MULTIPHASE, MULTICOMPONENT FLUID FLOW IN HOMOGENEOUS AND HETEROGENEOUS POROUS MEDIA*

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ÉCOULEMENT DE FLUIDES MULTICONSTITUANTS POLYPHASIQUES DANS DES MILIEUX POREUX HOMOGÈNES ET HÉTÉROGÈNES

L'écoulement polyphasique de plusieurs constituants à travers un milieu poreux est généralement décrit en introduisant des équations macroscopiques de conservation de la masse sous la forme d'équations de dispersion généralisées. Cette modélisation soulève plusieurs questions qui sont débattues dans cet article en se basant sur des résultats obtenus à partir d'une prise de moyenne volumique, couplée avec une simulation à l'échelle du pore de l'écoulement polyphasique. L'étude est limitée à un système binaire comportant deux phases et nous supposons que les équations de quantité de mouvement peuvent être résolues indépendamment des équations de diffusion/advection. L'hypothèse d'équilibre local est discutée et plusieurs contraintes d'échelles de longueur et de temps sont prises en compte.

Une des questions concerne l'influence sur les tenseurs de dispersion de la condition d'équilibre à l'échelle du pore à l'interface entre les différentes phases. Nos résultats montrent que ces phénomènes peuvent conduire à des variations significatives des coefficients de dispersion en rapport avec la dispersion passive, c'est-à-dire la dispersion sans flux de masse aux interfaces. Des équations macroscopiques sont alors obtenues dans le cas général ainsi que plusieurs équations locales de fermeture permettant de calculer les tenseurs de dispersion et d'autres propriétés à partir des géométries à l'échelle du pore, des vitesses et des caractéristiques des fluides. Des exemples de solutions de ces équations de fermeture sont donnés dans le cas de cellules unitaires représentatives à deux dimensions.

Les équations des écoulements biphasiques sont résolues de deux manières différentes : par une technique par éléments frontières ou une approche par réseau de Boltzmann modifié. Des solutions aux équations de fermeture associées aux équations de dispersion sont ensuite apportées au moyen d'une formulation par volumes finis des équations aux dérivées partielles. Les résultats montrent l'influence de la vitesse et de la saturation sur les paramètres effectifs. Ils mettent en évidence l'importance de la géométrie sur le comportement du tenseur de dispersion.

L'extension de ces résultats à une plus grande échelle incluant l'effet des hétérogénéités est proposée dans un cas limité correspondant à l'écoulement d'une phase, l'autre phase étant à la

saturation résiduelle. Une nouvelle équation de dispersion à grande échelle est obtenue, comportant un tenseur de dispersion à grande échelle que l'on peut déterminer à partir des caractéristiques d'hétérogénéité en passant par un système d'équations de fermeture. Les résultats sont étendus à un problème plus général d'écoulement biphasique, lorsque l'écoulement biphasique à grande échelle peut être supposé quasi statique. Des indications sont données concernant les difficultés associées aux écoulements soumis à des conditions fortement dynamiques et avec une dispersion anormale.

MULTIPHASE, MULTICOMPONENT FLUID FLOW IN HOMOGENEOUS AND HETEROGENEOUS POROUS MEDIA

The flow of several components and several phases through a porous medium is generally described by introducing macroscopic mass-balance equations under the form of generalized dispersion equations. This model raises several questions that are discussed in this paper on the basis of results obtained from the volume averaging method, coupled with pore-scale simulations of the multiphase flow. The study is limited to a binary, two-phase system, and we assume that the momentum equations can be solved independently from the diffusion/advection equations. The assumption of local-equilibrium is discussed and several length-scale and time-scale constraints are provided.

A key issue concerns the impact on the dispersion tensors of the pore-scale equilibrium condition at the interface between the different phases. Our results show that this phenomenon may lead to significant variations of the dispersion coefficients with respect to passive dispersion, i.e., dispersion without interfacial mass fluxes. Macroscopic equations are then obtained in the general case, and several local closure problems are provided that allow one to calculate the dispersion tensors and others properties, from the pore-scale geometry, velocities, and fluid characteristics. Examples of solutions of these closure problems are given in the case of two-dimensional representative unit cells.

The two-phase flow equations are solved in two different ways: a boundary element technique, or a modified lattice Boltzmann approach. Solutions of the closure problems associated with the dispersion equations are then given using a finite volume element formulation of the partial differential equations. The results show the influence of velocity and saturation on the effective parameters. They emphasize the importance of geometry on the behavior of the dispersion tensor.

Extension of these results to a larger-scale including the effect of heterogeneities is proposed in a limited case corresponding to the flow of one phase, the other phase being at residual saturation. A new large-scale dispersion equation is provided, which features a large-scale dispersion tensor that can be determined from the heterogeneity characteristics through a set of closure problems. Results are extended to a more general two-phase flow problem, when the large-scale two-phase flow can be assumed to be quasi-static. Indications are given on the difficulties associated with flow under large-scale dynamic conditions, with abnormal dispersion.

CIRCULACIÓN DE FLUIDOS MULTICOMPONENTES POLIFÁSICOS EN MEDIOS POROSOS HOMOGÉNEOS Y HETEROGÉNEOS

La circulación polifásica de diversos componentes a través de un medio poroso se describe, por lo general, introduciendo ecuaciones macroscópicas de conservación de las masas en forma de ecuaciones de dispersión generalizadas. Esta modelización viene a plantear varios problemas que serán tratados en el presente artículo fundándose para ello en los resultados conseguidos mediante una muestra de promedio volumétrico, acoplada con una simulación a escala del poro de la circulación polifásica. El estudio se limita a un sistema binario que consta de dos fases y se supone que las ecuaciones de cantidad de movimiento se pueden resolver independientemente de las ecuaciones de difusión/advención. Se pone en discusión la hipótesis de equilibrio local y se tienen debidamente en cuenta diversos imperativos de escalas de longitud y de tiempo.

El segundo aspecto del problema se refiere a la influencia sobre los tensores de dispersión de la condición de equilibrio a escala del poro, en el interfaz entre las distintas fases. Nuestros resultados vienen a demostrar que tales fenómenos pueden dar lugar a variaciones significativas de los coeficientes de dispersión en relación con la dispersión pasiva, o sea, la dispersión sin flujos de masa interfaciales. Se obtienen de este modo ecuaciones macroscópicas en el caso general y varias ecuaciones locales de clausura se obtienen a su vez, que permiten calcular los tensores de dispersión y otras propiedades a partir de geometrías a escala del poro, de las velocidades y de las características de los fluidos. Se indican diversos ejemplos de soluciones de estas ecuaciones de clausura en el caso de células unitarias representativas de dos dimensiones.

