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# Homogenization of Contaminant Transport in Fractured Porous Media

P. Royer, Laboratoire Sols, Solides, Structures, (UJF, INPG, CNRS), BP 53X, 38041  
Grenoble cedex, France, Pascale.Royer@hmg.inpg.fr

C. Serres, Institut de Protection et de Sûreté Nucléaire, Département d'Evaluation de la Sûreté,  
BP 6.92265 Fontenay-aux-Roses, France, Christophe.Serres@ipsn.fr

## 1 Introduction

In the scope of performance assessment of a deep geological repository for nuclear wastes, numerical simulations, and therefore accurate mathematical models are of importance for a better understanding of underground contaminant migration. A common feature of the potential geological formations selected in France for nuclear wastes repository is the presence of discontinuities at several length scales. As a result, flow and transport models must account for the fractured nature of 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 is more suitable for describing the large scale involved in the performance studies.

This work is aimed towards deriving the macroscopic governing equations of contaminant transport in a fractured porous medium. Such a medium is locally characterised by a representative elementary volume (REV) whose size is  $O(l)$  and that consists of a porous matrix domain,  $\Omega_m$  and a fracture domain,  $\Omega_f$ , whose common boundary is denoted  $\Gamma$  (figure 1).

At the local scale, (i.e. at the REV scale), contaminant transport is governed by the following equations.

In the fractures ( $\Omega_f$ ):

$$\mu \Delta \vec{v}_f - \vec{\nabla} p_f = \vec{0}, \quad (\text{Stokes equation}) \quad (1)$$

$$\vec{\nabla} \cdot \vec{v}_f = 0, \quad (\text{mass balance equation}) \quad (2)$$

$$\frac{\partial c_f}{\partial t} - \vec{\nabla} \cdot (\vec{D}_f \vec{\nabla} c_f - c_f \vec{v}_f) = 0, \quad (\text{diffusion-convection equation}) \quad (3)$$

where  $\vec{v}_f$ ,  $p_f$ ,  $c_f$  and  $\vec{D}_f$  are the velocity, pressure and concentration fields and the tensor of molecular diffusion in the fractures, respectively.

In the porous matrix ( $\Omega_m$ ):

$$\vec{v}_m = -\vec{K}_m \vec{\nabla} p_m, \quad (\text{Darcy's law}) \quad (4)$$

$$\vec{\nabla} \cdot \vec{v}_m = 0, \quad (\text{mass balance equation}) \quad (5)$$

$$\frac{\partial c_m}{\partial t} - \vec{\nabla} \cdot (\vec{D}_m \vec{\nabla} c_m - c_m \vec{v}_m) = 0, \quad (\text{diffusion-advection equation}) \quad (6)$$

where  $\vec{v}_m$ ,  $p_m$ ,  $c_m$  and  $\vec{D}_m$  are the velocity, pressure and concentration fields and the tensor of dispersion in the matrix, respectively.

On the boundary ( $\Gamma$ ):

$$\vec{v}_f \cdot \vec{n} = \vec{v}_m \cdot \vec{n} \quad (\text{continuity of fluxes}) \quad (7)$$

$$p_f = p_m \quad (\text{continuity of pressures}) \quad (8)$$

$$(\vec{d}_f \vec{\nabla} c_f) \cdot \vec{n} = (\vec{d}_m \vec{\nabla} c_m) \cdot \vec{n} \quad (\text{continuity of diffusive fluxes}) \quad (9)$$

$$c_f = c_m \quad (\text{continuity of concentrations}) \quad (10)$$

The essence of homogenization method is to determine an equivalent macroscopic behaviour by upscaling the local description. The purpose of the present study is to homogenize the local description (1-10), in order to determine the influence of the matrix-transport on the structure of the macroscopic transport equation.

