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Continuum Modelling of Contaminant Transport in Fractured Porous Media

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Abstract. This work is aimed towards deriving macroscopic models that describe pollutant migration through fractured porous media. A homogenisation method is used, that is, macroscopic models are deduced from the physical description over a representative elementary volume (REV), which consists of an open fracture surrounded by a porous matrix block. No specific geometry is at issue. The fractured porous medium is saturated by an incompressible fluid. At the REV's scale, the transport is assumed to be advective-diffusive in the porous matrix and due to convection and molecular diffusion in the fracture's domain. It is also assumed that there is no diffusion in the solid. We demonstrate that the macroscopic behaviour is described by a single-continuum model. Fluid flow is described by Darcy's law. Four macroscopic single-continuum models are obtained for the contaminant transport: a diffusive model, an advective-diffusive model and two advective-dispersive models. One of the two advective-dispersive models accounts for the advection process in the porous matrix. The domains of validity of these models are defined by means of the orders of magnitude of the local Péclet numbers in the porous matrix block and in the fracture's domain.

Key words: contaminant transport, fractured porous media, dual-porosity, continuum modelling, homogenisation.

1. Introduction

The focus of the present study is on the fundamentals of contaminant transport in fractured porous media. Such formations are composed of an interconnected network of fractures and blocks of porous medium. The practical applications are important as many natural formations are fractured, and accurate models are required for predicting the fate of pollutants in aquifers contaminated by industrial, agricultural and radioactive waste.

In the study of contaminant transport in fractured porous media, the bulk of the research effort has been devoted to the transport in discrete fracture network models. Some of this literature has been reviewed in Sahimi (1995) and Bear *et al.* (1993). These studies have proven to be useful for understanding transport

phenomena and discrete models are required when the continuum approach to the description of the transport problem is not applicable. However, the applicability of discrete models remains quite limited to field problems as they require the determination of the precise characteristics of the fracture network in its complete detail. Thus, in many practical field problems it is worth using continuum models when the conditions necessary to adopt this approach are met.

In the continuum approach, the transport problem is transformed from the microscopic level to a macroscopic scale at which the problem is expressed in terms of averages of the microscopic quantities. The need to know the exact local characteristics of the whole domain is circumvented by the use of these average quantities. The averages are taken over a representative elementary volume (REV). The size of this REV must be larger than the heterogeneity size and much smaller than the macroscopic length-scale. It follows that the continuum approach is applicable to a fractured porous medium provided that an REV can be determined. Two kinds of continuum approaches may be distinguished: (i) phenomenological approaches with which the form of the macroscopic model is postulated on the basis of physical considerations and experimental results; (ii) upscaling methods with which the macroscopic model is rigorously derived by starting with the physical behaviour at the REV's scale. Despite the applications, very few studies exist on continuum modelling of contaminant transport in fractured porous media. A comprehensive review of studies based on the use of continuum phenomenological models can be found in Berkowitz *et al.* (1988). Two kinds of continuous models have been used: the double-continuum models and the single-continuum models. In the double-continuum models, the fractured porous medium is represented as two distinct and interacting continua, one consisting of the network of fractures and the other of the porous blocks. The interaction between both continua is formulated by an exchange function. This concept was originally proposed by Barenblatt and Zheltov (1960) for describing fluid flow in a fractured porous medium. For transport of contaminants, double-continuum models have been employed in Bibby (1981) and Huyakorn *et al.* (1983). In the single-continuum approach, the whole fractured porous domain is represented as an equivalent porous medium. Berkowitz *et al.* (1988) underlined that in many cases a single conceptualization may be sufficient, but no firm evidence exists whether one or the other approach should be used.

In this study, we demonstrate that when considering, at the REV's scale, the flow of an incompressible fluid and the transport by advection and diffusion in the porous matrix with no diffusion in the solid, and by convection and molecular diffusion in the fracture's domain, the macroscopic model is a single-continuum model. We apply the homogenisation theory which is a rigorous method of upscaling by multiple scales expansions. No specific geometry is at issue, the work is aimed towards deriving the most general models. The REV consists of an open fracture surrounded by a porous matrix block.

After introducing the method, we analyse the local description and define the ranges of dimensionless parameters. The order-of-magnitude analysis of these

parameters leads to the determination of four distinct cases which are defined by means of the orders of magnitude of the local Péclet numbers, Pe_f and Pe_m , in the fracture's domain and in the porous matrix, respectively. Then we employ the homogenisation method systematically. The fluid flow is first analysed and leads to Darcy's law. Four macroscopic single-continuum transport models are finally obtained: a diffusive model, an advective-diffusive model and two advective-dispersive models. One of the two advective-dispersive models accounts for the advection process in the porous matrix.

2. An Introduction to Homogenisation

2.1. CONCEPT OF HOMOGENISABILITY

Modelling physical processes in heterogeneous media such as transport in porous media turns out to be a difficult task, as the complete description and solution at the microscopic level of the physical phenomenon being considered is impossible. Nonetheless, the internal disorder may allow continuum modelling, that is, the derivation of a large-scale continuous description. In other words, a physical process evolving in a heterogeneous medium can, under specific conditions, be macroscopically described by means of equations with transfer coefficients that are independent of the macroscopic boundary conditions. The essence of homogenisation techniques is to derive such equivalent macroscopic continuous behaviours by upscaling the so-called 'local description', that is, the physical description at the heterogeneity scale.

Homogenisation is possible if the density of heterogeneities is sufficiently high. For a material with a random structure, this intuitive condition entails the existence of a REV, which is large compared to the heterogeneity size and small compared to the macroscopic size. Thus, the fundamental assumption behind homogenisation is the separation of scales, which can be expressed as follows:

$$l \ll L,$$

where l is the characteristic size of the REV and L is the characteristic macroscopic length. Note that, even if not always explicitly stated, this fundamental assumption of separation of scales is common to all continuum approaches including all homogenisation techniques. The concept of homogenisability is, therefore, linked to the notion of separation of scales. Non-homogenisable situations can occur as the condition of separation of scales is not always satisfied. But in these situations, the physical phenomenon cannot be described by means of a macroscopic equivalent continuum model.

2.2. HOMOGENISATION FOR PERIODIC STRUCTURES

In the present study, we use the method of homogenisation for periodic structures – also called method of multiple scales – that has been introduced by Bensoussan

et al. (1978) and Sanchez-Palencia (1980). The method of multiple scales is based on two assumptions: (i) the separation of scales; (ii) the periodicity.

As alluded to above, the fundamental assumption is the separation of scales. The key parameter of this method is the length-scale ratio

$$\varepsilon = \frac{l}{L} \ll 1, \quad (2.1)$$

in which l is the microscopic characteristic length and L is the macroscopic characteristic length.

The medium is also assumed to be periodic and the period, Ω , is $O(l)$. As natural media are never periodic, it raises the question whether this assumption is a strong restriction or not. The condition of periodicity with the multiple scale method is actually the counterpart of the condition of local stationarity with statistic methods. The advantage of the multiple scale method is that, thanks to the condition of periodicity, no preliminary assumption on the form of the macroscopic equations is required. The macroscopic model results only from the physics being chosen at the local scale. Note that for a periodic medium, the REV is fully determined as it is merely the period. This method is thus a powerful tool for rigorously deriving the macroscopic behaviour of the problem being considered by starting with the detailed micro-scale physical description.

2.3. METHODOLOGY

2.3.1. Introduction

In this study, we use the approach suggested in Auriault (1991), with which the problem is tackled in a physical manner. Indeed, it offers the additional benefit that homogenisability conditions are explicitly stated. Thus, besides the macroscopic model, its domain of validity is also provided. The methodology is based on the use of the dimensionless numbers that arise from the local description. The domain of validity of the derived macroscopic model is given by means of orders of magnitude of the local dimensionless numbers.

2.3.2. Separation of Space Variables

Using the two characteristic lengths, l and L , two dimensionless space variables are defined

$$\vec{y} = \frac{\vec{X}}{l}, \quad (2.2)$$

$$\vec{x} = \frac{\vec{X}}{L}, \quad (2.3)$$

where \vec{X} is the physical space variable. If the condition of separation of scales is satisfied ($\varepsilon \ll 1$), then \vec{y} and \vec{x} appear as two independent space variables:

\vec{y} is the microscopic space variable and describes the local scale; whereas \vec{x} is the macroscopic variable. As a consequence, the unknown field quantities being considered (e.g. pressure, velocity, concentration, ...) are, a priori, functions of both space variables \vec{y} and \vec{x} . Furthermore, invoking the differentiation rule of multiple variables, the gradient operator with respect to the physical space variable, $\vec{\nabla}_X$, is written as

$$\vec{\nabla}_X = \frac{1}{l} \vec{\nabla}_y + \frac{1}{L} \vec{\nabla}_x, \quad (2.4)$$

where $\vec{\nabla}_y$ and $\vec{\nabla}_x$ are the gradient operators with respect to \vec{y} and \vec{x} , respectively.

2.3.3. Normalisation

The purpose of normalisation is to express the local description in a dimensionless form and then to analyse the orders of magnitude of the dimensionless parameters that arise from this new writing. The dimensionless writing is obtained by defining a dimensionless counterpart for all physical variables as follows:

$$\phi = \frac{\Phi}{\Phi_c},$$

in which Φ is a given physical variable, ϕ is its dimensionless counterpart and Φ_c is a characteristic value of Φ .

