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CONTAMINANT TRANSPORT IN FRACTURED POROUS MEDIA

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RESUME : Le but de cette étude est de déterminer les modèles mathématiques qui décrivent la migration de polluants en milieux poreux fracturés. On utilise une méthode d'homogénéisation, c'est à dire que les modèles macroscopiques sont rigoureusement déduits de la description physique à l'échelle d'un Volume Elementaire Représentatif (VER). Pour pouvoir appliquer l'homogénéisation, la condition fondamentale de séparation des échelles doit vérifiée : $l/L = \varepsilon \ll 1$. Dans le cadre de cette étude, l désigne la longueur caractéristique du VER , c'est à dire la taille caractéristique de l'échelle des fractures et L est la taille caractéristique macroscopique. On utilise l'approche introduite dans (Auriault, 1991). Cette méthodologie est basée sur la définition puis l'évaluation des nombres adimensionnels issus de la description à l'échelle du VER. On montre que le comportement macroscopique dépend du régime local de transport, lequel est caractérisé par le nombre de Péclet dans les fractures. On obtient quatre modèles macroscopiques de transport de soluté en milieux poreux fracturés.

ABSTRACT : This work is aimed towards deriving mathematical models that describe pollutant migration through fractured porous media. A homogenisation method is used, i .e. macroscopic models are rigorously deduced from the physical description which is valid within a Representative Elementary Volume (REV). The fundamental addumption behind homogenisation is the separation of scales which is expressed by : $l/L = \varepsilon \ll 1$. In the present work, l denotes the characteristic size of the REV, i.e. at the fracture's scale and L is the characteristic macroscopic size. The approach introduced in (Auriault, 1991) is used. This methodology is on the basis of definition and estimation of dimensionless numbers arising from the description at the REV's scale. It is shown that the macroscopic behaviour strongly depends upon the local transport regime characterised by the Péclet number in the fractures. Four distinct macroscopic models for solute transport in fractured porous media are derived.

KEYWORDS: Solute transport, fractured porous media, homogenisation.

I. INTRODUCTION.

The present work is aimed towards deriving the macroscopic equations that govern solute transport in fractured porous media. The medium is assumed to be locally characterised by a Representative Elementary Volume (REV). It consists of a porous matrix domain, Ω_m , and of a fracture domain, Ω_f , whose common boundary is denoted by Γ (Figure 1).

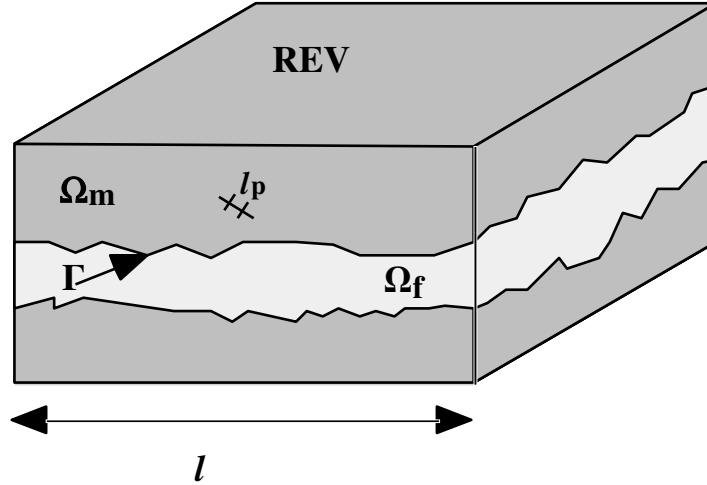


Figure 1: Periodic cell of the fractured porous medium

The macroscopic models are derived via homogenisation: they are rigorously deduced from the physical description at the REV's scale. The fundamental assumption behind all homogenisation techniques is that the scales must be separated. This fundamental condition is expressed as: $l/L = \varepsilon \ll 1$, where l is the characteristic length of the REV and L is the characteristic macroscopic length. In the present study we use the method of homogenisation for periodic structures - also called method of multiple scales - that was introduced by (Bensoussan et al., 1978) and (Sanchez-Palencia, 1980). The key parameter of the method is the length-scale ratio ε . The medium is also assumed to be periodic and the period, Ω , is $O(l)$. This assumption is not a restriction: it actually allows derivation of the macroscopic description and of the effective coefficients without any preliminary assumption on the form of the macroscopic behaviour.