The fundamental assumption behind homogenization theory is that the scales are separated:

$$l \ll L,$$

where  $l$  and  $L$  are the characteristic lengths at the heterogeneity scale and at the macroscopic scale, respectively. As this definition conjures up a geometrical separation of scales, we shall draw attention to the fact that this fundamental condition must also be checked regarding the phenomenon.

In this study, we use the method of homogenization for periodic structures, introduced by Bensoussan et al. (1978) and Sanchez-Palencia (1980). The key parameter of the model is the small parameter

$$\varepsilon = \frac{l}{L} \ll 1,$$

which is a measure of the separation of scales.

We also assume the medium to be periodic. This assumption is actually not a restriction: it allows determination of the macroscopic behaviour without any prerequisite on the form of the macroscopic equations. In the case of a periodic medium, the REV is merely the period.

In this study, we use the approach suggested in (Auriault, 1991), by which the problem is tackled in a physical rather than mathematical manner. Indeed, it offers the additional benefit that the conditions under which homogenization does apply are expressly stated. This formulation of the method is on the basis of definition and estimation of the non-dimensional numbers arising from

the local description under consideration. This fundamental step is called normalization and is aimed at specifying all cases that can be homogenized.

## 2 Normalization

The purpose of this section is to define the set of non-dimensional numbers that characterize the local description (1-9) and then to estimate them with respect to the small parameter  $\varepsilon$ . From equations (1) and (3), we can define

$$F_f = \frac{|\mu \Delta \bar{v}_f|}{|\bar{\nabla} p_f|}, \quad N_f = \frac{\left| \frac{\partial c_f}{\partial t} \right|}{|\bar{d} \bar{\nabla} c_f|}, \quad Pe_f = \frac{|c_f \bar{v}_f|}{|\bar{d} \bar{\nabla} c_f|} \quad (\text{Peclet number in the fractures}).$$

Similarly, equations (4) and (6) introduce

$$Q_m = \frac{|\tilde{K}_m \bar{\nabla} p_m|}{|\bar{v}_m|}, \quad N_m = \frac{\left| \frac{\partial c_m}{\partial t} \right|}{|\bar{d} \bar{\nabla} c_m|}, \quad Pe_m = \frac{|c_m \bar{v}_m|}{|\bar{d} \bar{\nabla} c_m|} \quad (\text{Peclet number in the porous matrix}).$$

Finally, from the boundary conditions (7) and (9) we get the two following non-dimensional numbers:

$$\frac{|\bar{v}_m \cdot \bar{n}|}{|\bar{v}_f \cdot \bar{n}|}, \quad \frac{|(\bar{d}_m \bar{\nabla} c_m) \cdot \bar{n}|}{|(\bar{d}_f \bar{\nabla} c_f) \cdot \bar{n}|}.$$

For estimating these non-dimensional numbers, let us consider  $L$  as the reference characteristic length. This arbitrary choice does not affect the final result. Thus, the numbers to be estimated in powers of  $\varepsilon$  are the following:

$$F_f = \frac{\mu V_{f_c}}{L \delta P}, \quad N_f = \frac{L^2}{D_{f_c} T_f}, \quad Pe_f = \frac{V_{f_c} L}{D_{f_c}}, \quad (\text{in the fractures})$$

( $V_{f_c}$  and  $D_{f_c}$  are characteristic values of the velocity and the molecular diffusion, respectively and  $\delta P$  is a characteristic macroscopic pressure drop).

$$Q_m = \frac{l_p^2}{L^2} \times \frac{V_{f_c}}{V_{m_c}} \times F_f^{-1}, \quad N_m = \frac{D_{f_c}}{D_{m_c}} \times N_f D_{f_c}, \quad Pe_m = \frac{V_{m_c}}{V_{f_c}} \times Pe_f, \quad (\text{in the porous matrix})$$

( $l_p$  is the characteristic length at the pore scale).

$$\frac{V_{m_c}}{V_{f_c}}, \frac{D_{m_c}}{D_{f_c}},$$

(on the boundary)

The goals of the analysis are two-fold:

- i) To define the conditions for which homogenization can be applied (homogenizable cases)
- ii) To draw the cases for which the matrix-influence is maximum.