The dimensionless writing of the equations requires the choice of a reference length. Let us arbitrarily choose L as the reference length. Thus, according to (2.4), the corresponding dimensionless operator gradient, $\vec{\nabla}$, is given by

$$\vec{\nabla} = L \vec{\nabla}_X = \varepsilon^{-1} \vec{\nabla}_y + \vec{\nabla}_x. \quad (2.5)$$

For a transient process a reference time is also required.

The approach consists in estimating all dimensionless numbers with respect to the small parameter ε . A dimensionless number Q is said to be order of ε^q when

$$\varepsilon^{q+1} \ll Q \ll \varepsilon^{q-1}. \quad (2.6)$$

2.3.4. Derivation of the Macroscopic Description

The homogenisation method of multiple scales is based on the fundamental statement that if the scales are well separated ($\varepsilon \ll 1$), then all physical variables can be looked for in the form of asymptotic expansions in powers of ε

$$\phi(\vec{y}, \vec{x}) = \phi^0(\vec{y}, \vec{x}) + \varepsilon \phi^1(\vec{y}, \vec{x}) + \varepsilon^2 \phi^2(\vec{y}, \vec{x}) + \dots, \quad (2.7)$$

in which functions ϕ^i are \vec{y} -periodic and dimensionless.

The method consists in incorporating these asymptotic expansions in the dimensionless local description. This leads to approximate governing equations and

boundary-conditions at the successive orders, which together with the condition of periodicity define boundary-value problems in the periodic cell. Once solved, their average over the period yields the macroscopic behaviour.

The purpose of the present work is to apply this method for deriving the models for contaminant transport in fractured porous media.

3. Contaminant Transport in Fractured Porous Media: Local-Scale Analysis

3.1. MEDIUM DESCRIPTION

The system considered in this study is a macroscopic volume of a densely fractured porous medium whose characteristic size is L and in which we investigate the transport of a contaminant. The medium is periodic, of period Ω , and has a scale length l which is small compared to L

$$\varepsilon = \frac{l}{L} \ll 1. \quad (3.1)$$

Within the periodic cell Ω , which is sketched on Figure 1, we denote by Ω_f the fracture's domain, by Ω_m the porous matrix domain and by Γ their common boundary. \vec{X} represents the physical space variable of the medium. We consider the dimensionless variables \vec{y} and \vec{x} defined by Equations (2.2) and (2.3). The separation of scales (3.1) implies that \vec{y} and \vec{x} are two separated space variables, that is, that both variables are necessary for describing the medium. As a consequence, the unknown field quantities are functions of both space variables and the gradient operator with respect to \vec{X} takes the form (2.4).

3.2. LOCAL BEHAVIOUR

3.2.1. In the Fractures (Ω_f)

The fracture's domain is saturated by water and the presence of a solute in water gives rise to convection and molecular diffusion. The fluid is assumed to be Newtonian and incompressible. We further assume that the flow is slow. Fluid flow in Ω_f is, therefore, described by Stokes equation

$$\mu \Delta_X \vec{V}_f - \vec{\nabla}_X P_f = \vec{0}, \quad (3.2)$$

where μ represents the viscosity, while Δ_X and $\vec{\nabla}_X$ are the Laplacian and the gradient operators with respect to the physical variable, \vec{X} , respectively. Symbols \vec{V}_f and P_f represent the fluid velocity and the fluid pressure, respectively.

For an incompressible fluid, the mass-balance equation is written as

$$\vec{\nabla}_X \cdot \vec{V}_f = 0. \quad (3.3)$$

The migration of the solute diluted in the liquid is described by the convection-diffusion equation

$$\frac{\partial C_f}{\partial \tau} - \vec{\nabla}_X \cdot (\tilde{d}_f \vec{\nabla}_X C_f - C_f \vec{V}_f) = 0, \quad (3.4)$$

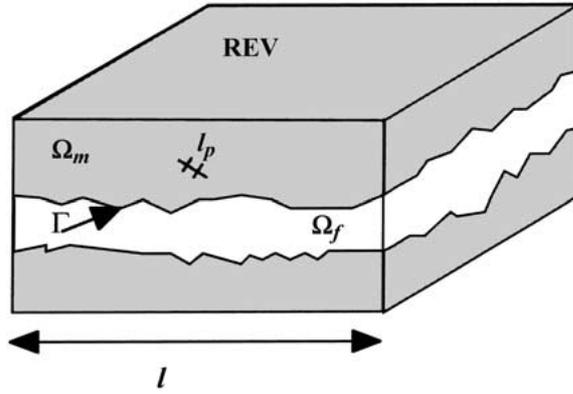


Figure 1. Periodic cell of the fractured porous medium.

in which τ represents the time, while C_f is the solute concentration in the fractures and \tilde{d}_f is the tensor of molecular diffusion.

3.2.2. In the Porous Matrix (Ω_m)

Fluid flow in the porous matrix is described by Darcy's law

$$\vec{V}_m = -\tilde{\kappa}_m \vec{\nabla}_X P_m, \quad (3.5)$$

where $\tilde{\kappa}_m$ is the permeability tensor of the porous matrix, \vec{V}_m and P_m represent the fluid velocity and the fluid pressure in the porous matrix, respectively.

The mass-balance equation is written as

$$\vec{\nabla}_X \cdot \vec{V}_m = 0. \quad (3.6)$$

The presence of the solute in the liquid gives rise to diffusion and convection in the micropores. We assume that there is no diffusion within the solid skeleton. Solute transport at the porous matrix scale is described by the advection-diffusion equation

$$\phi_m \frac{\partial C_m}{\partial \tau} - \vec{\nabla}_X \cdot (\tilde{d}_m \vec{\nabla}_X C_m - C_m \vec{V}_m) = 0, \quad (3.7)$$

in which C_m is the solute concentration in the porous matrix, and \tilde{d}_m represents the effective diffusion tensor. ϕ_m is the matrix porosity and is assumed to be such that $\phi_m = O(\varepsilon^0)$, which according to (2.6) means that $\phi_m \gg \varepsilon$.

Note that as a continuous model is considered at the porous matrix scale, the pore length-scale, l_p , is necessarily small compared to the period size: $l_p \ll l$.

3.2.3. Boundary Conditions (Γ)

Fluid flow and solute transport occur over the interface between the porous matrix and the fractures. Boundary conditions must, therefore, describe the continuity of fluid velocities

$$\vec{V}_f = \vec{V}_m \quad \text{on } \Gamma, \quad (3.8)$$

the continuity of pressures

$$P_f = P_m \quad \text{on } \Gamma, \quad (3.9)$$

the continuity of concentrations

$$C_f = C_m \quad \text{on } \Gamma, \quad (3.10)$$

and the continuity of solute fluxes, which according to (3.8) and (3.10) reduces to the continuity of diffusive fluxes

$$(\tilde{d}_f \vec{\nabla}_X C_f) \cdot \vec{n} = (\tilde{d}_m \vec{\nabla}_X C_m) \cdot \vec{n} \quad \text{on } \Gamma, \quad (3.11)$$

in which \vec{n} denotes a unit normal vector to Γ .

Equations (3.2) through (3.11) describe the behaviour at the local scale, that is over the period Ω . The purpose of the next step is to normalise this local description.

3.3. NORMALISATION

Normalisation of the local description consists in defining a dimensionless counterpart for each quantity by using characteristic quantities (see § 2.3.3). This requires the choice of a reference length and of a reference time. We arbitrarily choose L , the macroscopic characteristic length and T_f , the characteristic time of contaminant transfer in the fractures as the reference length and the reference time, respectively. According to the transport regime, T_f is either related to the diffusion or to the convection process. Equations (3.2)–(3.11) may be placed in a dimensionless form by introducing the new variables. The resulting dimensionless equations are

$$\frac{\mu V_{fc}}{L \delta P} \Delta \vec{v}_f - \vec{\nabla} p_f = \vec{0}, \quad (3.12)$$

$$\vec{\nabla} \cdot \vec{v}_f = 0, \quad (3.13)$$

$$\frac{L^2}{D_{fc} T_f} \frac{\partial c_f}{\partial t} - \vec{\nabla} \cdot \left(\tilde{D}_f \vec{\nabla} c_f - \frac{L V_{fc}}{D_{fc}} c_f \vec{v}_f \right) = 0, \quad (3.14)$$

$$\vec{v}_m = - \frac{l_p^2 \delta P}{\mu V_{mc} L} \tilde{K}_m \vec{\nabla} p_m, \quad (3.15)$$

$$\vec{\nabla} \cdot \vec{v}_m = 0, \quad (3.16)$$

$$\frac{\phi_m L^2}{D_{m_c} T_f} \frac{\partial c_m}{\partial t} - \vec{\nabla} \cdot \left(\tilde{D}_m \vec{\nabla} c_m - \frac{L V_{m_c}}{D_{m_c}} c_m \vec{v}_m \right) = 0, \quad (3.17)$$

$$\vec{v}_f|_{\Gamma} = \frac{V_{m_c}}{V_{f_c}} \vec{v}_m|_{\Gamma}, \quad (3.18)$$

$$p_f|_{\Gamma} = p_m|_{\Gamma}, \quad (3.19)$$

$$c_f|_{\Gamma} = c_m|_{\Gamma}, \quad (3.20)$$

$$[(\tilde{D}_f \vec{\nabla} c_f) \cdot \vec{n}]_{\Gamma} = \frac{D_{m_c}}{D_{f_c}} [(\tilde{D}_m \vec{\nabla} c_m) \cdot \vec{n}]_{\Gamma}. \quad (3.21)$$

Thus, the dimensionless writing introduces eight dimensionless numbers

$$\begin{aligned} F_f &= \frac{\mu V_{f_c}}{L \delta P}, & N_f &= \frac{L^2}{D_{f_c} T_f}, & \text{Pe}_f &= \frac{L V_{f_c}}{D_{f_c}}, \\ Q_m &= \frac{l_p^2 \delta P}{\mu V_{m_c} L}, & N_m &= \frac{\phi_m L^2}{D_{m_c} T_f}, & \text{Pe}_m &= \frac{L V_{m_c}}{D_{m_c}}, \\ v &= \frac{V_{m_c}}{V_{f_c}}, & d &= \frac{D_{m_c}}{D_{f_c}}. \end{aligned}$$

Pe_f and Pe_m are the Péclet numbers in the fracture's domain and in the porous matrix domain, respectively.

