows: for $i = 1,\cdots,N$, $\alpha = g,o,w$, and $(x,y) \in \Omega \times \partial Q_m$,

$$c^0_{i\alpha,m}(x,y,t) = c^0_{i\alpha,f}(x,t), \tag{4.5a}$$

$$\begin{aligned} &p^0_{\alpha,m}(x,y,t) \\ &\quad = \psi_\alpha(c^0_{1\alpha,f},\cdots,c^0_{N\alpha,f};\psi^{-1}_\alpha(c^0_{1\alpha,f},\cdots,c^0_{N\alpha,f};p^0_{\alpha,f}) - Z^0_{\mathbf{ref},\alpha} + y_3), \end{aligned} \tag{4.5b}$$

where the pressure distribution reference $Z^0_{\mathbf{ref},\alpha}$ is given by

$$\begin{aligned} &\frac{1}{|Q_m|}\int_{Q_m}\phi_m\rho_\alpha(c^0_{1\alpha,f},\cdots,c^0_{N\alpha,f};\psi_\alpha(c^0_{1\alpha,f},\cdots,c^0_{N\alpha,f}; \\ &\qquad\qquad \psi^{-1}_\alpha\left(c^0_{1\alpha,f},\cdots,c^0_{N\alpha,f};p^0_{\alpha,f}\right) - Z^0_{\mathbf{ref},\alpha} + y_3))\,dy \\ &\quad = \phi_m\rho_\alpha(c^0_{1\alpha,f},\cdots,c^0_{N\alpha,f};p^0_{\alpha,f}). \end{aligned} \tag{4.5c}$$

Again, the monotonicity assumption ensures a unique solution to (4.5c) for $Z^0_{\mathbf{ref},\alpha}$, $\alpha = g,o,w$ (for incompressible α-phase fluid, we set $Z^0_{\mathbf{ref},\alpha} = 0$).

The macroscopic model says that the fracture system, being highly permeable, quickly comes into chemical and mechanical equilibrium on the fracture spacing scale locally. This equilibrium is defined in terms of the concentrations and the "chemical equilibrium pseudo-potential," and it is reflected in the matrix equations through the boundary conditions (4.5a) and (4.5b). Note also that mass is conserved between the matrix and fracture systems, since fluid flow out of the matrix appears in the fractures through the integral in (4.3k).

5. Formal Homogenization. In this section we consider the formal homogenization from the microscopic model to the macroscopic one. Many of the techniques have been used in [4, 7, 12, 13, 16, 23, 15]. We recall the asymptotic relations

$$x = x^\varepsilon_c(x) + \varepsilon y, \quad \nabla \sim \varepsilon^{-1}\nabla_y + \nabla_x. \tag{5.1}$$

The solutions are then assumed (formally) to have the asymptotic form

$$\Psi^\varepsilon_f(x,t) \sim \sum_{\ell=0}^{\infty}\varepsilon^\ell\Psi^\ell_f(x,y,t), \quad (x,y) \in \Omega \times Q_f, \tag{5.2a}$$

$$\Psi^\varepsilon_m(x,t) \sim \sum_{\ell=0}^{\infty}\varepsilon^\ell\Psi^\ell_m(x,y,t), \quad (x,y) \in \Omega \times Q_m, \tag{5.2b}$$

for generic functions Ψ^ε_f and Ψ^ε_m associated with the fracture and matrix systems, respectively. Each of the functions Ψ^ℓ_f is assumed to be periodic in $y \in Q_f$. The functions we need to expand are p_α, s_α, and $c_{i\alpha}$. Functions of Ψ^ε_f or Ψ^ε_m can be expanded by Taylor's Theorem as

$$\begin{aligned} \varphi(\xi^\varepsilon) &= \varphi(\xi^0) + \varphi'(\xi^0)(\xi^\varepsilon - \xi^0) + \cdots \\ &\equiv \varphi(\xi^0) + \varepsilon\varphi^1 + \varepsilon^2\varphi^2 + \cdots, \quad \xi = \Psi_f \text{ or } \Psi_m, \end{aligned} \tag{5.3}$$