Las ecuaciones de las circulaciones bifásicas se pueden resolver de dos formas distintas : una técnica, por elementos de fronteras o bien, por un enfoque por red de Boltzmann modificada. Acto seguido, se proporcionan las soluciones para las ecuaciones de clausura asociadas a las ecuaciones de dispersión, por medio de una formulación por volúmenes finitos de las ecuaciones diferenciales con derivadas parciales. Los resultados demuestran la influencia de la velocidad y de la saturación sobre los parámetros efectivos. Tales resultados evidencian la importancia de la geometría sobre el comportamiento del tensor de dispersión.

Se propone así la ampliación de estos resultados a una mayor escala que incluye el efecto de las heterogeneidades en un caso límite que corresponde a la circulación de una fase, mientras que la otra fase se encuentra en saturación residual. Se propone una nueva ecuación de dispersión a gran escala que incluye un tensor de dispersión a gran escala que se puede determinar a partir de las características de heterogeneidad, pasando por un sistema de ecuaciones de clausura. Los resultados se amplían a un problema más general de circulación bifásica, cuando la circulación bifásica a gran escala se puede suponer en estado cuasiestático. Se dan indicaciones relativas a las dificultades asociadas a las circulaciones sometidas a condiciones ampliamente dinámicas y con una dispersión anormal.

INTRODUCTION

The mathematical modeling of multiphase, multi-component flows in porous media represents a very complex task. General formulations have been proposed heuristically, based on the assumption of local equilibrium [1, 2, 3, 4]. A complete theory that, from the pore-scale equations, deduces the macroscopic equations at some Darcy's scale and includes the effect of the heterogeneities in a subsequent large-scale up-scaling, has not yet been fully developed. The present work is restricted to the case of a binary two-phase flow and we derive the problems to be solved following two successive up-scaling procedures. An extension of a previous work [5] in which one of the phases was supposed to be completely immobile is first proposed through the pore-scale to Darcy-scale up-scaling problem. The possibility of a large-scale up-scaling is then investigated.
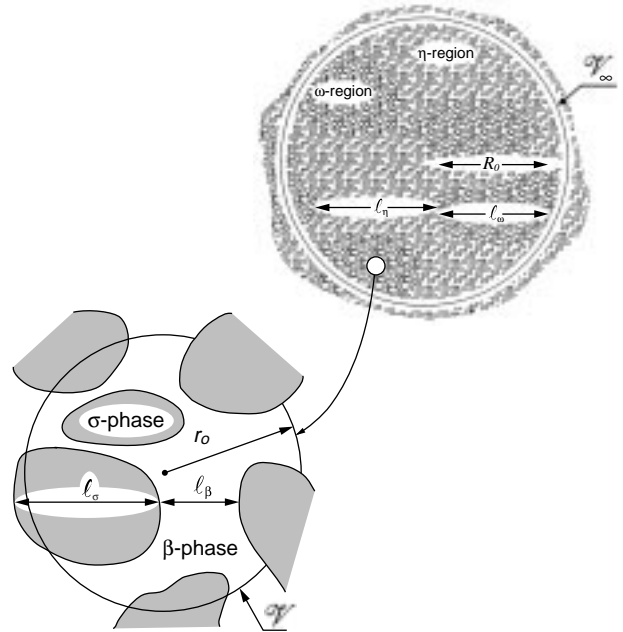
1 DARCY-SCALE PROBLEM

The problem under consideration is illustrated in Figure 1, where we have suggested that the porous medium could be affected by heterogeneities at a larger scale than that leading to the introduction of a Darcy-scale description. Two phases are flowing in the medium and the system involves only two chemical species. We assume further that the properties of neither phase depend upon the concentration. As a consequence, the two-phase flow problem can be de-coupled from the diffusion/advection problem. The two-phase flow problem has already been attacked from many different points of view and we refer the reader to the literature on the subject (see for instance [6, 7, 8, 9]). We simply recall that the theory leading to the classical generalized Darcy's law requires that the pore-scale flow be quasi-static and we will use this assumption below for pore-scale, two-phase flow solutions. First, a theoretical development that starts with the pore-scale diffusion/advection equations to obtain generalized dispersion equations through the use of a volume averaging technique is presented in this section. The dispersion tensors can be obtained from a set of pore-scale "closure" problems and their numerical solutions are provided on a model porous medium, as an example.

Figure 1

Two-phase flow in a porous medium.

1.1 Theory

The theory presented in this section follows previous developments found in the literature [10, 11, 5, 12] and we simply list the major steps below.

We start with the pore-scale equations for a given component and for the β-phase, leading to the following boundary value problem:

$$\frac{\partial c_\beta}{\partial t} + \nabla \cdot (\mathbf{v}_\beta c_\beta) = \nabla \cdot (D \nabla c_\beta) \qquad (1)$$

$$B.C.\ 1 \qquad c_\beta = C_\beta^{eq} \qquad \text{at } A_{\beta\gamma} \qquad (2)$$

$$B.C.\ 2 \qquad \mathbf{n} \cdot D \nabla c_\beta = 0 \qquad \text{at } A_{\beta\sigma} \qquad (3)$$

The boundary condition Equation (2) corresponds to the thermodynamic equilibrium condition. Similar equations exist for the γ-phase, but they are de-coupled as a consequence of Equation (2). Because of the assumptions made, the velocity field in Equation (1) is a known field. The Darcy-scale equation will be obtained by using a volume averaging method. The different averaged values used are given below:

$$\mathbf{V}_\beta = \langle \mathbf{v}_\beta \rangle = \frac{1}{V} \int_{V_\beta} \mathbf{v}_\beta \, \mathrm{d}V = \frac{V_\beta}{V} \langle \mathbf{v}_\beta \rangle^\beta = \varepsilon_\beta \mathbf{U}_\beta \quad (4)$$

$$\langle c_\beta \rangle = \frac{1}{V} \int_{V_\beta} c_\beta \, dV = \frac{V_\beta}{V} \langle c_\beta \rangle^\beta = \varepsilon_\beta \langle c_\beta \rangle^\beta = \varepsilon_\beta C_\beta \quad (5)$$

With these definitions, the total mass balance equation for the β-phase is written as:

$$\frac{\partial \varepsilon_\beta}{\partial t} + \nabla \cdot \mathbf{V}_\beta = - \frac{1}{V} \int_{A_{\beta\gamma}} \mathbf{n} \cdot (\mathbf{v}_\beta - \mathbf{w}_{\beta\gamma}) \, dA \quad (6)$$

where $\mathbf{w}_{\beta\gamma}$ is the velocity of the interface between the β and γ phases. In this equation, the volume fraction ε_β is often replaced by εS_β, where ε is the porosity and S_β is the β-phase saturation. The volume averaging of Equation (1) leads to:

$$\frac{\partial \varepsilon_\beta C_\beta}{\partial t} + \nabla \cdot \langle \mathbf{v}_\beta c_\beta \rangle = \nabla \cdot \langle D \nabla c_\beta \rangle$$
$$- \frac{1}{V} \int_{A_{\beta\gamma}} \mathbf{n} \cdot \left[C_\beta^{eq} (\mathbf{v}_\beta - \mathbf{w}_{\beta\gamma}) - D \nabla c_\beta \right] dA \quad (7)$$

where the integral term on the right hand side of the equation is a direct consequence of the spatial averaging theorems [13].