In this work, we use the approach introduced in (Auriault, 1991), by which the problem is tackled in a physical rather than mathematical manner. This methodology is on the basis of definition and estimation of dimensionless numbers arising from the description at the REV's scale. The domains of validity of the derived macroscopic descriptions are provided by means of the orders of magnitude of the local dimensionless numbers.

II. DIMENSIONLESS LOCAL DESCRIPTION.

The medium is saturated by water in which a solute is diluted. In the fracture's domain, fluid flow is described by Stokes equations and solute transport by the diffusion-convection equation. In the porous matrix the filtration of the liquid is described by Darcy's law and

solute transport is supposed to be governed by a diffusion-advection equation. The latter equation results from diffusion in the solid and from diffusion and convection in the pores. Note that the behaviour, at the porous matrix scale, of the process of diffusion in both the solid and the micropores and of convection in the micropores, may be very different from that considered here. In particular, this behaviour is conditioned by the order of magnitude of the diffusion coefficient ratio (Auriault and Lewandowska, 1997).

When cast in a dimensionless form (using L as the reference characteristic length and T_f , the characteristic time of the transport process in the fractures as the reference characteristic time) the equations that govern fluid flow and solute transport are the following:

• In Ω_f

$$F_f \quad \Delta \frac{\rho}{\omega} - \nabla \cdot \pi_\phi = 0 \quad \omega \eta \epsilon \rho \epsilon \quad \Phi_\phi = \frac{\mu \zeta_\phi}{\Lambda \delta \Pi}$$

(μ : viscosity; \dot{v}_f : fluid velocity in the fractures; P_f : fluid pressure in the fractures; δP : characteristic macroscopic pressure drop; V_{f_c} : characteristic value of \dot{v}_f)

$$\dot{v}_f \cdot \dot{v}_f = 0$$

$$N_f \quad \frac{\partial \chi_\phi}{\partial \tau} - \nabla \cdot (\tilde{D}_\phi \nabla \chi_\phi - \Pi \epsilon_\phi \chi_\phi \frac{\rho}{\omega}) = 0 \quad \omega \eta \epsilon \rho \epsilon \quad N_\phi = \frac{\lambda}{T_\phi \Delta_\phi} \quad \Pi \epsilon_\phi = \frac{\Lambda \zeta_{\phi_z}}{\Delta_\phi}$$

(c_f : solute concentration in the fractures; \tilde{D}_f : tensor of molecular diffusion in the fractures; D_{f_c} : characteristic value of \tilde{D}_f ; Pe_f : Péclet number in the fractures)

• In Ω_m

$$r \quad \dot{v}_m = -\Theta_\mu \tilde{K}_\mu \nabla \pi_\mu \quad \omega \eta \epsilon \rho \epsilon \quad \Theta_\mu = \frac{\lambda^2 \delta \Pi}{\mu \zeta_{\mu_z} \Lambda}$$

(\dot{v}_m : fluid velocity in the porous matrix; P_m : fluid pressure in the porous matrix; l_p : characteristic pore-size; l_p^2 / μ : estimation of the permeability; \tilde{K}_m : dimensionless permeability tensor of the porous matrix)

$$\dot{v}_m \cdot \dot{v}_m = 0$$

$$N_m \quad \frac{\partial \chi_\mu}{\partial \tau} - \nabla \cdot (\tilde{D}_\mu \nabla \chi_\mu - \Pi \epsilon_\mu \chi_\mu \frac{\rho}{\omega}) = 0 \quad \omega \eta \epsilon \rho \epsilon \quad N_\mu = \frac{\lambda}{\Delta_{\mu_z} T_\phi} \quad \Pi \epsilon_\mu = \frac{\Lambda \zeta_{\mu_z}}{\Delta_{\mu_z}}$$

(c_m : solute concentration in the porous matrix; \tilde{D}_m : tensor of effective diffusion in the porous matrix; D_{m_c} : characteristic value of \tilde{D}_m ; Pe_m : Péclet number in the porous matrix)

• On Γ

$$\frac{r}{v_f} = \frac{\rho}{\omega \tilde{\omega}} \quad \tilde{\omega} = \frac{\zeta_{\mu\chi}}{\zeta_{\phi}}$$

$$p_f = \pi_{\mu}$$

$$c_f = \chi_{\mu}$$

$$(\tilde{D}_f^r \nabla \chi_{\phi}) \cdot \hat{v} = \delta (\tilde{\Delta} \nabla \chi_{\mu}) \cdot \hat{v} \quad \delta = \frac{\Delta_{\mu\chi}}{\Delta_{\phi\chi}}$$