for some $\varphi^1, \varphi^2, \cdots$. Finally, by the change of variables $X = x_c^\varepsilon(x) + \varepsilon y$,

$$\int_{Q_m^\varepsilon(x)} \varphi(\xi^\varepsilon(X))\, dX = \varepsilon^3 \int_{Q_m} \varphi(\xi^\varepsilon(x_c^\varepsilon(x) + \varepsilon y))\, dy \tag{5.4a}$$
$$\sim \varepsilon^3 \int_{Q_m} \Big(\varphi(\xi^0(x,y)) + \sum_{\ell=1}^{\infty} \varepsilon^\ell \varphi^\ell(x,y)\Big) dy,$$

$$\int_{\partial Q_m^\varepsilon(x)} \varphi(\xi^\varepsilon(X))\, d\sigma(X) = \varepsilon^2 \int_{\partial Q_m} \varphi(\xi^\varepsilon(x_c^\varepsilon(x) + \varepsilon y))\, d\sigma(y) \tag{5.4b}$$
$$\sim \varepsilon^2 \int_{\partial Q_m} \Big(\varphi(\xi^0(x,y)) + \sum_{\ell=1}^{\infty} \varepsilon^\ell \varphi^\ell(x,y)\Big) d\sigma(y).$$

We substitute the formal asymptotic expansions given by (5.1)–(5.4) into (3.1)–(3.4) and equate coefficients of like powers of ε. The process is rather long and somewhat tedious, but it leads to our macroscopic model, which is the set of equations for the leading terms in the expansions. The derivation of the equations (4.3d)–(4.3j), (4.4a)–(4.4j), and (4.5a) is straightforward and therefore omitted. (We remark that the matrix equations are of the usual form because of (5.1) and our scaling, i.e., Property (P2)). Special emphasis is placed on obtaining the equations (4.3a)–(4.3c), (4.3k), and (4.5b)–(4.5c).

From the ε^{-1}-terms of (3.1a), (3.1b), and (3.3a), and the ε^{-2}-term of (3.1c), we have

$$v_{\alpha,f}^{-1} = -\frac{k_f^* k_{r,\alpha,f}^0}{\mu_{\alpha,f}^0} \nabla_y p_{\alpha,f}^0, \qquad (x,y) \in \Omega \times Q_f, \tag{5.5a}$$

$$J_{i\alpha,f}^{-1} = -\rho_{\alpha,f}^0 D_{i\alpha,f}^* \nabla_y c_{i\alpha,f}^0, \qquad (x,y) \in \Omega \times Q_f, \tag{5.5b}$$

$$\nabla_y \cdot \sum_{\beta=g}^{w} (c_{i\beta,f}^0 \rho_{\beta,f}^0 v_{\beta,f}^{-1} + J_{i\beta,f}^{-1}) = 0, \quad (x,y) \in \Omega \times Q_f, \tag{5.5c}$$

$$\sum_{\beta=g}^{w} (c_{i\beta,f}^0 \rho_{\beta,f}^0 v_{\beta,f}^{-1} + J_{i\beta,f}^{-1}) \cdot \nu = 0, \qquad (x,y) \in \Omega \times \partial Q_m. \tag{5.5d}$$

This, together with (4.3d)–(4.3j), is a steady-state system without sources and gravity. For a physical meaningful set of data, the periodic solution of this system is clearly constant in y; that is, for $i = 1, \cdots, N$, $\alpha = g, o, w$,

$$p_{\alpha,f}^0 = p_{\alpha,f}^0(x,t) \text{ only}, \tag{5.6a}$$

$$s_{\alpha,f}^0 = s_{\alpha,f}^0(x,t) \text{ only}, \tag{5.6b}$$

$$c_{i\alpha,f}^0 = c_{i\alpha,f}^0(x,t) \text{ only}, \tag{5.6c}$$

and then, by (4.3j), (5.5a), and (5.5b),

$$\chi_{i\alpha,f}^0 = \chi_{i\alpha,f}^0(x,t) \text{ only}, \tag{5.6d}$$

$$v_{\alpha,f}^{-1} = 0, \tag{5.6e}$$

$$J_{i\alpha,f}^{-1} = 0. \tag{5.6f}$$

Therefore, all terms containing $\nabla_y p^0_{\alpha,f}$, $\nabla_y s^0_{\alpha,f}$, and $\nabla_y c^0_{i\alpha,f}$ drop out in the analysis below. This considerably simplifies the rest of our calculations.

