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A Large-Scale Model for Dissolution in Heterogeneous Porous Media

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Abstract

Dissolution of pore-scale soluble substances occurs in applications from environmental hydrogeology to CO2 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 Damkhler 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 Dary-scale continua (liquid and soluble material). This latter term involves an exchange coefficient that will determine, through a Darcy-scale Damkhler number, the thickness of the dissolution front propagating into the porous medium.

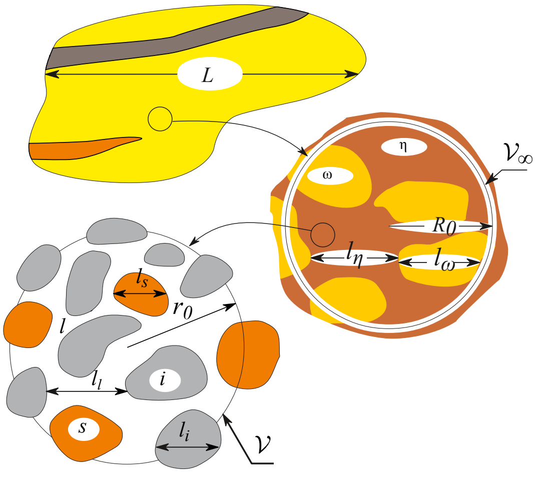


Figure 1: Multiple-scale features and averaging volumes

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

$$\nabla \cdot \left(\varepsilon_T (1-S)\, \mathbf{U}_l\right) = 0 \tag{1}$$

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

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

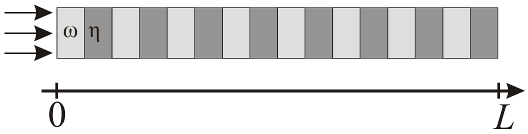
The large-scale model is obtained in the case of a separation of scales characterized the following inequality

$$l_i, l_s, l_l \ll l_\omega, l_\eta \ll l_d \ll L \tag{4}$$

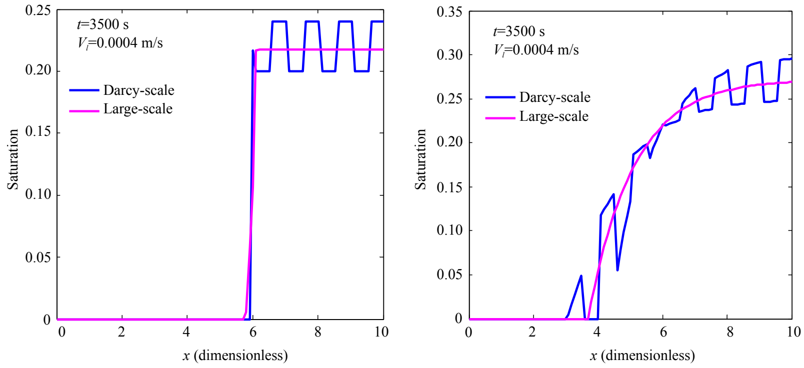
where l_i, l_s, l_l refers to the pore-scale, l_ω, l_η to the Darcy-scale heterogeneities, l_d to the thickness of the dissolution front, and L to the large-scale domain, and which is enforced in the case of small Damkhler numbers. The theory allows to develop a large-scale model involving large-scale averages denoetd by a starred variable. For illustration, the large-scale mass balance equation is given by

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

where the large-scale coefficient α^* is obtained from the resolution of a special closure problem. The theory is tested over different types of heterogenous media. An example of the application to a stratifed porous system is shown Fig. 2 which represent the direct Darcy-scale numerical results and the large-scale prediction. On 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.



(a) Stratified system



(b) Case of local equilibrium dissolution, high Da

(c) Case of local non-equilibrium dissolution, low Da

Figure 2: Dissolution of a partially soluble stratified porous medium

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