The phenomenon is thus governed by a large number of dimensionless parameters. The purpose of the order-of-magnitude analysis presented below is to assess the effect of each of these parameters and to sort out the transport regimes that can physically exist and that can be homogenised. The orders of magnitude of these dimensionless parameters are estimated with respect to powers of ε .

3.4. ORDER-OF-MAGNITUDE ANALYSIS

3.4.1. Order-of-Magnitude of v

v arises from boundary condition (3.18) and is the characteristic velocity ratio

$$v = \frac{V_{m_c}}{V_{f_c}}. \quad (3.22)$$

In an order-of-magnitude sense, Stokes equation in the fractures (3.2) and Darcy's law in the porous matrix (3.5) read

$$V_{f_c} = \mathcal{O}\left(\frac{l_p^2 \delta P}{\mu L}\right), \quad V_{m_c} = \mathcal{O}\left(\frac{l_p^2 \delta P}{\mu L}\right).$$

Thus, we get

$$v = \frac{V_{m_c}}{V_{f_c}} = \mathcal{O}\left(\frac{l_p^2}{l^2}\right), \quad (3.23)$$

where l_p is the characteristic pore-size.

3.4.2. Order-of-Magnitude of d

d emerges from Equation (3.21) that characterizes the continuity of solute fluxes and is defined as

$$d = \frac{D_{m_c}}{D_{f_c}}. \quad (3.24)$$

The tensor of effective diffusion in the porous matrix is such that

$$D_{m_c} = \mathcal{O}(\phi_m \tau_m D_{\text{mol}}). \quad (3.25)$$

D_{mol} represents the characteristic molecular diffusion in the micropores, τ_m is the tortuosity. The porosity ϕ_m has been assumed to be such that $\phi_m = \mathcal{O}(\varepsilon^0)$. Usual values of tortuosities vary from 0.1 for clays to 0.7 for sands (De Marsily, 1986). Thus, in general cases we have $\phi_m \tau_m = \mathcal{O}(\varepsilon^0)$.

In the fractures, \tilde{D}_f is the tensor of molecular diffusion

$$D_{f_c} = \mathcal{O}(D_{\text{mol}}). \quad (3.26)$$

Therefore, in general cases the order of magnitude of d is

$$d = \mathcal{O}\left(\frac{D_{m_c}}{D_{f_c}}\right) = \mathcal{O}(\varepsilon^0). \quad (3.27)$$

3.4.3. Order-of-Magnitude of F_f

F_f arises from Stokes equation in the fractures (3.12) and is defined by

$$F_f = \frac{\mu V_{f_c}}{L \delta P}. \quad (3.28)$$

Stokes equation indicates that the local flow is generated by a macroscopic pressure gradient, which in an order-of-magnitude sense reads

$$\frac{\mu V_{f_c}}{l^2} = \mathcal{O}\left(\frac{\delta P}{L}\right),$$

and from which we deduce

$$F_f = \frac{\mu V_{f_c}}{L \delta P} = \frac{\mu V_{f_c} L}{l^2 \delta P} \times \frac{l^2}{L^2} = \mathcal{O}(1) \times \mathcal{O}(\varepsilon^2) = \mathcal{O}(\varepsilon^2). \quad (3.29)$$

3.4.4. Order-of-Magnitude of Q_m

Q_m results from the normalisation of Darcy's law in the porous matrix (3.15) and is defined as

$$Q_m = \frac{l_p^2 \delta P}{\mu V_{m_c} L}. \quad (3.30)$$

Q_m can be expressed with respect to F_f as follows:

$$Q_m = \frac{l_p^2 \delta P}{\mu V_{m_c} L} = F_f^{-1} \times \frac{l_p^2}{L^2} \times \frac{V_{f_c}}{V_{m_c}}, \quad (3.31)$$

which according to (3.23) gives

$$Q_m = O(\varepsilon^0). \quad (3.32)$$

3.4.5. Orders-of-Magnitude of N_f and Pe_f

Both numbers, N_f and Pe_f , arise from the convective-diffusive equation in the fractures (3.14). Their orders of magnitude are actually linked. They are defined by

$$N_f = \frac{L^2}{T_f D_{f_c}}, \quad (3.33)$$

$$Pe_f = \frac{L V_{f_c}}{D_{f_c}}. \quad (3.34)$$

The possible orders of magnitude for Pe_f , which correspond to three distinct transport regimes in the fracture's domain, are the following:

$$\begin{aligned} Pe_f &\leq O(\varepsilon) \text{ (predominant diffusion),} \\ Pe_f &= O(\varepsilon^0) \text{ (equivalent diffusion and convection),} \\ Pe_f &= O(\varepsilon^{-1}) \text{ (predominant convection).} \end{aligned} \quad (3.35)$$

It can easily be shown that when $Pe_f < O(\varepsilon)$, the macroscopic behaviour is the same as in the case $Pe_f = O(\varepsilon)$. When $Pe_f > O(\varepsilon^{-1})$, the situation is non-homogenisable. The above results on the possible orders of Pe_f have been demonstrated in Auriault and Adler (1995) in the case of a single-porosity medium and remain valid at the fracture's scale in the present problem. We will, therefore, successively consider the following orders of magnitude for Pe_f :

$$Pe_f = O(\varepsilon), O(\varepsilon^0), O(\varepsilon^{-1}). \quad (3.36)$$

Now, let us define

$$T_{d_f} = \frac{L^2}{D_{f_c}} \text{ (characteristic time of diffusion in the fractures),} \quad (3.37)$$

$$T_{c_f} = \frac{L}{V_{f_c}} (\text{characteristic time of convection in the fractures}). \quad (3.38)$$

It follows that N_f and Pe_f can be expressed as time-scale ratios:

$$N_f = \frac{T_{d_f}}{T_f}, \quad (3.39)$$

$$\text{Pe}_f = \frac{T_{d_f}}{T_{c_f}}, \quad (3.40)$$

Noticing that

$$\begin{aligned} T_f &= T_{d_f} \quad \text{when } \text{Pe}_f = \text{O}(\varepsilon) \text{ (predominant diffusion),} \\ T_f &= T_{d_f} = T_{c_f} \quad \text{when } \text{Pe}_f = \text{O}(\varepsilon^0) \\ &\quad \text{(equivalent diffusion and convection),} \\ T_f &= T_{c_f} \quad \text{when } \text{Pe}_f = \text{O}(\varepsilon^{-1}) \text{ (predominant convection),} \end{aligned}$$

we get, according to (3.39) and (3.40)

$$\begin{aligned} N_f &= \text{O}(1) \quad \text{when } \text{Pe}_f = \text{O}(\varepsilon), \text{O}(1), \\ N_f &= \text{O}(\varepsilon^{-1}) \quad \text{when } \text{Pe}_f = \text{O}(\varepsilon^{-1}). \end{aligned} \quad (3.41)$$

3.4.6. Orders-of-Magnitude of N_m and Pe_m

Both dimensionless numbers arise from the normalisation of the advection-diffusion equation in the porous matrix (3.17). They are defined by

$$N_m = \frac{\phi m L^2}{D_{m_c} T_f}, \quad (3.42)$$

$$\text{Pe}_m = \frac{L V_{m_c}}{D_{m_c}}. \quad (3.43)$$

The orders of magnitude of N_m and Pe_m can be deduced from those of N_f and Pe_f , respectively, as follows:

$$N_m = \text{O}(d^{-1} N_f), \quad (3.44)$$

$$\text{Pe}_m = \frac{V_{m_c}}{V_{f_c}} d^{-1} \text{Pe}_f. \quad (3.45)$$

According to (3.27), we get

$$N_m = \text{O}(N_f), \quad (3.46)$$

$$\frac{\text{Pe}_m}{\text{Pe}_f} = \text{O}\left(\frac{V_{m_c}}{V_{f_c}}\right). \quad (3.47)$$

The order of magnitude of N_m is, therefore, deduced from the order of Pe_f and from (3.41). The determination of the order of Pe_m depends on the order of Pe_f and requires the knowledge of $\text{O}(V_{m_c}/V_{f_c})$.