In order to obtain a closed form of Equation (7), it is convenient to introduce Gray's decomposition of the pore-scale variables [14] given by:

$$c_\beta = C_\beta + \tilde{c}_\beta \quad ; \quad \mathbf{v}_\beta = \mathbf{U}_\beta + \tilde{\mathbf{v}}_\beta \quad (8)$$

Equation (7) after subtraction of Equation (6) becomes:

$$\varepsilon_\beta \frac{\partial C_\beta}{\partial t} + \mathbf{V}_\beta \cdot \nabla C_\beta + \nabla \cdot \langle \tilde{\mathbf{v}}_\beta \tilde{c}_\beta \rangle = \nabla \cdot \langle D \nabla c_\beta \rangle$$
$$+ \left[\frac{1}{V} \int_{A_{\beta\gamma}} \mathbf{n} \cdot (\mathbf{v}_\beta - \mathbf{w}_{\beta\gamma}) \, dA \right] (C_\beta - C_\beta^{eq}) \quad (9)$$
$$+ \frac{1}{V} \int_{A_{\beta\gamma}} \mathbf{n} \cdot \left[D \nabla c_\beta \right] dA$$

In previous developments by Zanotti and Carbonell [11] and Quintard and Whitaker [5], conditions like:

$$\mathbf{n} \cdot \mathbf{v}_\beta = \mathbf{n} \cdot \mathbf{w}_{\beta\gamma} = 0$$

were used at the interface between the two phases. In addition, in [11] saturation gradients were assumed to be zero. The originality of this paper resides in the fact that saturation gradients that were already included in [5] are now expanded to include terms involving the interface velocity, leading to a development that seems more consistent with the multiphase behavior of our system.

In order to get a governing equation for the concentration deviation, we divide Equation (9) by ε_β and subtract the result in equation from Equation (1). We obtain:

$$\frac{\partial \tilde{c}_\beta}{\partial t} + \tilde{\mathbf{v}}_\beta \cdot \nabla C_\beta + \mathbf{v}_\beta \cdot \nabla \tilde{c}_\beta - \varepsilon_\beta^{-1} \nabla \cdot \langle \tilde{\mathbf{v}}_\beta \tilde{c}_\beta \rangle$$
$$= \nabla \cdot \left(D \nabla \tilde{c}_\beta \right) - \varepsilon_\beta^{-1} D \nabla \cdot \left[\frac{1}{V} \int_{A_{\beta\sigma} + A_{\beta\gamma}} \mathbf{n} \tilde{c}_\beta dA \right]$$
$$- \varepsilon_\beta^{-1} \left[\frac{1}{V} \int_{A_{\beta\gamma}} \mathbf{n} \cdot (\mathbf{v}_\beta - \mathbf{w}_{\beta\gamma}) \, dA \right] (C_\beta - C_\beta^{eq}) \quad (10)$$
$$- \varepsilon_\beta^{-1} \frac{1}{V} \int_{A_{\beta\sigma} + A_{\beta\gamma}} \mathbf{n} \cdot \left[D \nabla \tilde{c}_\beta \right] dA$$

In this paper we follow the development proposed in [5] in order to obtain a representation of the concentration deviation in terms of the source terms that appear in Equation (10). We have:

$$\tilde{c}_\beta = \mathbf{b}_\beta \cdot \nabla C_\beta - s_\beta (C_\beta - C_\beta^{eq}) \quad (11)$$

and we choose the mapping quantities, $\mathbf{b}_\beta$ and s_β, in order to obtain a good approximation of the coupled Equations (9) and (10). Following ideas also developed in [5], we obtain:

Problem I

$$\tilde{\mathbf{v}}_\beta + \mathbf{v}_\beta \cdot \nabla \mathbf{b}_\beta = \nabla \cdot (D \nabla \mathbf{b}_\beta) - \varepsilon_\beta^{-1} \mathbf{u}_\beta \quad (12)$$

$$B.C.\ 1 \quad \mathbf{b}_\beta = 0 \quad \text{at } A_{\beta\gamma} \quad (13)$$

$$B.C.\ 2 \quad \mathbf{n} \cdot \nabla \mathbf{b}_\beta + \mathbf{n} = 0 \quad \text{at } A_{\beta\sigma} \quad (14)$$

$$\mathbf{b}_\beta(\mathbf{r} + \mathbf{l}_i) = \mathbf{b}_\beta(\mathbf{r}) \quad (15)$$

$$\langle \mathbf{b}_\beta \rangle = 0 \quad (16)$$

$$\mathbf{u}_\beta = \frac{1}{V} \int_{A_{\beta\sigma} + A_{\beta\gamma}} \mathbf{n} \cdot \left[D \nabla \mathbf{b}_\beta \right] dA - D \nabla \varepsilon_\beta \quad (17)$$

Problem II

$$\mathbf{v}_\beta \cdot \nabla s_\beta = \nabla \cdot (D \nabla s_\beta) - \varepsilon_\beta^{-1} \alpha \qquad (18)$$

$$B.C.\ 1 \qquad s_\beta = 1 \qquad \text{at } A_{\beta\gamma} \qquad (19)$$

$$B.C.\ 2 \qquad \mathbf{n} \cdot \nabla s_\beta = 0 \qquad \text{at } A_{\beta\sigma} \qquad (20)$$

$$s_\beta(\mathbf{r} + \mathbf{l}_i) = s_\beta(\mathbf{r}) \qquad (21)$$

$$\langle s_\beta \rangle = 0 \qquad (22)$$

$$\alpha = \frac{1}{V} \int_{A_{\beta\sigma} + A_{\beta\gamma}} \mathbf{n} \cdot \left[D \nabla s_\beta \right] dA \qquad (23)$$

Equations (15) and (21) correspond to periodicity conditions and here we have classically assumed that the porous medium can be locally described by a pseudo-periodic system.