III. ESTIMATION OF THE NON-DIMENSIONAL NUMBERS.

• Estimation of $v = \frac{\zeta_{\mu\chi}}{\zeta_{\phi}}$

From Stokes equation in the fractures and Darcy's law in the porous matrix we deduce that V_{f_c} and V_{m_c} are such that:

$$V_{f_c} = O\left(\frac{\lambda \delta \Pi}{\mu \Lambda}\right) \quad \zeta_{\mu\chi} = O\left(\frac{\lambda^2 \delta \Pi}{\mu \Lambda}\right).$$

Thus, we get:

$$v = \frac{\zeta_{\mu\chi}}{\zeta_{\phi}} = O\left(\frac{\lambda^2}{\lambda}\right)$$

• Estimation of $d = \frac{\Delta_{\mu\chi}}{\Delta_{\phi}}$

The tensor of effective diffusion in the porous matrix, D_{m_c} , characterises both the diffusion in the solid and the diffusion in the micropores. Therefore

$$D_{m_c} = \alpha(\Delta_s) + \alpha(\Delta_{\mu o \lambda} \times \tau_m) = \alpha(\Delta_{\mu o \lambda}).$$

(D_s : characteristic diffusion coefficient in the solid; D_{mol} : characteristic molecular diffusion in the micropores; τ_m : tortuosity).

In the fractures, D_f is the tensor of molecular diffusion. Thus

$$D_f = \alpha(\Delta_{\mu o \lambda})$$

We therefore deduce that

$$d = \frac{\Delta_{\mu\chi}}{\Delta_{\phi}} = O(1).$$

• Estimation of $F_f = \frac{\mu \zeta_{\phi}}{\Lambda \delta \Pi}$

The local flow is generated by a macroscopic pressure gradient, which leads to the following estimation:

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

from which we deduce:

$$F_f = O(\varepsilon^2).$$

- Estimation of $Q_m = \frac{\lambda_h^2 \delta \Pi}{\mu \zeta_{\mu_x} \Lambda}$

Q_m can be expressed with respect to F_f as follows:

$$Q_m = \Phi_\phi^{-1} \times \frac{\lambda}{\Lambda} = O(1)$$

- Estimation of $N_f = \frac{\Lambda}{T_\phi \Delta_\phi}$ and $Pe_f = \frac{\Lambda \zeta_{\phi_x}}{\Delta_\phi}$

The orders of magnitude of N_f and Pe_f are actually linked. In effect, both numbers can be expressed as characteristic time ratios as follows:

$$N_f = \frac{T_{\delta_\phi}}{T_\phi} \quad \Pi \varepsilon_\phi = \frac{T_{\delta_\phi}}{T_{\lambda_\phi}},$$

in which

$$T_{d_f} = \frac{\Lambda}{\Delta_\phi} \text{ is the characteristic time of diffusion in the fractures,}$$

$$T_{c_f} = \frac{\Lambda}{\zeta_\phi} \text{ is the characteristic time of convection in the fractures.}$$

Thus, we have:

$$\begin{cases} N_f = O(1) & \text{if } T_\phi = T_{\delta_\phi} \\ N_\phi = O(\Pi \varepsilon_\phi) & \text{if } T_\phi = T_{\lambda_\phi} \end{cases}$$

- Estimation of $N_m = \frac{\Lambda}{T_\phi \Delta_{\mu_x}}$ and $Pe_m = \frac{\Lambda \zeta_{\mu_x}}{\Delta_{\mu_x}}$

The orders of magnitude of N_m and Pe_m can be deduced from those of N_f and Pe_f :

$$N_m = \delta^{-1} N_\phi$$

$$Pe_m = O\left(\frac{\lambda_h^2}{\lambda}\right) \times \delta^{-1} \Pi \varepsilon_\phi$$

IV. DEFINITION OF CASES OF INTEREST.

The dimensionless description depends upon the orders of magnitude of Pe_f and that of l_p/l .

