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# A Large-Scale Model for Dissolution in Heterogeneous Porous Media

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**Key words:** upscaling, Large-scale model, Darcy-scale heterogeneity, Dissolution

## Abstract

Dissolution of pore-scale soluble substances occurs in applications from environmental hydrogeology to CO<sub>2</sub> storage. Development of Darcy-scale models has been widely discussed. This paper proposes an upscaling algorithm to develop large-scale models taking into account Darcy-scale heterogeneities. The theory is based on a comparison between the characteristic length-scale of the Darcy-scale heterogeneities and the length-scale of the dissolution front controlled by a Darcy-scale Damkehler number. The obtained large-scale model is shown to confront favorably to Darcy-scale direct numerical simulations.

## Introduction

In this paper we consider the dissolution of a soluble material (NAPL, deposited mineral) trapped in a porous structure as illustrated Fig. 1. The first upscaling development leading to a Darcy-scale description has received a lot of attention in the literature. The reader may refer to the theoretical work in [1, 2] for the development of local non-equilibrium models involving several Darcy-scale effective properties, in particular an active dispersion tensor and a source term corresponding to the mass exchange between the two Darcy-scale continua (liquid and soluble material). This latter term involves an exchange coefficient that will determine, through a Darcy-scale Damkehler number, the thickness of the dissolution front propagating into the porous medium.

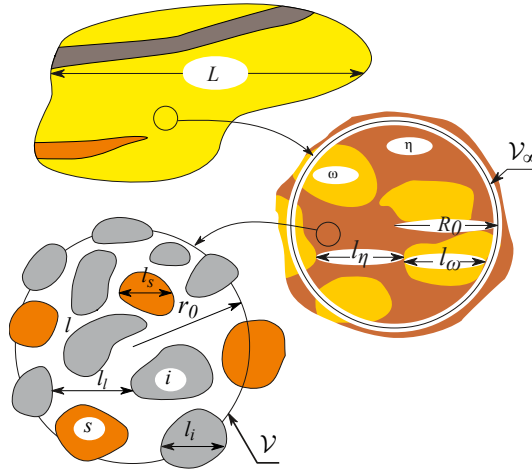


Figure 1: Multiple-scale features and averaging volumes

We consider here a simple version of this Darcy-scale model corresponding to the following Darcy-scale equations:

$$\nabla \cdot (\varepsilon_T (1 - S) \mathbf{U}_l) = 0 \quad (1)$$

$$\frac{\partial (\varepsilon_T (1 - S) C_l)}{\partial t} + \nabla \cdot (\varepsilon_T (1 - S) \mathbf{U}_l C_l) = -\alpha (C_l - C_{eq}) \quad (2)$$

$$\varepsilon_T \frac{\partial S}{\partial t} = \frac{\rho_l}{\rho_s} \alpha (C_l - C_{eq}) \quad (3)$$

The large-scale model is obtained in the case of a separation of scales characterized the following inequality

$$l_i, l_s, l_l \ll l_\omega, l_\eta \ll l_d \ll L \quad (4)$$

where  $l_i, l_s, l_l$  refers to the pore-scale,  $l_\omega, l_\eta$  to the Darcy-scale heterogeneities,  $l_d$  to the thickness of the dissolution front, and  $L$  to the large-scale domain, and which is enforced in the case of small Damkehler numbers. The

theory allows to develop a large-scale model involving large-scale averages denoted by a starred variable. For illustration, the large-scale mass balance equation is given by

$$\frac{\partial}{\partial t} (\{\varepsilon_T\} (1 - S^*) C_l^*) + \nabla \cdot (\{\varepsilon_T\} (1 - S^*) \mathbf{U}_l^* C_l^*) = -\alpha^* (C_l^* - C_{eq}) \quad (5)$$

where the large-scale coefficient  $\alpha^*$  is obtained from the resolution of a special closure problem. The theory is tested over different types of heterogeneous media. An example of the application to a stratified porous system is shown Fig. 2 which represent the direct Darcy-scale numerical results and the large-scale prediction. One sees that the large-scale prediction works very well, even for very sharp fronts, i.e., larger Damkhler numbers that one would expect from the constraint Eq. 4.

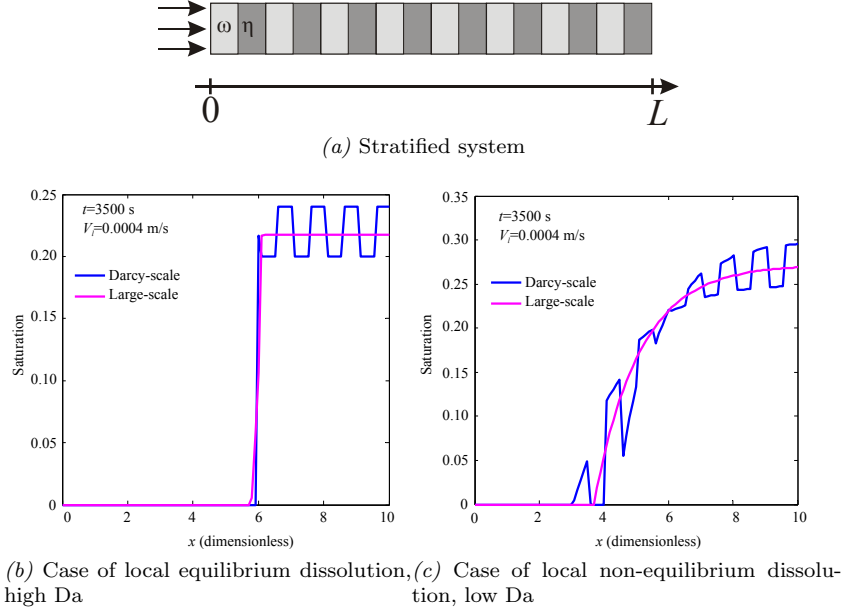


Figure 2: Dissolution of a partially soluble stratified porous medium

## References

- [1] M. Quintard and S. Whitaker. Convection, dispersion, and interfacial transport of contaminants: Homogeneous porous media. *Advances in Water Resources*, **17**, 221–239, (1994).
- [2] J. Guo, M. Quintard, and F. Laouafa. Dispersion in Porous Media with Heterogeneous Nonlinear Reactions. *Transport in Porous Media*, **109**, 541–570, (2015).