In the solution of closure problems I and II, we will use results for the two-phase flow closure problems. In fact, in the derivation of generalized Darcy's laws [7, 8, 9], the flow at the closure level, for the determination of the macroscopic flow properties, is assumed to be quasi-static. This basically means that velocity and interfaces are stationary and we will make the same assumption here. In the next section, we explain how these problems can be solved. Once the closure problems I and II have been obtained, the macroscopic equation can be derived by introducing the decomposition, Equation (11), into the averaged equation, Equation (9). This finally leads to the following macroscopic equation:

$$\varepsilon_\beta \frac{\partial C_\beta}{\partial t} + \mathbf{V}_\beta \cdot \nabla C_\beta - \nabla \cdot \left(\mathbf{d}_\beta \left(C_\beta - C_\beta^{eq} \right) \right) - \mathbf{u}_\beta \cdot \nabla C_\beta$$

$$= \nabla \cdot (\mathbf{D}_\beta \cdot \nabla C_\beta) - \alpha \left(C_\beta - C_\beta^{eq} \right) \qquad (24)$$

$$- (C_\beta - C_\beta^{eq}) \left(\frac{\partial \varepsilon_\beta}{\partial t} + \nabla \cdot \mathbf{V}_\beta \right)$$

where some additional convective terms that seem to play a minor role have been discarded [5]. The effective dispersion tensor in Equation (24) is given by:

$$\mathbf{D}_\beta = \varepsilon_\beta D \mathbf{I} + D \frac{1}{V} \int_{A_{\beta\sigma} + A_{\beta\gamma}} \mathbf{n}\, \mathbf{b}_\beta\, dA - \langle \widetilde{\mathbf{v}}_\beta \mathbf{b}_\beta \rangle \qquad (25)$$

while the "velocity-like" coefficient $\mathbf{d}_\beta$ is given by:

$$\mathbf{d}_\beta = - D \frac{1}{V} \int_{A_{\beta\sigma} + A_{\beta\gamma}} \mathbf{n}\, s_\beta\, dA + \langle \widetilde{\mathbf{v}}_\beta s_\beta \rangle \qquad (26)$$

For reasons invoked above, we believe that this form is more consistent than the one proposed in [5]. However, additional terms like $\mathbf{d}_\beta$ and $\mathbf{u}_\beta$ have not been considered so far in the literature. Discarding these terms leads to a more classical form, namely:

$$\frac{\partial \varepsilon_\beta C_\beta}{\partial t} + \nabla \cdot (\mathbf{V}_\beta C_\beta) = \nabla \cdot (\mathbf{D}_\beta \cdot \nabla C_\beta)$$

$$- \alpha \left(C_\beta - C_\beta^{eq} \right) \qquad (27)$$

Close attention to Equation (25) indicates that the dispersion tensor, which directly depends on the $\mathbf{b}_\beta$-field, may be affected by the boundary condition, Equation (13), at the interface between the two phases in the closure problem. If there were no mass flux at the β-γ interface, this boundary condition would be replaced by a boundary condition similar to the one corresponding to *passive* dispersion, i.e.:

$$\mathbf{n} \cdot \nabla \mathbf{b}_\beta + \mathbf{n} = 0 \qquad \text{at } A_{\beta\gamma} \qquad (28)$$

Therefore, it is expected that the values of the passive and active dispersion tensors may be slightly different, which has already been illustrated on a simple configuration in [5].

From a macroscopic point of view, the mass exchange coefficient α quantifies the flux of the species diffusing in the β-phase through the β-γ interface. For instance, in the limit of very large values of α, the macroscopic concentration in the β-phase, C_β, approaches the equilibrium concentration, i.e.:

$$C_\beta \approx C_\beta^{eq} \qquad (29)$$

This situation is referred to as local equilibrium. It is hence of prime interest to be able to determine both $\mathbf{D}_\beta$ and α. This, in fact, is an attractive feature of the theory developed here, since these quantities can be computed directly from the solution of closure problems I and II. The procedure for deriving such a solution is presented below, as are illustrative results on a model porous structure.

Numerical solutions

The procedure to solve these two closure problems starts with a stationary solution of the independent two-phase flow problem. This solution will provide the

required velocity fields and the position of the interface. This will give parameters needed to solve the two closure problems presented in this paper.

1.2 Two-Phase Flow Problem

We have used two different techniques to solve the two phase flow problems.

The first technique corresponds to a boundary integral element method. This method is very appealing if one is interested in computing immiscible two-phase, slow Stokes flows. Due to the reduction of the dimension of the problem, from 2 to 1 here, the method allows one precisely to locate and to describe the interface separating the two phases and does not require any computation of a linear system solution for in-field calculations [15]. This method has been successfully applied in a similar configuration [16] and was used here on the cell depicted in Figure 2. The stationary solution on this cell, obtained from an initial guess and an iterative procedure, depends on four parameters: the porosity, ε, the β-phase saturation, S_β, the aqueous to non-aqueous viscosity ratio, μ, and the capillary number, Ca. In the following, we illustrate our results with data obtained with:

$$\varepsilon = 0.7 \quad ; \quad \mu = 1 \quad ; \quad Ca = 1$$

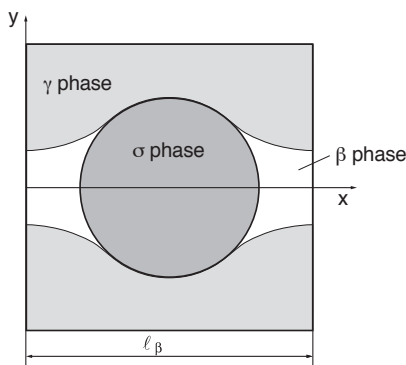and S_β ranging from 0.2 to 0.8.

Figure 2

Pore-scale unit cell.

