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# Continuous Models for Solute Transport in Fractured Porous media

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## Abstract

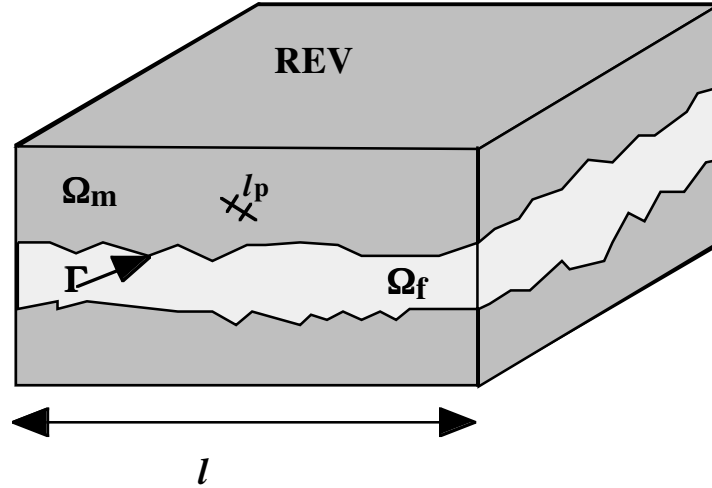
This work is aimed towards deriving mathematical models that describe pollutant migration through fractured porous media. A homogenisation method is used, i.e. macroscopic models are rigorously deduced from the physical description which is valid within a Representative Elementary Volume (REV). The fundamental assumption behind homogenisation is the separation of scales which is expressed by:  $l/L = \varepsilon \ll 1$ . In the present work,  $l$  is 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.

## 1. Introduction

Excavation of underground openings generates mechanical and hydrogeological disturbances of the host rock around the openings. The investigation of this excavation disturbed zone (EDZ) is of particular importance for the underground disposal of nuclear radioactive waste since its impact on the radionuclide migration from the waste to a potential outlet has to be investigated. According to a work performed in France - Tournemire research site for methodological studies in clay formation – (Boisson, 1998), the EDZ developed in indurated clays presents reactivation or/and creation of fractures as it can be observed in crystalline rocks. Oversimplified and conservative integrated approaches have led to represent the EDZ as a continuous high-permeability zone. The simulation of detailed retention phenomena like matrix diffusion will allow to move from conservative approaches to more realistic approaches. In an integrated performance assessment approach, numerical simulation and therefore accurate mathematical models are of importance for simulating flow and transport in media that account for the fracturing that may affect the host rock. The modelling strategy developed at IPSN (French Institute for Nuclear Safety and Protection) gives a great importance to continuum approaches, as it presents advantages for describing large time and space scales involved in the performance assessment studies.

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,  $\Omega_m$ , and of a fracture domain,  $\Omega_f$ , whose common boundary is denoted by  $\Gamma$  (see figure). 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  $\varepsilon$ . The medium is also assumed to be periodic and the period,  $\Omega$ , 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.



## 2. 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  $\Omega_f$

$$F_f \Delta \vec{v}_f - \vec{\nabla} p_f = \vec{0} \quad \text{where} \quad F_f = \frac{\mu V_{f_c}}{L \delta P}$$

( $\mu$ : viscosity;  $\vec{v}_f$ : fluid velocity in the fractures;  $p_f$ : fluid pressure in the fractures;  $\delta P$ : characteristic macroscopic pressure drop;  $v_{f_c}$ : characteristic value of  $\vec{v}_f$ )

$$\vec{\nabla} \cdot \vec{v}_f = 0$$

$$N_f \frac{\partial c_f}{\partial t} - \vec{\nabla} \cdot (\mathcal{D}_f \vec{\nabla} c_f - Pe_f c_f \vec{v}_f) = \vec{0} \quad \text{where} \quad N_f = \frac{L^2}{T_f D_{f_c}} \quad Pe_f = \frac{L V_{f_c}}{D_{f_c}}$$

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

- In  $\Omega_m$

$$\vec{v}_m = -Q_m \mathcal{K}_m \vec{\nabla} p_m \quad \text{where} \quad Q_m = \frac{l_p^2 \delta P}{\mu V_{m_c} L}$$

( $\vec{v}_m$ : fluid velocity in the porous matrix;  $p_m$ : fluid pressure in the porous matrix;  $l_p$ : characteristic pore-size;  $l_p^2 / \mu$ : estimation of the permeability;  $\mathcal{K}_m$ : dimensionless permeability tensor of the porous matrix)

$$\vec{\nabla} \cdot \vec{v}_m = 0$$

$$N_m \frac{\partial c_m}{\partial t} - \vec{\nabla} \cdot (\mathcal{D}_m \vec{\nabla} c_m - Pe_m c_m \vec{v}_m) = 0 \quad \text{where} \quad N_m = \frac{L^2}{D_{m_c} T_f} \quad Pe_m = \frac{LV_{m_c}}{D_{m_c}}$$

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

• On  $\Gamma$

$$\vec{v}_f = v \vec{v}_m \quad \text{where} \quad v = \frac{V_{m_c}}{V_{f_c}}$$

$$p_f = p_m$$

$$c_f = c_m$$

$$(\mathcal{D}_f \vec{\nabla} c_f) \cdot \vec{n} = d (\mathcal{D}_m \vec{\nabla} c_m) \cdot \vec{n} \quad \text{where} \quad d = \frac{D_{m_c}}{D_{f_c}}$$