From the ε^0-terms of (3.1a), (3.1b), and (3.3a), and the ε^{-1}-term of (3.1c), we observe that

$$v^0_{\alpha,f} = -\frac{k^*_f k^0_{r,\alpha,f}}{\mu^0_{\alpha,f}} \left(\nabla_y p^1_{\alpha,f} + \nabla_x p^0_{\alpha,f} - \rho^0_{\alpha,f} g\right), \quad (x,y) \in \Omega \times Q_f, \tag{5.7a}$$

$$J^0_{i\alpha,f} = -\rho^0_{\alpha,f} D^*_{i\alpha,f} \left(\nabla_y c^1_{i\alpha,f} + \nabla_x c^0_{i\alpha,f}\right), \qquad (x,y) \in \Omega \times Q_f, \tag{5.7b}$$

$$\nabla_y \cdot \sum_{\beta=g}^{w} (c^0_{i\beta,f} \rho^0_{\beta,f} v^0_{\beta,f} + J^0_{i\beta,f}) = 0, \qquad (x,y) \in \Omega \times Q_f, \tag{5.7c}$$

$$\sum_{\beta=g}^{w} (c^0_{i\beta,f} \rho^0_{\beta,f} v^0_{\beta,f} + J^0_{i\beta,f}) \cdot \nu = 0, \qquad (x,y) \in \Omega \times \partial Q_m. \tag{5.7d}$$

Therefore, for $i = 1, \cdots, N$ and with

$$F_i(x,y,t) = \sum_{\beta=g}^{w} \left(c^0_{i\beta,f} \rho^0_{\beta,f} \frac{k^*_f k^0_{r,\beta,f}}{\mu^0_{\beta,f}} p^1_{\beta,f} + \rho^0_{\beta,f} D^*_{i\beta,f} c^1_{i\beta,f} \right), \tag{5.8a}$$

by (5.6), we have

$$\nabla_y^2 F_i(x,y,t) = 0, \quad (x,y) \in \Omega \times Q_f, \tag{5.8b}$$

$$\nabla_y F_i \cdot \nu = -\sum_{\beta=g}^{w} \left(c^0_{i\beta,f} \rho^0_{\beta,f} \frac{k^*_f k^0_{r,\beta,f}}{\mu^0_{\beta,f}} \left(\nabla_x p^0_{\beta,f} - \rho^0_{\beta,f} g\right) + \rho^0_{\beta,f} D^*_{i\beta,f} \nabla_x c^0_{i\beta,f} \right) \cdot \nu, \quad (x,y) \in \Omega \times \partial Q_m. \tag{5.8c}$$

Apply (4.1) to see that the solution can be written as

$$F_i(x,y,t) = \sum_{j=1}^{3} \sum_{\beta=g}^{w} \left(c^0_{i\beta,f} \rho^0_{\beta,f} \frac{k^*_f k^0_{r,\beta,f}}{\mu^0_{\beta,f}} \left(\frac{\partial p^0_{\beta,f}}{\partial x_j} - \rho^0_{\beta,f} g_j \right) + \rho^0_{\beta,f} D^*_{i\beta,f} \frac{\partial c^0_{i\beta,f}}{\partial x_j} \right) \omega_j(y) + \theta_i(x,t), \tag{5.9}$$

for some functions θ_i of x and t, $i = 1, \cdots, N$. Since only y-derivatives of $F_i(x,y,t)$ will be needed below, θ_i need not be evaluated.