The second technique is a new lattice Boltzmann formulation. The system is characterized by a coarse-grained, conserved order parameter that takes characteristic values in the bulk phases and varies continuously in a narrow interfacial region. The relaxation of the order parameter field is driven by local minimization of the free energy. This results in a "Cahn-Hilliard" type equation for the evolution of the order parameter field, with the driving force being the gradient of the chemical potential. The fluid velocity satisfies a modified Navier-Stokes equation that includes an explicit coupling term to the order parameter. This coupling term gives rise to capillary forces. From a numerical point of view, the governing equations are applicable throughout the entire domain, avoiding the need for iterative solution for the location of the moving interface, which is necessary in classical formulations. In three-dimensions and for complex geometries, direct numerical integration of the multiphase equations is generally infeasible. These equations are solved numerically using a lattice Boltzmann technique. Sets of distribution functions representing the mean populations of the particles on a lattice and the order parameter, are allowed to relax to equilibrium according to a Boltzmann equation which is discrete in both space and time. The collision operator is approximated by a single time relaxation form. The equilibrium distribution functions are chosen so that the appropriate dynamic equations are recovered in the limit. The local nature of the formulation makes it highly amenable to massively parallel processing. These advantages make possible the study of multiphase flows in irregular three-dimensional geometries.

An example of the velocity field obtained for the unit cell in Figure 2 is shown in Figure 3.
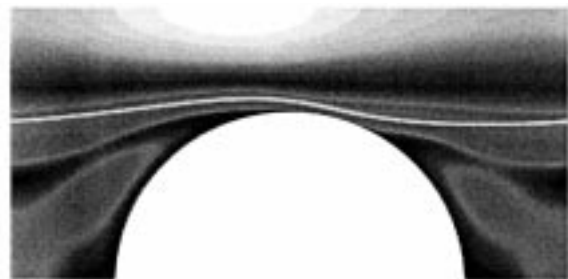

Figure 3

Velocity field, v_β, for $\varepsilon_\beta = 0.45$.

1.3 Dispersion Problem

The closure problems presented in this section are solved by following numerical procedures that are described in [5, 17, 18, 12]. Solutions have been

obtained for the two-phase flow calculations presented above. Results for different saturations are given in Figures 4, 5 and 6.
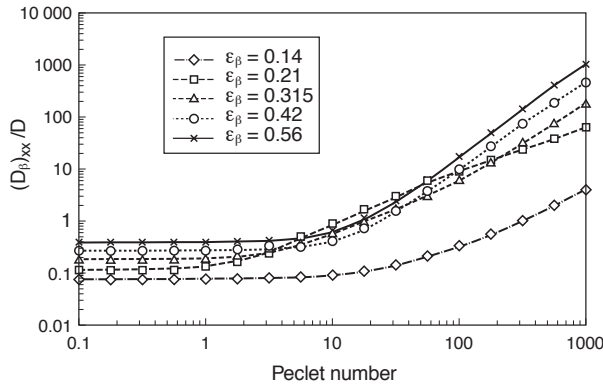

Figure 4

Longitudinal dispersion coefficient versus the unit cell Peclet number and for various saturations.
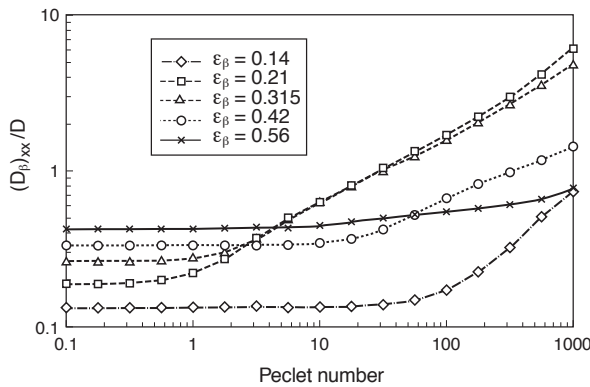

Figure 5

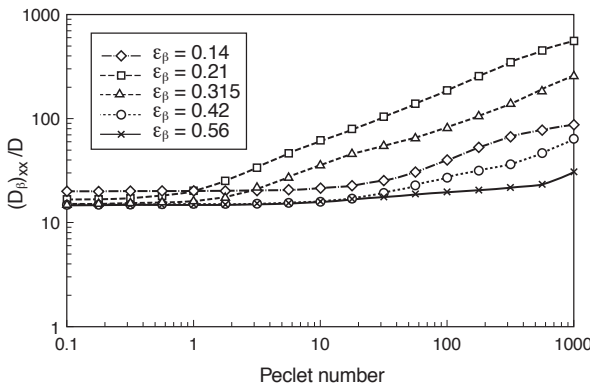Transversal dispersion coefficient versus the unit cell Peclet number and for various saturations.

Figure 6

Mass exchange coefficient versus the unit cell Peclet number and for various saturations.

These results are useful to understand the complex relationship between the effective properties and the averaged velocity and saturation.

2 LARGE-SCALE PROBLEM

In this section, we are interested in the flow over a heterogeneous porous medium similar to the one represented in Figure 7. In a first attempt to deal with this problem within the framework of the volume averaging method, we assume that the exchange term associated with the flux between the two-phases has negligible effect on the concentration field. We also assume, at first, that the γ-phase is at residual saturation and we will extend results obtained in this limit to a more general situation afterwards.
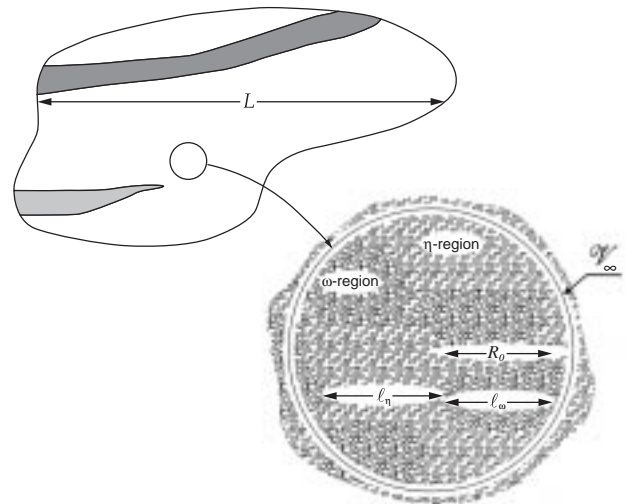

Figure 7

Two-region model of a heterogeneous porous medium.