### 3. Estimation of the Dimensionless Numbers

• Estimation of  $v = \frac{V_{m_c}}{V_{f_c}}$

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:

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

Thus, we get:

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

• Estimation of  $d = \frac{D_{m_c}}{D_{f_c}}$

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

Therefore

$$D_{m_c} = O(D_s) + O(D_{mol} \times \tau_m) = O(D_{mol}) \quad \text{and} \quad D_f = O(D_{mol}).$$

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

We therefore deduce that

$$d = \frac{D_{m_c}}{D_{f_c}} = O(1).$$

• Estimation of  $F_f = \frac{\mu V_{f_c}}{L \delta P}$

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  $Q_m = \frac{l_p^2 \delta P}{\mu V_{m_c} L}$

$Q_m$  can be expressed with respect to  $F_f$  as follows:

$$Q_m = F_f^{-1} \times \frac{l^2}{L^2} = O(1)$$

- Estimation of  $N_f = \frac{L^2}{T_f D_{f_c}}$  and  $Pe_f = \frac{LV_{f_c}}{D_{f_c}}$

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:

$$N_f = \frac{T_{d_f}}{T_f} \quad Pe_f = \frac{T_{d_f}}{T_{c_f}},$$

in which

$T_{d_f} = \frac{L^2}{D_{f_c}}$  is the characteristic time of diffusion in the fractures,

$T_{c_f} = \frac{L}{V_{f_c}}$  is the characteristic time of convection in the fractures.

Thus, we have:

$$\begin{cases} N_f = O(1) & \text{if } T_f = T_{d_f} \\ N_f = O(Pe_f) & \text{if } T_f = T_{c_f} \end{cases}$$

- Estimation of  $N_m = \frac{L^2}{T_f D_{m_c}}$  and  $Pe_m = \frac{LV_{m_c}}{D_{m_c}}$

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

$$N_m = d^{-1} N_f \quad Pe_m = O\left(\frac{l_p^2}{l^2}\right) \times d^{-1} Pe_f$$

#### 4. Definition of the 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:

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

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

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

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 -  $Pe_f < O(\varepsilon)$  - or lead to a non-homogenisable situation (i.e. when there is no equivalent macroscopic continuous description) -  $Pe_f > O(\varepsilon^{-1})$  -.

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 (Royet et al., 1996)):

$$\frac{l_p}{l} = O(\varepsilon^{1/2}); \quad \frac{l_p}{l} = O(\varepsilon); \quad \frac{l_p}{l} = O(\varepsilon^2)$$

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:

$$Pe_m = O\left(\frac{l_p^2}{l^2}\right) \times d^{-1} Pe_f = O\left(\frac{l_p^2}{l^2}\right) \times O(Pe_f)$$

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

$$Pe_m = O(\varepsilon^{-1}) \times O\left(\frac{l_p^2}{l^2}\right).$$

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

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

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

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

## 5. 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  $\varepsilon$ :

$$\phi = \phi^0(\vec{y}, \vec{x}) + \varepsilon \phi^1(\vec{y}, \vec{x}) + \varepsilon^2 \phi^2(\vec{y}, \vec{x}) + \dots \quad (\phi = \vec{v}_f, p_f, c_f, \vec{v}_m, p_m, c_m)$$

in which the functions  $\phi^i$  are  $\Omega$ -periodic and where  $\vec{y}$  and  $\vec{x}$  are the microscopic and the macroscopic dimensionless space variables, respectively, and are defined by:

$$\vec{y} = \frac{\vec{X}}{l} \quad \vec{x} = \frac{\vec{X}}{L} = \varepsilon \vec{y} \quad (\vec{X} : \text{physical space variable}).$$

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  $\varepsilon$ , 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

$$\vec{\nabla}_f \cdot \vec{v}_f = -\vec{\mathcal{D}}_f \vec{\nabla} P$$

$$\vec{\nabla} \cdot \vec{v}_f = 0$$

### Solute transport

$$\text{Case I: } \frac{\partial C}{\partial t} - \vec{\nabla} \cdot (\vec{\mathcal{D}}_{eff} \vec{\nabla} C) = 0 \quad (\text{purely diffusive behaviour})$$

$$\text{Case II: } \frac{\partial C}{\partial t} - \vec{\nabla} \cdot (\vec{\mathcal{D}}_{eff} \vec{\nabla} C - C \vec{v}_f) = 0 \quad (\text{convection-diffusion})$$

$$\text{Case III.a: } \frac{\partial C}{\partial t} - \varepsilon \vec{\nabla} \cdot [\vec{\mathcal{D}}_{disp} \vec{\nabla} C - \frac{1}{\varepsilon} C (\vec{v}_f + \varepsilon \vec{v}_m)] = 0 \quad (\text{dispersion - influence of the porous matrix -})$$

$$\text{Case III.b: } \frac{\partial C}{\partial t} - \varepsilon \vec{\nabla} \cdot (\vec{\mathcal{D}}_{disp} \vec{\nabla} C - \frac{1}{\varepsilon} C \vec{v}_f) = 0 \quad (\text{dispersion})$$

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

## 6. 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  $\mathbf{D}_{eff}$  (models I and II) and  $\mathbf{D}_{disp}$  (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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