3.4.7. Interpretation and Definition of Cases of Interest

According to the above estimations, the dimensionless local description may now be written as follows:

$$\varepsilon^2 \Delta \vec{v}_f - \vec{\nabla} p_f = \vec{0} \quad \text{in } \Omega_f, \quad (3.48)$$

$$\vec{\nabla} \cdot \vec{v}_f = 0 \quad \text{in } \Omega_f, \quad (3.49)$$

$$N_f \frac{\partial c_f}{\partial t} - \vec{\nabla} \cdot (\tilde{D}_f \vec{\nabla} c_f - \text{Pe}_f c_f \vec{v}_f) = 0 \quad \text{in } \Omega_f, \quad (3.50)$$

$$\vec{v}_m = -\tilde{K}_m \vec{\nabla} p_m \quad \text{in } \Omega_m, \quad (3.51)$$

$$\vec{\nabla} \cdot \vec{v}_m = 0 \quad \text{in } \Omega_m, \quad (3.52)$$

$$N_m \frac{\partial c_m}{\partial t} - \vec{\nabla} \cdot (\tilde{D}_m \vec{\nabla} c_m - \text{Pe}_m c_m \vec{v}_m) = 0 \quad \text{in } \Omega_m, \quad (3.53)$$

$$\vec{v}_f = \frac{\text{Pe}_m}{\text{Pe}_f} \vec{v}_m \quad \text{on } \Gamma, \quad (3.54)$$

$$p_f = p_m \quad \text{on } \Gamma, \quad (3.55)$$

$$c_f = c_m \quad \text{on } \Gamma, \quad (3.56)$$

$$(\tilde{D}_f \vec{\nabla} c_f) \cdot \vec{n} = (\tilde{D}_m \vec{\nabla} c_m) \cdot \vec{n} \quad \text{on } \Gamma, \quad (3.57)$$

in which, according to (2.5), the dimensionless gradient operator, $\vec{\nabla}$, is written as

$$\vec{\nabla} = \varepsilon^{-1} \vec{\nabla}_y + \vec{\nabla}_x. \quad (3.58)$$

Thus, the local description (3.48)–(3.57) depends upon the orders of magnitude of Pe_f , Pe_m , N_f , N_m . We have already determined the orders of magnitude of interest for Pe_f (3.36), from which the orders of N_f (3.41) and of N_m (3.46) can be deduced. The order of Pe_m is an important parameter of the problem as it characterizes the transport regime in the porous matrix and, as a result, may condition the macroscopic behaviour. According to (3.47), the order of Pe_m is obtained from the orders of Pe_f and v . According to (3.23), we have

$$v = \frac{V_{m_c}}{V_{f_c}} = \text{O}\left(\frac{l_p^2}{l^2}\right).$$

The continuous model for describing the phenomenon in the porous matrix is valid provided $l_p \ll l$, and thus $V_{m_c} \ll V_{f_c}$. Let a priori consider the following possible orders of magnitude for v :

$$v = O(\varepsilon), O(\varepsilon^2), O(\varepsilon^3), \dots \quad (3.59)$$

The cases of interest are defined from the possible combinations between the orders of Pe_m and Pe_f . According to the three situations defined in (3.35), to relationship (3.47) and to the possible orders for v (3.59), the transport regimes in the porous matrix and in the fracture's domain can be combined in the four following ways:

- Case I: $Pe_f \leq O(\varepsilon)$ and $Pe_m < O(\varepsilon)$.
Predominant diffusion in the fractures,
predominant diffusion in the porous matrix.
- Case II: $Pe_f = O(\varepsilon^0)$ and $Pe_m \leq O(\varepsilon)$.
Equivalent diffusion and convection in the fractures,
predominant diffusion in the porous matrix.
- Cases III: $Pe_f = O(\varepsilon^{-1})$.
Predominant convection in the fractures.
 - ★Case III.a: $Pe_m = O(\varepsilon^0)$.
Equivalent diffusion and advection in the porous matrix
 - ★Case III.b: $Pe_m \leq O(\varepsilon)$.
Predominant diffusion in the porous matrix

Cases I and II show that when $Pe_f = O(\varepsilon)$ or $Pe_f = O(\varepsilon^0)$, the transport regime remains of predominant diffusion type in the porous matrix (i.e. $Pe_m < \varepsilon^0$), whatever the order of v is. Case III, corresponding to $Pe_f = O(\varepsilon^{-1})$, is split into two sub-cases which lead to two distinct transport regimes in the porous matrix:

$$Pe_f = O(\varepsilon^{-1}) : \begin{cases} v = O(\varepsilon) \Rightarrow Pe_m = O(\varepsilon^0). \\ \text{(equivalent diffusion and advection in the porous matrix),} \\ v \leq O(\varepsilon^2) \Rightarrow Pe_m \leq O(\varepsilon) \\ \text{(predominant diffusion in the porous matrix).} \end{cases}$$

The homogenisation procedure may now be applied in each of the four cases defined above. All physical (and dimensionless) variables, $\vec{v}_f, p_f, c_f, \vec{v}_m, p_m, c_m$, are looked for in the form of asymptotic expansions in powers of ε

$$\vec{v}_f(\vec{y}, \vec{x}) = \vec{v}_f^0(\vec{y}, \vec{x}) + \varepsilon \vec{v}_f^1(\vec{y}, \vec{x}) + \varepsilon^2 \vec{v}_f^2(\vec{y}, \vec{x}) + \dots, \quad (3.60)$$

$$p_f(\vec{y}, \vec{x}) = p_f^0(\vec{y}, \vec{x}) + \varepsilon p_f^1(\vec{y}, \vec{x}) + \varepsilon^2 p_f^2(\vec{y}, \vec{x}) + \dots, \quad (3.61)$$

$$c_f(\vec{y}, \vec{x}, t) = c_f^0 + \varepsilon c_f^1(\vec{y}, \vec{x}, t) + \varepsilon^2 c_f^2(\vec{y}, \vec{x}, t) + \dots, \quad (3.62)$$

$$\vec{v}_m(\vec{y}, \vec{x}) = \vec{v}_m^0(\vec{y}, \vec{x}) + \varepsilon \vec{v}_m^1(\vec{y}, \vec{x}) + \varepsilon^2 \vec{v}_m^2(\vec{y}, \vec{x}) + \dots, \quad (3.63)$$

$$p_m(\vec{y}, \vec{x}) = p_m^0(\vec{y}, \vec{x}) + \varepsilon p_m^1(\vec{y}, \vec{x}) + \varepsilon^2 p_m^2(\vec{y}, \vec{x}) + \dots, \quad (3.64)$$

$$c_m(\vec{y}, \vec{x}, t) = c_m^0(\vec{y}, \vec{x}, t) + \varepsilon c_m^1(\vec{y}, \vec{x}, t) + \varepsilon^2 c_m^2(\vec{y}, \vec{x}, t) + \dots, \quad (3.65)$$

where the functions $\vec{v}_f^i, p_f^i, c_f^i, \vec{v}_m^i, p_m^i, c_m^i$ are Ω -periodic.

Then, the method consists in incorporating these expansions, together with the expression of the dimensionless gradient operator (3.58) in the set of dimensionless Equations (3.48) through (3.57). The identification at the successive orders of ε allows the construction of appropriate boundary-value problems. Solving these boundary-value problems leads to the macroscopic behaviour. Application of this procedure for analysing the distinct fluid flow and solute transport problems is presented in the two next sections.

4. Homogenisation of Fluid Flow

Fluid flow is described by Equations (3.48), (3.49), (3.51), (3.52), and boundary conditions (3.54) and (3.55). Substituting expansions (3.60), (3.63), (3.64) and (3.64) into these equations and invoking the differentiation rule (3.58), we get a set of perturbation equations

$$\vec{\nabla}_y p_f^0 = \vec{0}, \quad (4.1)$$

$$\Delta_y \vec{v}_f^0 - \vec{\nabla}_y p_f^1 - \vec{\nabla}_x p_f^0 = \vec{0}, \quad (4.2)$$

\vdots

$$\vec{\nabla}_y \cdot \vec{v}_f^0 = 0, \quad (4.3)$$

$$\vec{\nabla}_y \cdot \vec{v}_f^1 + \vec{\nabla}_x \cdot \vec{v}_f^0 = 0, \quad (4.4)$$

\vdots

$$\vec{\nabla}_y p_m^0 = \vec{0}, \quad (4.5)$$

\vdots

$$\vec{v}_m^0 = -\tilde{K}_m(\vec{\nabla}_y p_m^1 + \vec{\nabla}_x p_m^0), \quad (4.6)$$

\vdots

$$\vec{\nabla}_y \cdot \vec{v}_m^0 = \vec{0}, \quad (4.7)$$

\vdots

$$\vec{v}_f^0 = \vec{0} \quad \text{on } \Gamma, \quad (4.8)$$

$$\vec{v}_f^1 = \begin{cases} \vec{v}_m^0 & \text{if } v = O(\varepsilon), \\ \vec{0} & \text{if } v = O(\varepsilon^2), \end{cases} \quad (4.9)$$

\vdots

$$p_f^0 = p_m^0 \quad \text{on } \Gamma, \quad (4.10)$$

⋮

$$\vec{v}_f^i, \vec{v}_m^i, p_f^i, p_m^i \quad \text{are } \Omega\text{-periodic.}$$