From the ε^0-term of (3.1c) and the ε^1-term of (3.3a), we see that

$$\begin{aligned}(5.10a)\qquad &\phi_f^* \frac{\partial}{\partial t}\sum_{\beta=g}^{w}(c^0_{i\beta,f}\rho^0_{\beta,f}s^0_{\beta,f})\\ &\quad+\nabla_y\cdot\sum_{\beta=g}^{w}(c^0_{i\beta,f}\rho^0_{\beta,f}v^1_{\beta,f}+c^0_{i\beta,f}\rho^1_{\beta,f}v^0_{\beta,f}+c^1_{i\beta,f}\rho^0_{\beta,f}v^0_{\beta,f}+J^1_{i\beta,f})\\ &\quad+\nabla_x\cdot\sum_{\beta=g}^{w}(c^0_{i\beta,f}\rho^0_{\beta,f}v^0_{\beta,f}+J^0_{i\beta,f})\\ &\quad=0,\quad (x,y)\in\Omega\times Q_f,\end{aligned}$$

$$\begin{aligned}(5.10b)\qquad &\sum_{\beta=g}^{w}(c^0_{i\beta,f}\rho^0_{\beta,f}v^1_{\beta,f}+c^0_{i\beta,f}\rho^1_{\beta,f}v^0_{\beta,f}+c^1_{i\beta,f}\rho^0_{\beta,f}v^0_{\beta,f}+J^1_{i\beta,f})\cdot\nu\\ &\quad=\sum_{\beta=g}^{w}(c^0_{i\beta,m}\rho^0_{\beta,m}v^0_{\beta,m}+J^0_{i\beta,m})\cdot\nu,\quad (x,y)\in\Omega\times\partial Q_m.\end{aligned}$$

Locally average (5.10a) and use the definition of ϕ_f, (4.2a), to obtain

$$\begin{aligned}(5.11)\qquad &\phi_f\frac{\partial}{\partial t}\sum_{\beta=g}^{w}(c^0_{i\beta,f}\rho^0_{\beta,f}s^0_{\beta,f})\\ &\quad+\frac{1}{|Q|}\int_{Q_f}\nabla_y\cdot\sum_{\beta=g}^{w}(c^0_{i\beta,f}\rho^0_{\beta,f}v^1_{\beta,f}+c^0_{i\beta,f}\rho^1_{\beta,f}v^0_{\beta,f}+c^1_{i\beta,f}\rho^0_{\beta,f}v^0_{\beta,f}+J^1_{i\beta,f})\,dy\\ &\quad+\nabla_x\cdot\left(\frac{1}{|Q|}\int_{Q_f}\sum_{\beta=g}^{w}(c^0_{i\beta,f}\rho^0_{\beta,f}v^0_{\beta,f}+J^0_{i\beta,f})\,dy\right)=0.\end{aligned}$$

We now apply the divergence theorem to the first integral of (5.11), use (5.10b), make a second application of the divergence theorem, and use (4.4c); that is,

$$\begin{aligned}(5.12)\qquad &\frac{1}{|Q|}\int_{Q_f}\nabla_y\cdot\sum_{\beta=g}^{w}(c^0_{i\beta,f}\rho^0_{\beta,f}v^1_{\beta,f}+c^0_{i\beta,f}\rho^1_{\beta,f}v^0_{\beta,f}+c^1_{i\beta,f}\rho^0_{\beta,f}v^0_{\beta,f}+J^1_{i\beta,f})\,dy\\ &\quad=\frac{1}{|Q|}\int_{\partial Q_f}\sum_{\beta=g}^{w}(c^0_{i\beta,f}\rho^0_{\beta,f}v^1_{\beta,f}+c^0_{i\beta,f}\rho^1_{\beta,f}v^0_{\beta,f}+c^1_{i\beta,f}\rho^0_{\beta,f}v^0_{\beta,f}+J^1_{i\beta,f})\cdot\nu\,d\sigma(y)\\ &\quad=-\frac{1}{|Q|}\int_{\partial Q_m}\sum_{\beta=g}^{w}(c^0_{i\beta,m}\rho^0_{\beta,m}v^0_{\beta,m}+J^0_{i\beta,m})\cdot\nu\,d\sigma(y)\\ &\quad=-\frac{1}{|Q|}\int_{Q_m}\nabla_y\cdot\sum_{\beta=g}^{w}(c^0_{i\beta,m}\rho^0_{\beta,m}v^0_{\beta,m}+J^0_{i\beta,m})\,dy\\ &\quad=\frac{1}{|Q|}\int_{Q_m}\phi_m\frac{\partial}{\partial t}\sum_{\beta=g}^{w}(c^0_{i\beta,m}\rho^0_{\beta,m}s^0_{\beta,m})\,dy\\ &\quad\equiv -q_{m,i}.\end{aligned}$$

Here, we have used periodicity to see that no contribution arises from the integral over ∂Q, the outer boundary of Q_f, and the fact that the outer normal to $\partial Q_f \setminus \partial Q$ is opposite to that of ∂Q_m. This defines $q_{m,i}$ as in (4.3k).