We start with the following Darcy-scale dispersion equation for the β-phase:

$$\frac{\partial \varepsilon_\beta C_\beta}{\partial t} + \nabla \cdot (\mathbf{V}_\beta C_\beta) = \nabla \cdot (\mathbf{D}_\beta \cdot \nabla C_\beta) \qquad (30)$$

where C_β is the intrinsic averaged concentration and $\mathbf{V}_\beta$ is the filtration velocity. The velocity field will be affected by the heterogeneities in the system, but it can be determined independently from the dispersion problem. The dispersion tensor is thus position-dependent, i.e., the function expressing the dependence with the velocity depends on the position. Large-scale

averages are defined over a large-scale averaging volume V_∞ as:

$$\{C_\beta\} = \frac{1}{V_\infty} \int_{V_\infty} C_\beta \, dV \qquad (31)$$

Taking the large-scale average of Equation (30) leads to:

$$\frac{\partial (\{\varepsilon_\beta\} \{C_\beta\})}{\partial t} + \nabla \cdot (\{\mathbf{V}_\beta\} \{C_\beta\}) + \nabla \cdot \{\widetilde{\mathbf{V}}_\beta \widetilde{C}_\beta\}$$

$$= \nabla \cdot (\{\mathbf{D}_\beta\} \cdot \nabla \{C_\beta\} + \{\mathbf{D}_\beta \cdot \nabla \widetilde{C}_\beta\}) \qquad (32)$$

where we have introduced the following large-scale decompositions:

$$C_\beta = \{C_\beta\} + \widetilde{C}_\beta \quad ; \quad \mathbf{V}_\beta = \{\mathbf{V}_\beta\} + \widetilde{\mathbf{V}}_\beta \qquad (33)$$

The Darcy-scale equation for the concentration deviation is obtained by subtracting Equation (32) from Equation (30), which yields:

$$\frac{\partial (\varepsilon_\beta C_\beta - \{\varepsilon_\beta\} \{C_\beta\})}{\partial t} + \nabla \cdot (\mathbf{V}_\beta \widetilde{C}_\beta)$$

$$+ \nabla \cdot (\widetilde{\mathbf{V}}_\beta \{C_\beta\}) - \nabla \cdot \{\widetilde{\mathbf{V}}_\beta \widetilde{C}_\beta\}$$

$$= \nabla \cdot (\mathbf{D}_\beta \cdot \nabla \widetilde{C}_\beta) + \nabla \cdot (\widetilde{\mathbf{D}}_\beta \cdot \nabla \{C_\beta\})$$

$$- \nabla \cdot (\{\mathbf{D}_\beta \cdot \nabla \widetilde{C}_\beta\}) \qquad (34)$$

where we have adopted the notation:

$$\widetilde{\mathbf{D}}_\beta = \mathbf{D}_\beta - \{\mathbf{D}_\beta\} \qquad (35)$$

Equations (32) and (34) have to be solved simultaneously in order to provide a complete solution of the problem, which is a tremendous task, in general. However, assuming that the different length-scale and time-scale associated with the Darcy-scale and the large-scale problems are conveniently separated, the time derivative in Equation (34) can be discarded, as can terms corresponding to derivatives of large-scale averages such as $\nabla \cdot (\{\mathbf{D}_\beta \cdot \nabla \widetilde{C}_\beta\})$ and $\nabla \cdot \{\widetilde{\mathbf{V}}_\beta \widetilde{C}_\beta\}$.

Taking this into account, Equation (34) becomes:

$$\nabla \cdot (\mathbf{V}_\beta \widetilde{C}_\beta) + \nabla \cdot (\widetilde{\mathbf{V}}_\beta \{C_\beta\})$$

$$= \nabla \cdot (\mathbf{D}_\beta \cdot \nabla \widetilde{C}_\beta) + \nabla \cdot (\widetilde{\mathbf{D}}_\beta \cdot \nabla \{C_\beta\}) \qquad (36)$$

and a representation of the concentration deviation can be written as:

$$\widetilde{C}_\beta = \mathbf{b}_\beta^* \cdot \nabla \{C_\beta\} + ... \qquad (37)$$

where the dots are a reminder that second order terms have been neglected. In this equation the mapping vector $\mathbf{b}_\beta^*$ has to be chosen so as to cancel all first order terms with respect to $\nabla \{C_\beta\}$ in Equation (36). Therefore, it must obey the following "closure" problem.

Large-Scale Closure Problem

$$\mathbf{V}_\beta \cdot \nabla \mathbf{b}_\beta^* + \widetilde{\mathbf{V}}_\beta = \nabla \cdot (\mathbf{D}_\beta \cdot \nabla \mathbf{b}_\beta^*) + \nabla \cdot \widetilde{\mathbf{D}}_\beta \qquad (38)$$

$$\mathbf{b}_\beta^*(\mathbf{r} + \mathbf{l}_i) = \mathbf{b}_\beta^*(\mathbf{r}) \qquad (39)$$

$$\{\mathbf{b}_\beta^*\} = 0 \qquad (40)$$

where we have used the fact that the velocity field is divergence free. In these equations, two source terms will generate large-scale dispersion effects. The first one is associated with the velocity fluctuations, while the other is associated with the variations of the dispersion tensor. The last equation, Equation (40), corresponds to the fact that the average of the deviation is zero, while Equation (39) assumes that the medium can be described locally by a periodic system. This last assumption has been discussed thoroughly in the literature and has been proved to be useful even for disordered systems (see [19] for an illustration). Introducing the decomposition in Equation (32) leads to the following large-scale dispersion equation:

$$\frac{\partial (\{\varepsilon_\beta\} \{C_\beta\})}{\partial t} + \nabla \cdot (\{\mathbf{V}_\beta\} \{C_\beta\}) = \nabla \cdot (\mathbf{D}_\beta^* \cdot \nabla \{C_\beta\}) \qquad (41)$$

in which the large-scale dispersion tensor is given by:

$$\mathbf{D}_\beta^* = \{\mathbf{D}_\beta\} + \{\mathbf{D}_\beta \cdot \nabla \mathbf{b}_\beta^*\} - \{\widetilde{\mathbf{V}}_\beta \mathbf{b}_\beta^*\} \qquad (42)$$

2.1 Extension to Quasi-Static Two-Phase Flow

The problem of two-phase flow in heterogeneous media has received a great deal of attention in the literature, especially from the point of view of "homogenization" techniques [20, 21, 22, 23]. We start with the generalized Darcy's law, i.e.:

$$\frac{\partial \varepsilon_\alpha}{\partial t} + \nabla \cdot \mathbf{V}_\alpha = 0 \qquad \alpha = \beta, \gamma \qquad (43)$$

$$\mathbf{V}_\alpha = -\frac{\mathbf{K}_\alpha}{\mu_\alpha} \cdot \left(\nabla P_\alpha - \rho_\alpha \mathbf{g}\right) \qquad \alpha = \beta, \gamma \qquad (44)$$