It follows from (4.1), (4.5) and (4.10) that

$$p_f^0 = p_m^0 = p^0(\vec{x}). \quad (4.11)$$

Thus, at the first order the pressure field is the same in the fractures and in the porous matrix and does not depend on the local variable, \vec{y} . This result is actually a consequence of the separation of scales and means that, at the first order of approximation, the pressure is constant over the REV. We now note that Equations (4.2), (4.3), (4.8) define a linear boundary-value problem of variable \vec{y} and whose unknowns are \vec{v}_f^0 and p_f^1 . This boundary-value problem shows that \vec{v}_f^0 and p_f^1 are linear functions of $\vec{\nabla}_x p^0$. Therefore, we can write the solutions in the form

$$\vec{v}_f^0 = -\tilde{k}_f \vec{\nabla}_x p^0, \quad (4.12)$$

$$p_f^1 = -\vec{\chi}_f \cdot \vec{\nabla}_x p^0 + \bar{p}^1(\vec{x}), \quad (4.13)$$

in which \tilde{k}_f is a second-rank tensor, $\vec{\chi}_f$ is a vector and that are such that

$$-\frac{\partial k_{fij}}{\partial x_l \partial x_l} + \frac{\partial \chi_{fj}}{\partial y_i} - I_{ij} = 0 \quad \text{in } \Omega_f, \quad (4.14)$$

$$\frac{\partial k_{fij}}{\partial x_i} = 0 \quad \text{in } \Omega_f, \quad (4.15)$$

$$k_{fij} = 0 \quad \text{on } \Gamma, \quad (4.16)$$

k_{fij} and χ_{fj} are Ω -periodic.

For details related to the derivation of these solutions, the reader is referred to Ene and Sanchez-Palencia (1975), Sanchez-Palencia (1980), Auriault (1991). Next we average Equation (4.4) over the period. This step requires the use of boundary condition (4.9), which depends upon the order of v . In both cases we obtain

$$\vec{\nabla}_x \cdot \langle \vec{v}_f^0 \rangle_{\Omega_f} = 0, \quad (4.17)$$

where the average, over the period, of a quantity defined in Ω_f is defined by

$$\langle \cdot \rangle_{\Omega_f} = \frac{1}{|\Omega|} \int_{\Omega_f} \cdot \, d\Omega. \quad (4.18)$$

We shall now use the expression obtained for \vec{v}_f^0 (4.12) and the definition (4.18) of the average to obtain $\langle \vec{v}_f^0 \rangle_{\Omega_f}$. We deduce

$$\langle \vec{v}_f^0 \rangle_{\Omega_f} = -\tilde{K}_f \vec{\nabla}_x p^0, \quad (4.19)$$

in which

$$\tilde{K}_f = \langle \tilde{k}_f \rangle_{\Omega_f} = \frac{1}{|\Omega|} \int_{\Omega_f} \tilde{k}_f \, d\Omega. \quad (4.20)$$

Equation (4.19) is Darcy's law. The second-rank tensor \tilde{K}_f is the effective fracture permeability. It can be proved that \tilde{K}_f is symmetrical and positive. For determining \tilde{K}_f , the boundary-value problem (4.14)–(4.16), from which we get \tilde{k}_f , must be solved over the periodic cell. Therefore, \tilde{K}_f depends only on the geometry of the cell and on the fluid viscosity. The macroscopic behaviour of the flow of the fluid is, therefore, given by Equations (4.17) and (4.19), and can also be written as

$$\vec{\nabla}_x \cdot (\tilde{K}_f \vec{\nabla}_x p_f^0) = 0. \quad (4.21)$$

Thus, there is only one model for the fluid flow problem, which shows that the order of magnitude of Pe_m/Pe_f in boundary-condition (3.54) has no influence. We note that the flow in the matrix has no influence on this macroscopic behaviour. The influence of the porous matrix at the macroscopic scale is actually linked to the characteristic times of the flow in the porous matrix and in the fractures. Thus, in a dual-porosity medium a steady-state phenomenon has a single-porosity behaviour. In effect, investigation of the flow of an incompressible fluid in a deformable fractured porous medium (Auriault and Boutin, 1992, 1993) and of a highly compressible fluid in a rigid fractured porous medium (Royer and Auriault, 1994) have shown a strong influence of the flow in the porous matrix.

5. Homogenisation of Contaminant Transport

The mass transfer of the solute in the fluid is described by Equations (3.50), (3.53) and boundary conditions (3.54), (3.56) and (3.57). In this section we will successively consider the cases defined in Section 3.4.7 that correspond to distinct transport regimes in the fractures.

5.1. CASE I: PREDOMINANT DIFFUSION IN THE FRACTURES ($\text{Pe}_f \leq \text{O}(\varepsilon)$)

We consider here the case defined by

$$\begin{aligned} \text{Pe}_f &= \text{O}(\varepsilon), & \text{Pe}_m &= \text{O}(\varepsilon^2) \Rightarrow v = \frac{\text{Pe}_m}{\text{Pe}_f} = \text{O}(\varepsilon), \\ N_f &= \text{O}(N_m) = \text{O}(\varepsilon^0). \end{aligned}$$

We get the following set of perturbations expansions.

In Ω_f

$$\vec{\nabla}_y \cdot (\tilde{D}_f \vec{\nabla}_y c_f^0) = 0, \quad (5.1)$$

$$\vec{\nabla}_y \cdot [\tilde{D}_f (\vec{\nabla}_y c_f^1 + \vec{\nabla}_x c_f^0)] + \vec{\nabla}_x \cdot (\tilde{D}_f \vec{\nabla}_y c_f^0) = 0, \quad (5.2)$$

$$\begin{aligned} & \frac{\partial c_f^0}{\partial t} - \vec{\nabla}_y \cdot \left[\tilde{D}_f \left(\vec{\nabla}_y c_f^2 + \vec{\nabla}_x c_f^1 \right) - c_f^0 \vec{v}_f^0 \right] - \\ & - \vec{\nabla}_x \cdot \left[\tilde{D}_f \left(\vec{\nabla}_y c_f^1 + \vec{\nabla}_x c_f^0 \right) \right] = 0, \end{aligned} \quad (5.3)$$

⋮

In Ω_m

$$\vec{\nabla}_y \cdot \left(\tilde{D}_m \vec{\nabla}_y c_m^0 \right) = 0, \quad (5.4)$$

$$\vec{\nabla}_y \cdot \left[\tilde{D}_m \left(\vec{\nabla}_y c_m^1 + \vec{\nabla}_x c_m^0 \right) \right] + \vec{\nabla}_x \cdot \left(\tilde{D}_m \vec{\nabla}_y c_m^0 \right) = 0, \quad (5.5)$$

$$\begin{aligned} & \frac{\partial c_m^0}{\partial t} - \vec{\nabla}_y \cdot \left[\tilde{D}_m \left(\vec{\nabla}_y c_m^2 + \vec{\nabla}_x c_m^1 \right) \right] - \\ & - \vec{\nabla}_x \cdot \left[\tilde{D}_m \left(\vec{\nabla}_y c_m^1 + \vec{\nabla}_x c_m^0 \right) \right] = 0, \end{aligned} \quad (5.6)$$

⋮

On Γ

$$\vec{v}_f^0 = \vec{0}, \quad (5.7)$$

$$\vec{v}_f^1 = \vec{v}_m^0, \quad (5.8)$$

⋮

$$c_f^0 = c_m^0, \quad (5.9)$$

$$c_f^1 = c_m^1, \quad (5.10)$$

⋮

$$\left(\tilde{D}_f \vec{\nabla}_y c_f^0 \right) \cdot \vec{n} = \left(\tilde{D}_m \vec{\nabla}_y c_m^0 \right) \cdot \vec{n}, \quad (5.11)$$

$$\left[\tilde{D}_f \left(\vec{\nabla}_y c_f^1 + \vec{\nabla}_x c_f^0 \right) \right] \cdot \vec{n} = \left[\tilde{D}_m \left(\vec{\nabla}_y c_m^1 + \vec{\nabla}_x c_m^0 \right) \right] \cdot \vec{n}, \quad (5.12)$$

$$\left[\tilde{D}_f \left(\vec{\nabla}_y c_f^2 + \vec{\nabla}_x c_f^1 \right) \right] \cdot \vec{n} = \left[\tilde{D}_m \left(\vec{\nabla}_y c_m^2 + \vec{\nabla}_x c_m^1 \right) \right] \cdot \vec{n}, \quad (5.13)$$

⋮

We consider the first-order cell problem defined by (5.1), (5.4), (5.9) and (5.11), which has the formal solution

$$c_f^0 = c_m^0 = c^0(\vec{x}, t). \quad (5.14)$$

Thus, at the first order the concentration is independent of the local spatial variable and is the same field in the fractures and in the porous matrix.