The following orders of magnitude will be considered:

$$Pe_f = O(\varepsilon) \Rightarrow N_\phi = O(1) \quad (\text{predominant diffusion})$$

$$Pe_f = O(1) \Rightarrow N_\phi = O(1) \quad (\text{equivalent diffusion and convection})$$

$$Pe_f = O(\varepsilon^{-1}) \Rightarrow N_\phi = O(\varepsilon^{-1}) \quad (\text{predominant convection})$$

It has been shown (Auriault and Adler, 1995) that any other order of magnitude for Pe_f would either be equivalent to one of the cases investigated here - $Pe_f < \mathcal{O}(\varepsilon)$ - or lead to a non-homogenisable situation (i.e. when there is no equivalent macroscopic continuous description) - $Pe_f > \mathcal{O}(\varepsilon^{-1})$ -.

Former studies concerning various physical processes in fractured porous media have shown that three characteristic orders of magnitude may be considered for l_p/l (for example see (Royer et al., 1996)):

$$\begin{cases} \frac{l_p}{l} = \mathcal{O}(\varepsilon^{1/2}) \\ \frac{\lambda_k}{\lambda} = \mathcal{O}(\varepsilon) \\ \frac{\lambda_k}{\lambda} = \mathcal{O}(\varepsilon^2) \end{cases}$$

The order of magnitude of l_p/l may have an impact on the order of magnitude of Pe_m , which defines the solute transport regime in the porous matrix:

$$Pe_m = \mathcal{O}\left(\frac{\lambda_k^2}{\lambda^2}\right) \times \delta^{-1} \Pi \varepsilon_\phi = \mathcal{O}\left(\frac{\lambda_k^2}{\lambda^2}\right) \times \mathcal{O}(\Pi \varepsilon_\phi)$$

When $Pe_f = \mathcal{O}(\varepsilon)$ or $Pe_f = \mathcal{O}(1)$, we have $Pe_m < \mathcal{O}(1)$,

which shows that the transport regime will always be the same, namely a regime of predominant diffusion, whatever the order of l_p/l . Therefore, in these cases, the order of l_p/l has no effect.

In contrast, when $Pe_f = \mathcal{O}(\varepsilon^{-1})$ we have

$$Pe_m = \mathcal{O}(\varepsilon^{-1}) \times \mathcal{O}\left(\frac{\lambda_k^2}{\lambda^2}\right).$$

Thus, if $l_p/l = \mathcal{O}(\varepsilon^{1/2})$, then a Péclet number of $Pe_m = \mathcal{O}(1)$ is reached, which corresponds to a regime of equivalent diffusion and advection in the porous matrix; whereas if $l_p/l = \mathcal{O}(\varepsilon)$ or $l_p/l = \mathcal{O}(\varepsilon^2)$, we get $Pe_m < \mathcal{O}(1)$, i.e. a regime of predominant diffusion.

Thus, when $Pe_f = \mathcal{O}(\varepsilon^{-1})$, two orders of magnitude for l_p/l are of interest:

$$\frac{l_p}{l} = \mathcal{O}(\varepsilon^{1/2}) \quad \text{and} \quad \frac{\lambda_k}{\lambda} = \mathcal{O}(\varepsilon).$$

As a conclusion, the cases to be investigated are the following:

- Case I: $Pe_f = \mathcal{O}(\varepsilon)$; $N_\phi = \mathcal{O}(1)$; $\frac{\lambda_k}{\lambda} = \mathcal{O}(\varepsilon^{1/2})$.
- Case II: $Pe_f = \mathcal{O}(1)$; $N_\phi = \mathcal{O}(1)$; $\frac{\lambda_k}{\lambda} = \mathcal{O}(\varepsilon^{1/2})$.
- Case III: $Pe_f = \mathcal{O}(\varepsilon^{-1})$; $N_\phi = \mathcal{O}(\varepsilon^{-1})$.
 - Case III.1: $\frac{l_p}{l} = \mathcal{O}(\varepsilon^{1/2})$.

- Case III.2: $\frac{l_p}{l} = O(\varepsilon)$.

V. DERIVED SCALED-UP MODELS.

The homogenisation method of multiple scales is based upon 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 :

$$\dot{v}_f = \omega_\phi^0(\dot{\psi}, \dot{\xi}) + \varepsilon \omega_\phi^1(\dot{\psi}, \dot{\xi}) + \varepsilon^2 \omega_\phi^2(\dot{\psi}, \dot{\xi}) + \dots$$

$$p_f = \pi_\phi^0(\dot{\psi}, \dot{\xi}) + \varepsilon \pi_\phi^1(\dot{\psi}, \dot{\xi}) + \varepsilon^2 \pi_\phi^2(\dot{\psi}, \dot{\xi}) + \dots$$