$$P_\gamma - P_\beta = p_c\left(S_\beta\right) \qquad (45)$$

Large-scale averages are defined in Equation (31) The process of averaging the Darcy-scale equations leads, in general, to a very complicated problem, with time-dependent, non-local and dynamic properties. An illustrative example of such a treatment can be found in [23]. However, it has been pointed out in several works [21] and [22] that, for sufficiently large capillary effects, a simple closure problem can be proposed that leads to large-scale equations having the same form as the Darcy-scale equation. In this case, local variations of the saturation are small enough to be discarded in the closure problem, i.e., in Darcy-scale equations, while, of course, they remain in the large-scale averaged equations. We do not list here all the equations pertaining to this quasi-static theory that can be found in [23] since it is beyond the scope of this paper to discuss the domain of validity of such an assumption. However, it has been recognized [24] that the results can be applied in many practical instances to systems exhibiting large spatial and temporal gradients. Within the quasi-static theory, the local-scale closure problem specifies the saturation field over the representative unit cell as:

$$\varepsilon_\beta = p_c^{-1}(P_c^*) \qquad (46)$$

where P_c^* is the large-scale capillary pressure. This in turn specifies the multiphase permeabilities $\mathbf{K}_\alpha$. The large-scale pressure deviations can be expressed as:

$$\widetilde{P}_\alpha = P_\alpha - \{P_\alpha\} = \mathbf{f}_\alpha \cdot \left(\nabla \{P_\alpha\} - \rho_\alpha \mathbf{g}\right) \qquad (47)$$

where $\mathbf{f}_\alpha$ is specified by the following closure problem.

$$\nabla \cdot \left(\mathbf{K}_\alpha \cdot \nabla \mathbf{f}_\alpha\right) + \nabla \cdot \mathbf{K}_\alpha = 0 \qquad (48)$$

along with conditions similar to Equations (39) and (40). Finally, the resulting large-scale equations take the following form:

$$\frac{\partial \{\varepsilon_\alpha\}}{\partial t} + \nabla \cdot \{\mathbf{V}_\alpha\} = 0 \qquad (49)$$

$$\{\mathbf{V}_\alpha\} = -\frac{\mathbf{K}_\alpha^*}{\mu_\alpha} \cdot \left(\nabla \{P_\alpha\} - \rho_\alpha \mathbf{g}\right) \qquad (50)$$

where the large-scale multiphase permeability tensors are expressed as:

$$\mathbf{K}_\alpha^* = \{\mathbf{K}_\alpha\} + \{\mathbf{K}_\alpha \cdot \nabla \mathbf{f}_\alpha\} \qquad (51)$$

The average of Equation (46) can be used to build a large-scale capillary pressure relationship. With that in hand, along with Equations (44) and (47) one can obtain for a given large-scale capillary pressure and large-scale pressure gradient an estimate of the two velocity fields, $\mathbf{V}_\beta$ and $\mathbf{V}_\gamma$, which can be used to solve the dispersion problem.

If one could recover the concentration deviation equation, Equation (34), one would be faced with two different problems for $\widetilde{C}_\beta$ and $\widetilde{C}_\gamma$ similar to the one solved for the case where the γ-phase is at residual saturation. This is only possible if time-derivatives and large-scale gradients can be discarded in Equation (34). Since these assumptions have been used when introducing the quasi-static theory for the multiphase flow problem, it seems consistent to use these assumptions in order to get a simplified equation for the concentration deviation. Once again, we remind the reader that these assumptions are only used at the closure level, and that this does not mean that the flow is steady, nor that it has zero large-scale gradients. With these assumptions, Equations for $\widetilde{C}_\beta$ and $\widetilde{C}_\gamma$ can be solved independently. Each solution is similar to the development leading to Equations (36) to (42).

2.2 Numerical Solution and Examples

In this section we explain how these different closure problems can be solved in order to build dispersion tensor relationships as a function of the saturations and velocities for a given porous medium geometry.

Geometry is rendered discrete by using blocks on a cartesian grid. For the two-phase flow calculations, we used a numerical model discussed in [21]. For the closure problem associated with dispersion, the PDEs are solved by using approximations that are discussed in detail in [5] and [19]. The overall algorithm follows the steps described below:

– Choose of a large-scale capillary pressure;
– Solve for Equation (46);

– Calculate of the large-scale saturation;

– Solve for the closure problems, Equation (48);

– Calculate of the multiphase permeabilities, Equation (51);

– Choose of the large-scale pressure gradients;

– Calculate of the Darcy-scale closure velocity fields, by using Equations (47) and (44);

– Solve for the dispersion closure problems that are similar to Equations (38) through (40);

– Calculate of the multiphase dispersion tensors, Equation (42).

This process can be repeated to build a complete mapping of the multiphase permeabilities, large-scale capillary pressure, and multiphase dispersion tensors with respect to saturation and large-scale pressure gradients. This latter relationship can be replaced by a dependence on the velocities.

Steps 1 through 5 in the above procedure have been described in [21] and [19]. Results obtained for the unit cell shown in Figure 8 are presented in Figures 9, 10 and 11. Steps 6 and 7 do not pose any problem, and solutions are readily obtained. A solution of the closure problem for $\mathbf{b}_\beta^*$ (Step 8) is shown in Figure 12. Values of the large-scale dispersion coefficients for the β-phase are shown in Figures 13 and 14. For a given large-scale saturation, the plots show the expected dependence upon the large-scale Peclet number defined as:

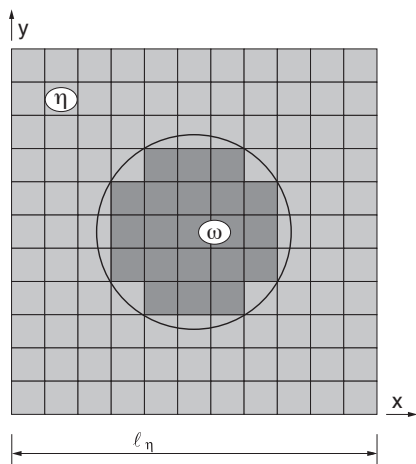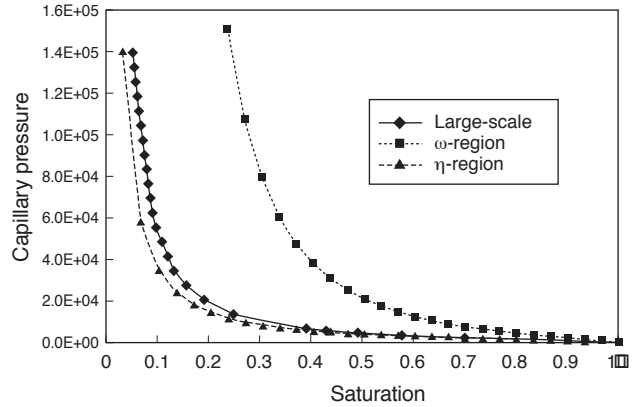$$Pe_\beta^{LS} = \frac{\{\mathbf{V}_\alpha\}\, l_\eta}{D_{ref}} \qquad (52)$$