It can be shown that the physics does impose (Auriault and Adler, 1995):  $F_f = O(\varepsilon^2)$ , and that a maximum influence of the matrix-transport is characterised by (Auriault, 1983), (Auriault and Lewandowska, 1995):

$$\frac{V_{m_c}}{V_{f_c}} = O(\varepsilon), \frac{D_{m_c}}{D_{f_c}} = O(\varepsilon^2).$$

Now, the equations describing the flow and the transport in the porous matrix are meaningful if  $l_p \ll l$ . Let us assume that  $\frac{l_p}{l} = O(\varepsilon)$ .

Therefore, the non-dimensional numbers related to the boundary conditions are defined by the above estimations. As for the non-dimensional numbers related to the porous matrix,  $Q_m$  is defined and  $N_m$  and  $Pe_m$  are such that:

$$N_m = O(\varepsilon^{-2})N_f, Pe_m = O(\varepsilon^{-1})Pe_f.$$

Note that the fact that a physical situation is homogenizable and that the influence of matrix-transport is maximum is, in particular, characterised by the order of magnitude:

$$\frac{Pe_m}{Pe_f} = O(\varepsilon^{-1}).$$

Now, it turns out that the orders of magnitude of  $Pe_f$  and  $N_f$  are linked and that three distinct orders of magnitude for  $Pe_f$  can be considered:

- i)  $Pe_f = O(\varepsilon)$  (dominant diffusion)
- ii)  $Pe_f = O(1)$  (equivalent diffusion and convection)
- iii)  $Pe_f = O(\varepsilon^{-1})$  (dominant convection)

Any other order of magnitude for  $Pe_f$  will lead to a non-homogenizable physical situation, i.e, a physical situation for which no continuous macroscopic description is conceivable. We have homogenized the local description corresponding to case ii). The macroscopic description is presented in the next section.

### 3 Scaled-up Model in the Case of Equivalent Diffusion and Convection in the Fractures

This case is characterised by the following estimations:

$$\begin{aligned} F_f &= O(\varepsilon^2), N_f = O(1), Pe_f = O(1). && \text{(in the fractures)} \\ Q_m &= O(\varepsilon), N_m = O(\varepsilon^{-2}), Pe_m = O(\varepsilon^{-1}). && \text{(in the porous matrix)} \\ \frac{V_{m\varepsilon}}{V_f} &= O(\varepsilon), \frac{D_{m\varepsilon}}{D_f} = O(\varepsilon^2) && \text{(on the boundary)} \end{aligned}$$

As a result, the non-dimensional local description is the following, in which all quantities are now non-dimensional quantities:

$$\varepsilon^2 \mu \Delta \bar{v}_f - \bar{\nabla} p_f = \bar{0} \quad \text{in } \Omega_f \quad (11)$$

$$\bar{\nabla} \cdot \bar{v}_f = 0 \quad \text{in } \Omega_f \quad (12)$$

$$\frac{\partial c_f}{\partial t} - \bar{\nabla} \cdot (\bar{d} \bar{\nabla} c_f - c_f \bar{v}_f) = 0 \quad \text{in } \Omega_f \quad (13)$$

$$\bar{v}_m = -\varepsilon \bar{K}_m \bar{\nabla} p_m \quad \text{in } \Omega_m \quad (14)$$

$$\bar{\nabla} \cdot \bar{v}_m = 0 \quad \text{in } \Omega_m \quad (15)$$

$$\frac{\partial c_m}{\partial t} - \bar{\nabla} \cdot (\varepsilon^2 \bar{d} \bar{\nabla} c_m - \varepsilon c_m \bar{v}_m) = 0 \quad \text{in } \Omega_m \quad (16)$$