For the second integral of (5.11), note that, by (5.7a), (5.7b), and (5.9), the jth component of the vector is

$$
\begin{aligned}
(5.13)\qquad & \sum_{\beta=g}^{w}(c^0_{i\beta,f}\rho^0_{\beta,f}v^0_{\beta,f,j}+J^0_{i\beta,f,j}) \\
&\quad = -\frac{\partial F_i}{\partial y_j}-\sum_{\beta=g}^{w}\left(c^0_{i\beta,f}\rho^0_{\beta,f}\frac{k^*_f k^0_{r,\beta,f}}{\mu^0_{\beta,f}}\left(\frac{\partial p^0_{\beta,f}}{\partial x_j}-\rho^0_{\beta,f}g_j\right)+\rho^0_{\beta,f}D^*_{i\beta,f}\frac{\partial c^0_{i\beta,f}}{\partial x_j}\right) \\
&\quad = -\sum_{\beta=g}^{w}\sum_{\ell=1}^{3}\left(\frac{\partial \omega_\ell}{\partial y_j}+\delta_{j,\ell}\right) \\
&\qquad\qquad \times\left(c^0_{i\beta,f}\rho^0_{\beta,f}\frac{k^*_f k^0_{r,\beta,f}}{\mu^0_{\beta,f}}\left(\frac{\partial p^0_{\beta,f}}{\partial x_\ell}-\rho^0_{\beta,f}g_\ell\right)+\rho^0_{\beta,f}D^*_{i\beta,f}\frac{\partial c^0_{i\beta,f}}{\partial x_\ell}\right).
\end{aligned}
$$

If we recall definitions (4.2b) and (4.2c) for k_f and $D_{i\alpha,f}$, and if we *define* $v_{\alpha,f}$ and $J_{i\alpha,f}$ by (4.3a)–(4.3b), then we have that

$$
(5.14)\qquad \frac{1}{|Q|}\int_{Q_f}\sum_{\beta=g}^{w}(c^0_{i\beta,f}\rho^0_{\beta,f}v^0_{\beta,f}+J^0_{i\beta,f})\,dy=\sum_{\beta=g}^{w}(c^0_{i\beta,f}\rho^0_{\beta,f}v_{\beta,f}+J_{i\beta,f}).
$$

Now (4.3c) follows from (5.11), (5.12), and (5.14).

Finally, we consider the matrix boundary conditions. Clearly, (4.5b) follows from (3.3c), since $(\varepsilon^{-1}-1)(x_3-x^\varepsilon_{c,3})=(1-\varepsilon)y$. As for (4.5c), note that from (3.4a)–(3.4b), and using (5.4b),

$$
\begin{aligned}
&\overline{c}^0_{i\alpha}=c^0_{i\alpha,f},\quad i=1,\cdots,N,\ \alpha=g,o,w, \\
&\overline{Z}^\varepsilon_\alpha\sim\frac{1}{|\partial Q_m|}\int_{\partial Q_m}\left[\psi^{-1}_\alpha(\overline{c}^0_{1\alpha},\cdots,\overline{c}^0_{N\alpha};p^0_{\alpha,f})-x^\varepsilon_{c,3}-\varepsilon y_3\right]d\sigma(y)+\mathcal{O}(\varepsilon).
\end{aligned}
$$

Since $x^\varepsilon_c+\varepsilon y=x$,

$$
\overline{Z}^0_\alpha=\psi^{-1}_\alpha(\overline{c}^0_{1\alpha},\cdots,\overline{c}^0_{N\alpha};p^0_{\alpha,f})-x_3,
$$

and (4.5c) follows from (3.4c) using (5.4a).

This completes our formal derivation of the macroscopic model by homogenization of the microscopic model.

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