Next we note that the problem defined by (5.2), (5.5), (5.10) and (5.12) constitutes a linear boundary-value problem for the concentration c^1 and leads to the solution

$$c^1 = \vec{\tau}^1 \cdot \vec{\nabla}_x c^0 + \bar{c}^1(\vec{x}, t), \quad (5.15)$$

where $\bar{c}^1(\vec{x}, t)$ is an arbitrary function. $\bar{\tau}^1$ is \vec{y} -periodic, continuous over Γ , average to zero for uniqueness

$$\langle \bar{\tau}^1 \rangle_{\Omega} = \frac{1}{|\Omega|} \int_{\Omega} \bar{\tau}^1 d\Omega = \vec{0}, \quad (5.16)$$

and is the solution to the following boundary-value problem:

$$\frac{\partial}{\partial y_i} \left(D_{fij} \left(I_{jk} + \frac{\partial \tau_k^1}{\partial y_j} \right) \right) = 0 \quad \text{in } \Omega_f, \quad (5.17)$$

$$\frac{\partial}{\partial y_i} \left(D_{mij} \left(I_{jk} + \frac{\partial \tau_k^1}{\partial y_j} \right) \right) = 0 \quad \text{in } \Omega_m, \quad (5.18)$$

$$D_{fij} \left(I_{jk} + \frac{\partial \tau_k^1}{\partial y_j} \right) n_i = D_{mij} \left(I_{jk} + \frac{\partial \tau_k^1}{\partial y_j} \right) n_i \quad \text{on } \Gamma. \quad (5.19)$$

In other words, τ_i^1 is the particular solution to the boundary-value problem defined by (5.2), (5.5), (5.10) and (5.12) when $\partial c^0 / \partial x_j \vec{e}_j = \vec{e}_i$.

Lastly we average (5.3) over Ω . After using the divergence theorem and boundary condition (5.13), the Ω -average of (5.6) is then required to obtain

$$\begin{aligned} \frac{\partial c^0}{\partial t} - \vec{\nabla}_x \cdot \langle \tilde{D}_f (\vec{\nabla}_y c^1 + \vec{\nabla}_x c^0) \rangle_{\Omega_f} - \\ - \vec{\nabla}_x \cdot \langle \tilde{D}_m (\vec{\nabla}_y c^1 + \vec{\nabla}_x c^0) \rangle_{\Omega_m} = 0, \end{aligned} \quad (5.20)$$

in which $\langle \cdot \rangle_{\Omega_f}$ is defined by (4.18) and $\langle \cdot \rangle_{\Omega_m}$, the average over the period of a quantity defined in Ω_m , is

$$\langle \cdot \rangle_{\Omega_m} = \frac{1}{|\Omega|} \int_{\Omega_m} \cdot d\Omega. \quad (5.21)$$

This can also be written as

$$\frac{\partial c^0}{\partial t} - \vec{\nabla}_x \cdot (\tilde{D}^* \vec{\nabla}_x c^0) = 0, \quad (5.22)$$

in which the tensor of effective diffusion is defined by

$$\begin{aligned} D_{ij}^* = \frac{1}{|\Omega|} \int_{\Omega_f} D_{fik} \left(\frac{\partial \tau_k^1}{\partial y_j} + I_{kj} \right) d\Omega + \\ + \frac{1}{|\Omega|} \int_{\Omega_m} D_{mik} \left(\frac{\partial \tau_k^1}{\partial y_j} + I_{kj} \right) d\Omega. \end{aligned} \quad (5.23)$$

The macroscopic behaviour of mass transfer of the solute is, therefore, described by Equation (5.22). We note that this behaviour is purely diffusive and

that the influence of the porous matrix appears only in the tensor of effective diffusion, \tilde{D}^* . It can be shown that \tilde{D}^* is a symmetrical positive-definite tensor that depends on the geometry of the periodic cell and on \tilde{D}_f and \tilde{D}_m . Note that \tilde{D}^* is derived from vector $\bar{\tau}^1$, which is independent of time (Auriault and Adler, 1995). This model is valid when $\text{Pe}_f \leq \text{O}(\varepsilon)$ and $\text{Pe}_m < \text{O}(\varepsilon)$.

5.2. CASE II: EQUIVALENT DIFFUSION AND CONVECTION IN THE FRACTURES ($\text{Pe}_f = \text{O}(\varepsilon^0)$)

The case under consideration here is defined by the following orders of magnitude:

$$\begin{aligned} \text{Pe}_f &= \text{O}(\varepsilon^0), & \text{Pe}_m &= \text{O}(\varepsilon) \Rightarrow v = \frac{\text{Pe}_m}{\text{Pe}_f} = \text{O}(\varepsilon), \\ N_f &= \text{O}(N_m) = \text{O}(\varepsilon^0). \end{aligned}$$

At the two first orders, we get the same boundary-value problems as in the previous case (§ 5.1). Thus, we have

$$c_f^0 = c_m^0 = c^0(\vec{x}, t), \quad (5.24)$$

$$c^1 = \bar{\tau}^1 \cdot \vec{\nabla}_x c^0 + \bar{c}^1(\vec{x}, t). \quad (5.25)$$

The mass-balance equation at the third order in Ω_f reads

$$\begin{aligned} \frac{\partial c_f^0}{\partial t} - \vec{\nabla}_y \cdot \left[\tilde{D}_f \left(\vec{\nabla}_y c_f^2 + \vec{\nabla}_x c_f^1 \right) - c_f^0 \vec{v}_f^1 - c_f^1 \vec{v}_f^0 \right] - \\ - \vec{\nabla}_x \cdot \left[\tilde{D}_f \left(\vec{\nabla}_y c_f^1 + \vec{\nabla}_x c_f^0 \right) - c_f^0 \vec{v}_f^0 \right] = 0. \end{aligned} \quad (5.26)$$

We then average (5.26) to obtain

$$\begin{aligned} \frac{\partial c^0}{\partial t} - \vec{\nabla}_x \cdot \langle \tilde{D}_f (\vec{\nabla}_y c^1 + \vec{\nabla}_x c^0) - c^0 \vec{v}_f^0 \rangle_{\Omega_f} - \\ - \vec{\nabla}_x \cdot \langle \tilde{D}_m (\vec{\nabla}_y c^1 + \vec{\nabla}_x c^0) \rangle_{\Omega_m} = 0, \end{aligned} \quad (5.27)$$

which can also be written as:

$$\frac{\partial c^0}{\partial t} - \vec{\nabla}_x \cdot (\tilde{D}^* \vec{\nabla}_x c^0 - c^0 \langle \vec{v}_f^0 \rangle_{\Omega_f}) = 0, \quad (5.28)$$

where \tilde{D}^* , and $\langle \vec{v}_f^0 \rangle_{\Omega_f}$ are defined by (5.23) and (4.19), respectively. Solute migration is, therefore, described by Equation (5.28). This behaviour is of convection-diffusion type. The tensor of effective diffusion is the same as in the previous case.

This model is valid when $\text{Pe}_f = \text{O}(\varepsilon^0)$ and $\text{Pe}_m \leq \text{O}(\varepsilon)$.

5.3. CASE III: PREDOMINANT CONVECTION IN THE FRACTURES
($\text{Pe}_f = \text{O}(\varepsilon^{-1})$)

We consider here the following orders of magnitude:

$$\text{Pe}_f = \text{O}(\varepsilon^{-1}) \Rightarrow N_f = \text{O}(N_m) = \text{O}(\varepsilon^{-1}).$$

As explained in Section 3.4.7, two cases must be considered.

CASE III.a. $\text{Pe}_m = \text{O}(\varepsilon^0) \Rightarrow v = \frac{\text{Pe}_m}{\text{Pe}_f} = \text{O}(\varepsilon).$

The perturbation equations are the following:

In Ω_f

$$\vec{\nabla}_y \cdot (\tilde{D}_f \vec{\nabla}_y c_f^0 - c_f^0 \vec{v}_f^0) = 0, \quad (5.29)$$

$$\begin{aligned} \frac{\partial c_f^0}{\partial t} - \vec{\nabla}_y \cdot [\tilde{D}_f (\vec{\nabla}_y c_f^1 + \vec{\nabla}_x c_f^0) - c_f^0 \vec{v}_f^1 - c_f^1 \vec{v}_f^0] - \\ - \vec{\nabla}_x \cdot (\tilde{D}_f \vec{\nabla}_y c_f^0 - c_f^0 \vec{v}_f^0) = 0, \end{aligned} \quad (5.30)$$

$$\begin{aligned} \frac{\partial c_f^1}{\partial t} - \vec{\nabla}_y \cdot [\tilde{D}_f (\vec{\nabla}_y c_f^2 + \vec{\nabla}_x c_f^1) - c_f^0 \vec{v}_f^2 - c_f^1 \vec{v}_f^1 - c_f^2 \vec{v}_f^0] - \\ - \vec{\nabla}_x \cdot [\tilde{D}_f (\vec{\nabla}_y c_f^1 + \vec{\nabla}_x c_f^0) - c_f^0 \vec{v}_f^1 - c_f^1 \vec{v}_f^0] = 0, \end{aligned} \quad (5.31)$$

⋮

In Ω_m

$$\vec{\nabla}_y \cdot (\tilde{D}_m \vec{\nabla}_y c_m^0) = 0, \quad (5.32)$$

$$\begin{aligned} \frac{\partial c_m^0}{\partial t} - \vec{\nabla}_y \cdot [\tilde{D}_m (\vec{\nabla}_y c_m^1 + \vec{\nabla}_x c_m^0) - c_m^0 \vec{v}_m^0] - \\ - \vec{\nabla}_x \cdot (\tilde{D}_m \vec{\nabla}_y c_m^0) = 0, \end{aligned} \quad (5.33)$$

$$\begin{aligned} \frac{\partial c_m^1}{\partial t} - \vec{\nabla}_y \cdot [\tilde{D}_m (\vec{\nabla}_y c_m^2 + \vec{\nabla}_x c_m^1) - c_m^0 \vec{v}_m^1 - c_m^1 \vec{v}_m^0] - \\ - \vec{\nabla}_x \cdot [\tilde{D}_m (\vec{\nabla}_y c_m^1 + \vec{\nabla}_x c_m^0) - c_m^0 \vec{v}_m^0] = 0, \end{aligned} \quad (5.34)$$