$$\bar{v}_f \cdot \bar{n} = \varepsilon \bar{v}_m \cdot \bar{n} \quad \text{on } \Gamma \quad (17)$$

$$p_f = p_m \quad \text{on } \Gamma \quad (18)$$

$$(\bar{d}_f \bar{\nabla} c_f) \cdot \bar{n} = \varepsilon^2 (\bar{d}_m \bar{\nabla} c_m) \cdot \bar{n} \quad \text{on } \Gamma \quad (19)$$

$$c_f = c_m \quad \text{on } \Gamma \quad (20)$$

Applying homogenization (Auriault, 1991) to this local description leads to the following macroscopic behaviour:

$$\bar{V}_f = -\bar{K}_f \bar{\nabla} P, \quad (21)$$

$$\bar{\nabla} \cdot \bar{V}_f = 0, \quad (22)$$

$$\bar{\nabla} \cdot (\bar{D}_f^* \bar{\nabla} C_f - C_f \bar{V}_f) = \frac{\partial C_f}{\partial t} - \underbrace{\int_{-\infty}^t \hat{H}(t-\tau) \frac{\partial^2 C_f}{\partial t^2} d\tau}_{\text{Coupling effect with the matrix-transport}} \quad (23)$$

$\bar{K}_f$  and  $\bar{D}_f^*$  are the effective tensors of permeability and dispersion, respectively. They are symmetrical tensors and depend only upon the geometry of the periodic cell.

The influence of the porous matrix appears only in the transport equation (23) and, in particular, through the memory function  $\hat{H}(t)$ . The convolution product

$$\int_{-\infty}^t \hat{H}(t-\tau) \frac{\partial^2 C_f}{\partial t^2} d\tau$$

shows that the behaviour, at a given time, depends on the history of the second time derivative of the concentration.

#### 4 Conclusions

We have investigated the problem of contaminant transport in a fractured porous medium. An important conclusion drawn from this study is that the macroscopic description strongly depends upon the values of a set of specific physical parameters. Thus, we have defined three homogenizable physical situations for which the influence of matrix-transport is maximum.

In the present work, we have homogenized only one of these physical situations, which corresponds to equivalent diffusion and convection in the fractures. The macroscopic behaviour exhibits strong memory effects.

In the framework of performance assessment of a potential repository site, besides providing a model of solute transport in a fractured porous rock, as the analysis is focused at a particular scale, the present study also offers guidelines for the site characterisation.

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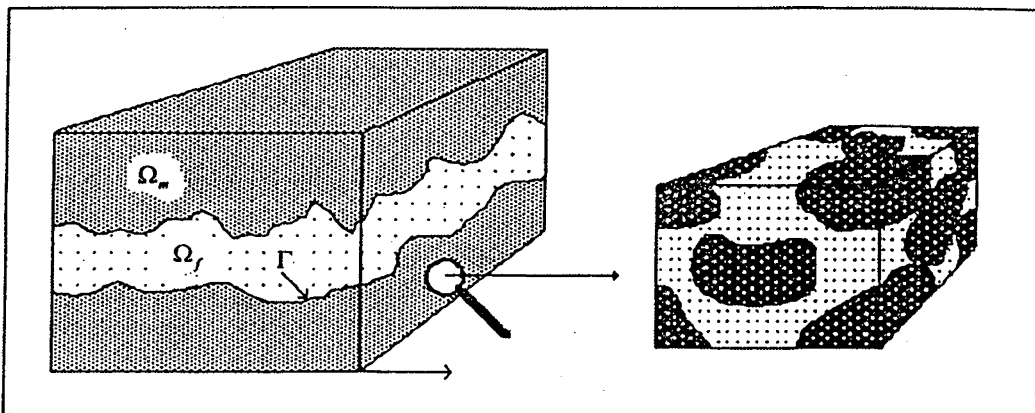


Figure 1: Periodic cell of the fractured porous medium.