Figure 9

Darcy-scale and large-scale capillary pressure curve.
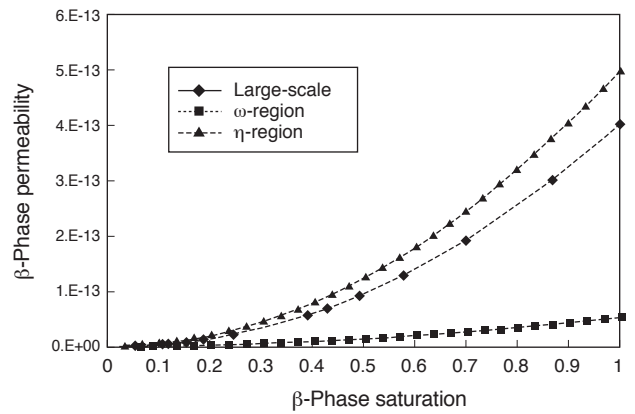
Figure 10

β-phase permeabilities.

Figure 8

Unit cell and representation of a coarse grid discretization.
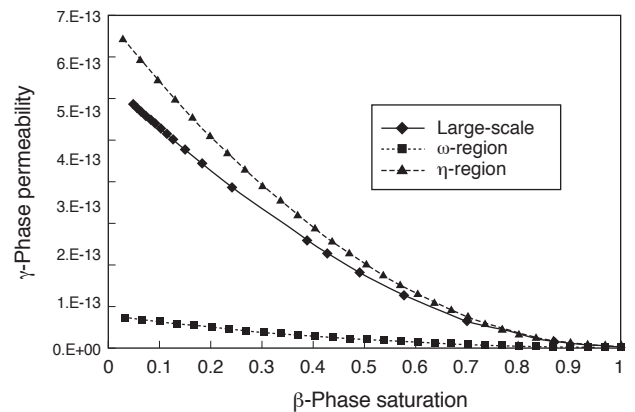

Figure 11

γ-phase permeabilities.
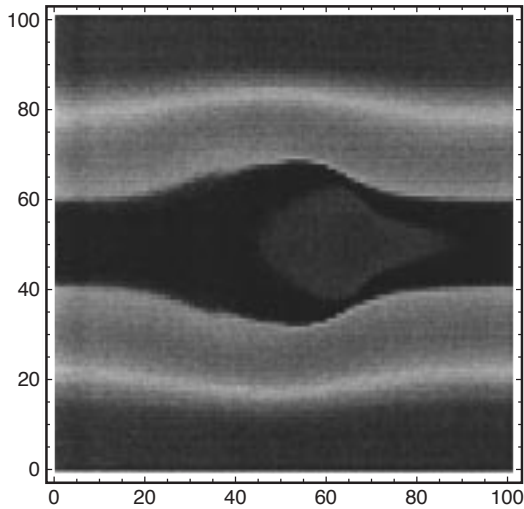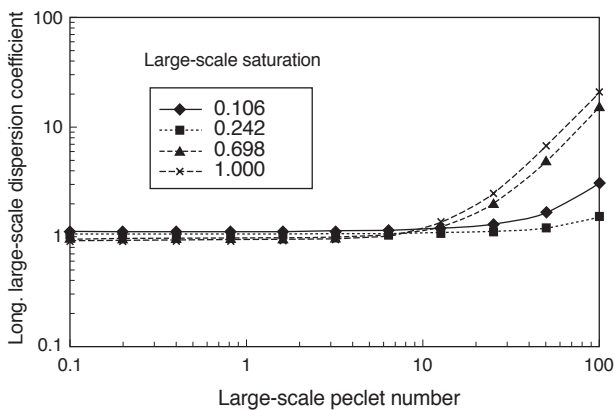
Figure 12

Field $(b_\beta^*)_x$.

Figure 13

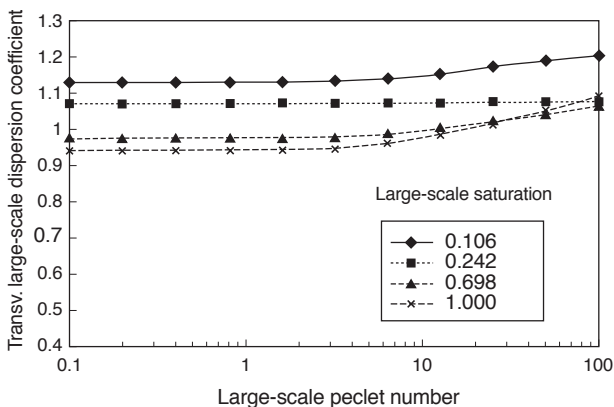Longitudinal β-phase large-scale dispersion coefficient.

Figure 14

Transversal β-phase large-scale dispersion coefficient.

However, the dependence on both the large-scale saturation and the Peclet number is quite complicated. For instance, the dispersion coefficient increases with saturation at low Peclet numbers, and behaves in an opposite way at large Peclet numbers. This is due to a complex influence of the large-scale saturation on the Darcy-scale values. Similar results can be obtained for the γ-phase, but it is beyond the scope of this paper to present a complete analysis of many cases. The emphasis is rather on the methodology and the tools that have been designed to deal with such problems.

CONCLUSION

In this paper, a complete up-scaling theory of a binary, two-phase flow in heterogeneous media has been proposed. Several assumptions have been made that allowed us to introduce a large-scale dispersion theory.

Among these assumptions, the most important ones are associated with the fact that large temporal and spatial gradient effects have been discarded, thus suppressing large-scale dynamic, non-local, anomalous behavior. In addition, the large-scale problem did not incorporate all the features of a multicomponent system.

If these constraints were removed, one would have to overcome difficulties associated with the treatment of equilibrium conditions. If the model assumes that local equilibrium does not exist at Darcy's scale, the expected large-scale behavior would be very complicated, with possible history effects. If the Darcy's scale model assumes local equilibrium, this does not mean that, due to large spatial gradients, the resulting large-scale model will feature partitioning equations corresponding to the equations valid at Darcy's scale. There is obviously a need for further theoretical development within the perspective of up-scaling theories described in this paper.

Even with the simplifying assumptions made here, the large-scale dispersion coefficients exhibit very complex behavior with respect to the large-scale saturation, and the large-scale Peclet number. Tools proposed in this paper can be used to quantify all the aspects of this complex physical phenomenon.

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