$$c_f = \chi_\phi^0(\dot{\psi}, \dot{\xi}) + \varepsilon \chi_\phi^1(\dot{\psi}, \dot{\xi}) + \varepsilon^2 \chi_\phi^2(\dot{\psi}, \dot{\xi}) + \dots$$

$$\dot{v}_m = \omega_\mu^0(\dot{\psi}, \dot{\xi}) + \varepsilon \omega_\mu^1(\dot{\psi}, \dot{\xi}) + \varepsilon^2 \omega_\mu^2(\dot{\psi}, \dot{\xi}) + \dots$$

$$p_m = \pi_\mu^0(\dot{\psi}, \dot{\xi}) + \varepsilon \pi_\mu^1(\dot{\psi}, \dot{\xi}) + \varepsilon^2 \pi_\mu^2(\dot{\psi}, \dot{\xi}) + \dots$$

$$c_m = \chi_\mu^0(\dot{\psi}, \dot{\xi}) + \varepsilon \chi_\mu^1(\dot{\psi}, \dot{\xi}) + \varepsilon^2 \chi_\mu^2(\dot{\psi}, \dot{\xi}) + \dots$$

in which the functions $\dot{v}_f^i, p_f^i, c_f^i, \dot{v}_m^i, p_m^i, c_m^i$ are Ω -periodic and where \dot{y} and \dot{x} are the microscopic and the macroscopic dimensionless space variables, respectively, and are defined by:

$$\dot{y} = \frac{\dot{r}}{\lambda},$$

$$\dot{x} = \frac{\dot{r}}{\Lambda} = \varepsilon \dot{\psi},$$

(\dot{X} : physical space variable).

The method consists in incorporating these asymptotic expansions in the non-dimensional local description. This leads to governing equations and boundary-conditions at the successive orders of ε , 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 derived macroscopic models are the following:

Fluid flow

$$\dot{V}_f = -\tilde{K}_\phi \dot{\nabla} \Pi$$

$$\dot{\nabla} \cdot \dot{V}_f = 0$$

Solute transport

$$\text{Case I: } \frac{\partial C}{\partial t} - \dot{\nabla} \cdot (\tilde{D}_{eff} \dot{\nabla} C) = 0$$

(purely diffusive

behaviour)

$$\text{Case II: } \frac{\partial C}{\partial t} - \dot{\nabla} \cdot (\tilde{D}_{eff} \dot{\nabla} C - C \dot{V}_f) = 0$$

(convection-diffusion)

$$\text{Case III.a: } \frac{\partial C}{\partial t} - \varepsilon \dot{\nabla} \cdot [\tilde{D}_{disp} \dot{\nabla} C - \frac{1}{\varepsilon} C (\dot{V}_f + \varepsilon \dot{V}_m)] = 0$$

(dispersion with influence of the porous matrix)

$$\text{Case III.b: } \frac{\partial C}{\partial t} - \varepsilon \dot{\nabla} \cdot (\tilde{D}_{disp} \dot{\nabla} C - \frac{1}{\varepsilon} C \dot{V}_f) = 0$$

(dispersion)

\tilde{K}_f is the effective permeability tensor. \tilde{D}_{eff} is the effective diffusion tensor and \tilde{D}_{disp} is the apparent dispersion tensor. They are defined by boundary-value problems to be solved over the REV. \tilde{K}_f is a symmetrical tensor and depends only upon the geometry of the REV. \tilde{D}_{eff} is also symmetrical and depends upon the cell-geometry and the molecular diffusion. \tilde{D}_{disp} is not symmetrical in the general case and depends upon the pressure gradient.

VI. CONCLUSION.

An important conclusion drawn from this study is that the macroscopic description strongly depends upon the local transport regime (Pe_f) and in a less extent upon the order of magnitude of l_p/l . Four distinct continuous models for solute transport in fractured porous media have been derived.

In fractured porous media, dual-porosity effects appear only when the characteristic times of the involved physical processes are very different in the porous matrix and in the fractures. Thus, since the flow is steady-state, there is no dual-porosity effect in the macroscopic fluid flow equations (single-porosity model for fluid flow). In contrast, since the solute transport process is time-dependent, dual-porosity effects are present in all macroscopic transport equations, through the expressions obtained for \tilde{D}_{eff} (models I and II) and \tilde{D}_{disp} (models IIIa and IIIb). An important feature of model IIIa is that it shows an influence of the advection in the porous matrix at the macroscopic scale.

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