⋮

On Γ

$$\vec{v}_f^0 = \vec{0}, \quad (5.35)$$

$$\vec{v}_f^1 = \vec{v}_m^0, \quad (5.36)$$

$$\vec{v}_f^2 = \vec{v}_m^1, \quad (5.37)$$

⋮

$$c_f^0 = c_m^0, \quad (5.38)$$

$$c_f^1 = c_m^1, \quad (5.39)$$

⋮

$$\left(\tilde{D}_f \vec{\nabla}_y c_f^0 \right) \cdot \vec{n} = \left(\tilde{D}_m \vec{\nabla}_y c_m^0 \right) \cdot \vec{n}, \quad (5.40)$$

$$\left[\tilde{D}_f \left(\vec{\nabla}_y c_f^1 + \vec{\nabla}_x c_f^0 \right) \right] \cdot \vec{n} = \left[\tilde{D}_m \left(\vec{\nabla}_y c_m^1 + \vec{\nabla}_x c_m^0 \right) \right] \cdot \vec{n}, \quad (5.41)$$

$$\left[\tilde{D}_f \left(\vec{\nabla}_y c_f^2 + \vec{\nabla}_x c_f^1 \right) \right] \cdot \vec{n} = \left[\tilde{D}_m \left(\vec{\nabla}_y c_m^2 + \vec{\nabla}_x c_m^1 \right) \right] \cdot \vec{n}, \quad (5.42)$$

⋮

Considering Equations (5.29), (5.32), (5.40), (5.35) and (5.38), we get

$$c_f^0 = c_m^0 = c^0(\vec{x}, t). \quad (5.43)$$

Integration of Equation (5.30) over the periodic cell yields

$$\frac{\partial c^0}{\partial t} = -\vec{\nabla}_x \cdot (c^0 \langle \vec{v}_f^0 \rangle_{\Omega_f}).$$

Using this expression for $\partial c^0 / \partial t$, Equations (5.30) and (5.33) reduce to

$$\begin{aligned} \vec{\nabla}_y \cdot \left[\tilde{D}_f \left(\vec{\nabla}_y c_f^1 + \vec{\nabla}_x c_f^0 \right) \right] - \vec{v}_f^0 \cdot \vec{\nabla}_y c_f^1 \\ = \vec{\nabla}_x c^0 \cdot (\vec{v}_f^0 - \langle \vec{v}_f^0 \rangle_{\Omega_f}), \end{aligned} \quad (5.44)$$

$$\vec{\nabla}_y \cdot \left[\tilde{D}_m \left(\vec{\nabla}_y c_m^1 + \vec{\nabla}_x c_m^0 \right) \right] = \langle \vec{v}_f^0 \rangle_{\Omega_f} \cdot \vec{\nabla}_x c^0. \quad (5.45)$$

From Equations (5.44) and (5.45), boundary conditions (5.36), (5.39) and (5.41), we deduce

$$c^1 = \bar{\tau}^{\text{III}} \cdot \vec{\nabla}_x c^0 + \bar{c}^1(\vec{x}, t), \quad (5.46)$$

where \bar{c}^1 is an arbitrary function. $\bar{\tau}^{\text{III}}$ is \vec{y} -periodic, continuous over Γ , average to zero for uniqueness

$$\langle \bar{\tau}^{\text{III}} \rangle_{\Omega} = 0, \quad (5.47)$$

and is the solution to the following boundary-value problem:

$$\begin{aligned} \frac{\partial}{\partial y_i} \left[D_{fij} \left(I_{jk} + \frac{\partial \tau_k^{\text{III}}}{\partial y_j} \right) \right] - v_{fi}^0 \frac{\partial \tau_k^{\text{III}}}{\partial y_i} \\ = (v_{fk}^0 - \langle v_{fk}^0 \rangle_{\Omega_f}) \quad \text{in } \Omega_f, \end{aligned} \quad (5.48)$$

$$\frac{\partial}{\partial y_i} \left[D_{mij} \left(I_{jk} + \frac{\partial \tau_k^{\text{III}}}{\partial y_j} \right) \right] = \langle v_{fk}^0 \rangle_{\Omega_f} \quad \text{in } \Omega_m, \quad (5.49)$$

$$\left[D_{fij} \left(I_{jk} + \frac{\partial \tau_k^{\text{III}}}{\partial y_j} \right) \right] \cdot \vec{n} = \left[D_{mij} \left(I_{jk} + \frac{\partial \tau_k^{\text{III}}}{\partial y_j} \right) \right] \cdot \vec{n} \quad \text{on } \Gamma. \quad (5.50)$$

An important feature of $\vec{\tau}^{\text{III}}$ is that it depends on $\vec{\nabla}_x p^0$.

Finally, the average over the period of equation (5.31) leads to

$$\begin{aligned} \frac{\partial \langle c^1 \rangle_{\Omega}}{\partial t} - \vec{\nabla}_x \cdot \langle \tilde{D}_f (\vec{\nabla}_y c^1 + \vec{\nabla}_x c^0) - c^0 \vec{v}_f^1 - c^1 \vec{v}_f^0 \rangle_{\Omega_f} - \\ - \vec{\nabla}_x \cdot \langle \tilde{D}_m (\vec{\nabla}_y c^1 + \vec{\nabla}_x c_m^0) - c^0 \vec{v}_m^0 \rangle_{\Omega_m} = 0, \end{aligned} \quad (5.51)$$

which, according to the expression obtained for c^1 (5.46), can also be written as

$$\begin{aligned} \frac{\partial \langle c^1 \rangle_{\Omega}}{\partial t} - \vec{\nabla}_x \cdot (\tilde{D}^{**} \vec{\nabla}_x c^0) + \\ + \vec{\nabla}_x \cdot [c^0 \langle \vec{v}_f^1 \rangle_{\Omega_f} + \bar{c}^1 \langle \vec{v}_f^0 \rangle_{\Omega_f} + c^0 \langle \vec{v}_m^0 \rangle_{\Omega_m}] = 0, \end{aligned} \quad (5.52)$$

where the effective tensor \tilde{D}^{**} is defined by

$$\begin{aligned} D_{ik}^{**} = \frac{1}{|\Omega|} \int_{\Omega_f} \left(D_{fij} \left(I_{jk} + \frac{\partial \tau_k^{\text{III}}}{\partial y_j} \right) - \tau_k^{\text{III}} v_{fi}^0 \right) d\Omega + \\ + \frac{1}{|\Omega|} \int_{\Omega_m} \left(D_{mij} \left(I_{jk} + \frac{\partial \tau_k^{\text{III}}}{\partial y_j} \right) \right) d\Omega. \end{aligned} \quad (5.53)$$

\tilde{D}^{**} depends on the velocity, and therefore on the pressure gradient. It is, therefore, a dispersion tensor. It can be shown that \tilde{D}^{**} is a positive-definite tensor but, in general cases, it is not a symmetrical tensor (Auriault and Adler, 1995).

We shall now use expression (4.6) to define $\langle \vec{v}_m^0 \rangle_{\Omega_m}$. Hence, by averaging we obtain

$$\langle \vec{v}_m^0 \rangle_{\Omega_m} = -\tilde{K}_m^* \vec{\nabla}_x p^0, \quad (5.54)$$

where \tilde{K}_m^* , the effective permeability tensor of the porous matrix, is given by

$$K_{mik}^* = \frac{1}{|\Omega|} \int_{\Omega_m} K_{mij} \left(I_{jk} + \frac{\partial \chi_{mk}}{\partial y_j} \right) d\Omega. \quad (5.55)$$

Now we define the average concentration field and average velocity fields by

$$\langle c \rangle_{\Omega} = \langle c^0 \rangle_{\Omega} + \varepsilon \langle c^1 \rangle_{\Omega} = c^0 + \varepsilon \bar{c}^1, \quad (5.56)$$

$$\langle \vec{v}_f \rangle_{\Omega_f} = \langle \vec{v}_f^0 \rangle_{\Omega_f} + \varepsilon \langle \vec{v}_f^1 \rangle_{\Omega_f}, \quad (5.57)$$

$$\langle \vec{v}_m \rangle_{\Omega_m} = \langle \vec{v}_m^0 \rangle_{\Omega_m}. \quad (5.58)$$

When neglecting the terms in ε^2 , the equation that governs the average concentration $\langle c \rangle_\Omega$ is

$$\begin{aligned} \frac{\partial \langle c \rangle_\Omega}{\partial t} - \varepsilon \vec{\nabla}_x \cdot (\tilde{D}^{**} \vec{\nabla}_x \langle c \rangle_\Omega) + \\ + \vec{\nabla}_x \cdot [\langle c \rangle_\Omega (\langle \vec{v}_f \rangle_{\Omega_f} + \varepsilon \langle \vec{v}_m \rangle_{\Omega_m})] = 0. \end{aligned} \quad (5.59)$$

This model describes a convective-dispersive behaviour. An important property of this macroscopic behaviour is that it depends upon the fluid velocity in the porous matrix. Note that the advection term due to the fluid velocity in the porous matrix is as important as the dispersion process as they are both of order ε . This model is valid only when $\text{Pe}_f = \text{O}(\varepsilon^{-1})$ and $\text{Pe}_m = \text{O}(\varepsilon^0)$.

$$\text{CASE III.b. } \text{Pe}_m = \text{O}(\varepsilon) \Rightarrow v = \frac{\text{Pe}_m}{\text{Pe}_f} = \text{O}(\varepsilon^2).$$

The first-order problem is identical to that obtained in Case III.1. Furthermore, it can easily be shown that the second-order problem leads to the same solution as in Case III.1. We, therefore, get

$$c_f^0 = c_m^0 = c^0(\vec{x}, t), \quad (5.60)$$

$$c^1 = \bar{\tau}^{\text{III}} \cdot \vec{\nabla}_x c^0 + \bar{c}^1(\vec{x}, t). \quad (5.61)$$

The mass-balance equation at the third order in Ω_f reads

$$\begin{aligned} \frac{\partial c_f^1}{\partial t} - \vec{\nabla}_y \cdot \left[\tilde{D}_f \left(\vec{\nabla}_y c_f^2 + \vec{\nabla}_x c_f^1 \right) - c_f^0 \vec{v}_f^2 - c_f^1 \vec{v}_f^1 - c_f^2 \vec{v}_f^0 \right] - \\ - \vec{\nabla}_x \cdot \left[\tilde{D}_f \left(\vec{\nabla}_y c_f^1 + \vec{\nabla}_x c_f^0 \right) - c_f^0 \vec{v}_f^1 - c_f^1 \vec{v}_f^0 \right] = 0. \end{aligned} \quad (5.62)$$

Its average over the period leads to

$$\frac{\partial \langle c^1 \rangle_\Omega}{\partial t} - \vec{\nabla}_x \cdot (\tilde{D}^{**} \vec{\nabla}_x c^0) + \vec{\nabla}_x \cdot [c^0 \langle \vec{v}_f^1 \rangle_{\Omega_f} + \bar{c}^1 \langle \vec{v}_f^0 \rangle_{\Omega_f}] = 0, \quad (5.63)$$

in which \tilde{D}^{**} is defined by (5.53).

The difference between Equation (5.63) and its counterpart in Case III.1 (5.52) is that the term \vec{v}_m^0 does not appear in (5.63). Therefore, the equation with respect to the average concentration field and average velocity fields is the following:

$$\frac{\partial \langle c \rangle_\Omega}{\partial t} - \varepsilon \vec{\nabla}_x \cdot (\tilde{D}^{**} \vec{\nabla}_x \langle c \rangle_\Omega) + \vec{\nabla}_x \cdot [\langle c \rangle_\Omega \langle \vec{v}_f \rangle_{\Omega_f}] = 0. \quad (5.64)$$

Fluid flow in the porous matrix has no effect on the macroscopic behaviour in this case. This model is valid when $\text{Pe}_f = \text{O}(\varepsilon^{-1})$ and $\text{Pe}_m \leq \text{O}(\varepsilon)$.

6. Conclusion

We have shown that the macroscopic fluid flow is described by Darcy's law, combined with the mass-balance equation, and in which the permeability is that of the fracture network. For the transport of contaminant, we have derived four macroscopic models and their domains of validity (Figure 2). These four macroscopic models are single-continuum models: they are single-concentration-field models. Thus, no fracture/matrix solute exchange term is involved, and as a consequence, there is no memory effects. Dual-porosity effects actually occur when the characteristic time of the phenomenon at the pore scale is of same order as the characteristic time in the fractures

$$\frac{T_p}{T_f} = O(1). \quad (6.65)$$

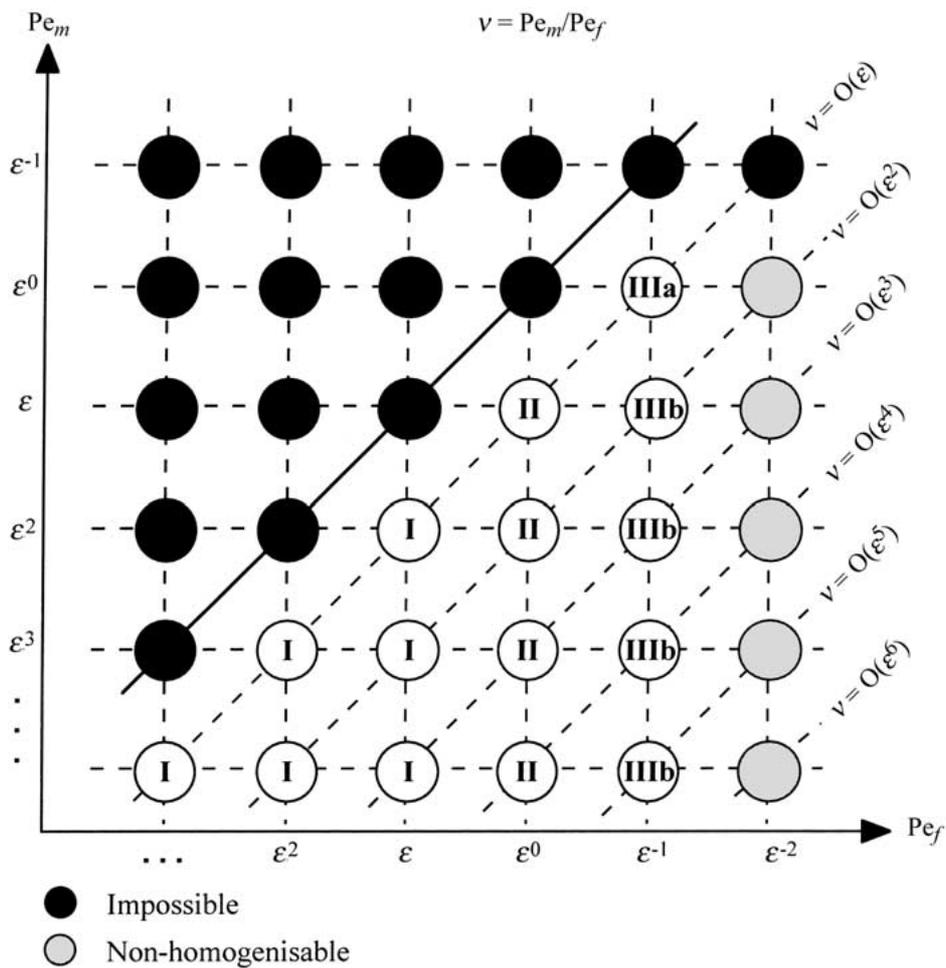


Figure 2. Macroscopic models with respect to the orders of magnitude of Pe_f and Pe_m .

In the present problem, T_p is the characteristic time of diffusion at the pore scale

$$T_p = \frac{l^2}{D_{p_c}} = O\left(\frac{l^2}{D_{\text{mol}}}\right),$$

and T_f is either T_{d_f} or T_{c_f} (see § 3.4.5).

Now, as the transport regime in the porous matrix is either predominantly diffusive or of equivalent diffusion and convection type, the characteristic time in the porous matrix is the characteristic time of diffusion

$$T_m = \frac{\phi_m L^2}{D_{m_c}} = O\left(T_p \times \frac{L^2}{l^2}\right) = O(\varepsilon^{-2} T_p).$$

The condition for obtaining memory effects (6.65) can thus also be written as

$$\frac{T_m}{T_f} = O(\varepsilon^{-2}). \quad (6.66)$$

Let now examine why this condition is not satisfied. By definition, N_m is such that (3.42)

$$N_m = \frac{\Phi_m L^2}{D_{m_c} T_f} = \frac{T_m}{T_f}.$$

According to (3.46) and (3.41), we have

$$N_m = \frac{T_m}{T_f} = \begin{cases} O(1) & \text{when } \text{Pe}_f = O(\varepsilon), O(1), \\ O(\varepsilon^{-1}) & \text{when } \text{Pe}_f = O(\varepsilon^{-1}). \end{cases} \quad (6.67)$$

Therefore, the order $T_m/T_f = O(\varepsilon^{-2})$ cannot be reached. We note that

$$\text{when } \text{Pe}_f = O(\varepsilon), O(1): T_f = T_{d_f} \Rightarrow \frac{T_m}{T_f} = O\left(\frac{D_{f_c}}{D_{m_c}}\right),$$

$$\text{when } \text{Pe}_f = O(\varepsilon^{-1}): T_f = T_{d_c} \Rightarrow \frac{T_m}{T_f} = O\left(\varepsilon^{-1} \frac{D_{f_c}}{D_{m_c}}\right).$$

Thus, the absence of memory effects is linked to the order of magnitude of D_{f_c}/D_{m_c} , which we have shown to be $O(\varepsilon^0)$ in general cases. The fact that for purely diffusive problems, this ratio must be $O(\varepsilon^2)$ for obtaining memory effects is a classical result of the homogenisation theory, which has first been demonstrated in Auriault (1983). Consequently, memory effects may occur for contaminant transport in a single porosity medium (e.g. a fractured non porous medium) provided that the solute does diffuse within the solid skeleton and that

$$\frac{D_s}{D_{\text{mol}}} = O(\varepsilon^2),$$

where D_s is the diffusivity in the solid (Auriault and Lewandowska, 1997).

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