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Q1 Upscaling diffusion waves in porous media

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HIGHLIGHTS

- Diffusion waves in porous media are studied.
- Upscaling is made with volume averaging methods.
- The upscaled equations governing diffusion waves are established.
- The effective diffusivities of diffusion waves are estimated.

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ABSTRACT

The aim of this work is to derive the effective-medium equations and to estimate the related effective diffusivities for diffusion waves in porous media. Effective diffusivities are estimated within the framework of the volume averaging method, where they are obtained from the solution of the associated closure problems in 2D and 3D periodic unit cells. The results showed that the transport of diffusion waves are governed by the diffusion and co-diffusion mechanisms of harmonic waves. In addition, numerical results showed that the effective diffusivities increase with frequency, while the effective co-diffusivities display a resonance-like behavior. Our results also indicate that geometry plays a more significant effect over the predictions of the co-diffusion coefficient at moderate frequencies and it mainly influences the predictions of the direct diffusivity at low frequencies (*i.e.*, $\omega^* \ll 1$).

1. Introduction

Q3 Consider the diffusion problem in a two-phase domain composed of a fluid phase (γ-phase) saturating the pores of a rigid porous medium (κ-phase) as sketched in Fig. 1. Assume that diffusion transport of a chemical species (species A) through the γ-phase is Fickian and it is governed by

$$\frac{\partial \rho_\gamma(\mathbf{x},t)}{\partial t} = \nabla\cdot\left[\mathscr{D}_\gamma \nabla \rho_\gamma(\mathbf{x},t)\right], \quad \text{in the } \gamma\text{-phase} \tag{1}$$

where $\rho_\gamma(\mathbf{x},t)$ is the density of the transported matter (*e.g.*, solutes, phonons, etc.) in the γ-phase, $\mathscr{D}_\gamma$ is the mixture diffusivity and $\mathbf{x}$ is a position vector. Assuming that the solid phase is impermeable to mass transport, we may impose the following boundary condition

$$-\mathbf{n}_{\gamma\kappa}\cdot\mathscr{D}_\gamma\nabla\rho_\gamma(\mathbf{x},t) = 0, \quad \text{at the } \gamma\kappa\text{-interface.} \tag{2}$$

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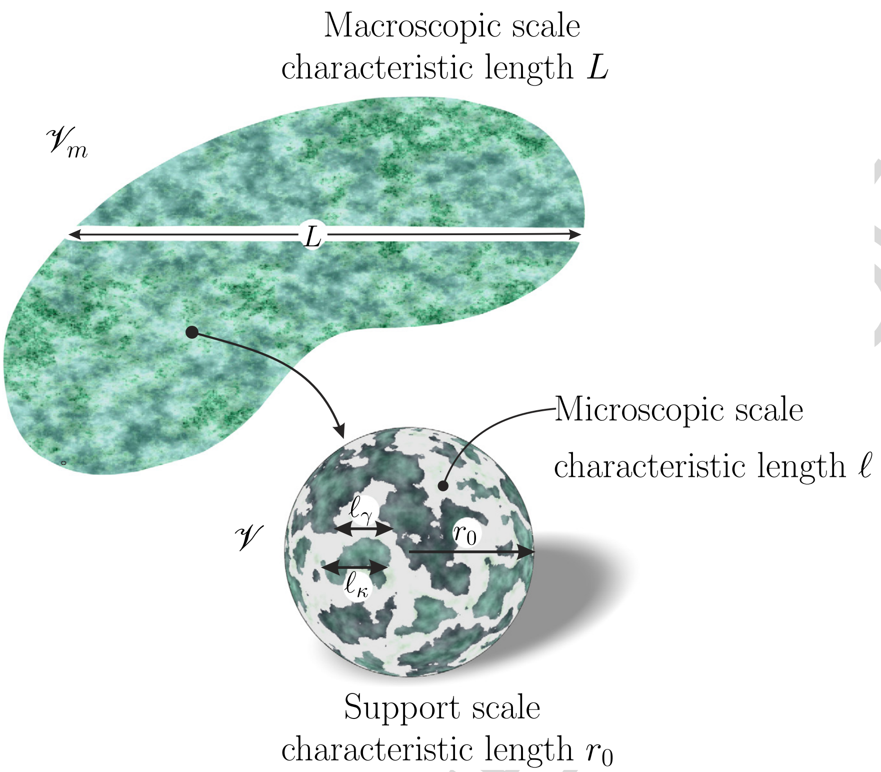

Fig. 1. Sketch of the system including the characteristic scales and lengths.

Eqs. (1) and (2) are valid in the entire macroscopic domain $\mathscr{V}_m$ sketched in Fig. 1. In the following, let us assume that the density $\rho_\gamma(\mathbf{x}, t)$ is a function of time in such a way that its variations can be expressed as an infinite Fourier time series of a fundamental frequency, ω:

$$\rho_\gamma(\mathbf{x}, t) = a(\mathbf{x}) + \sum_{k=1}^{\infty} b_k(\mathbf{x}) \sin(k\omega t) + c_k(\mathbf{x}) \cos(k\omega t) \tag{3}$$

where the harmonic coefficients $a(\mathbf{x})$, $b_k(\mathbf{x})$ and $c_k(\mathbf{x})$ are functions of position and have the same units as the density $\rho_\gamma(\mathbf{x}, t)$. In this way, the harmonic coefficients will be considered as density fractions of the total oscillatory density $\rho_\gamma(\mathbf{x}, t)$.

Density variations like those in Eq. (3) can arise when the density in some domain or boundary region is perturbed periodically. Hence, the harmonic oscillations $\sin(k\omega t)$ and $\cos(k\omega t)$ can be conceived as *diffusion waves* propagating in a non-uniform medium [1]. These waves cannot be beamed, lack of wave fronts and do not travel very fast. Diffusion waves appear in the context of thermal waves, physics of plasma waves, turbid media, among others [2]. Solute density waves can be detected in the mass transfer mechanisms involved in stratified media [3,4], electrolytes [5], membranes [6], and cardiac arrhythmias [7]. In some instances (*e.g.*, biological tissues) the transport medium is not uniform, but it can be considered as a composite medium with permeable and non-permeable fractions like the porous medium sketched in Fig. 1. Furthermore, under certain growth conditions, cell populations move like traveling waves at constant speed as noted by Kennedy and Aris [8]. This effect can be used for *in situ* bioremediation processes of contaminated soils using chemosensitive bacteria (*cf.* [9]). In such case, the presence of the non-permeable κ-phase can lead, via accumulation–depletion effects [1], to complex density patterns in the γ-phase domain.

Commonly, pseudo-homogeneous or effective-medium representations of the transport phenomena in porous media are obtained to estimate the effective transport properties of the underlying mechanisms [10]. This means that the essential features of transport phenomena taking place at the microscale are captured by effective-medium coefficients and the system can be conceived as a new continuum. Handling the infinite number of oscillatory components in the Fourier time series in Eq. (3) is, in general, not a trivial problem. In many instances, the consideration of the fundamental oscillatory components $\sin(k\omega t)$ and $\cos(k\omega t)$ can provide valuable information about the effective transport properties as functions of frequency. In this regard, given a porous medium configuration, the problem to be addressed is to derive a pseudo-homogeneous (*i.e.*, effective medium) representation of the harmonic components of the density $\rho_\gamma(\mathbf{x}, t)$. The harmonic balance of Eq. (3) in the governing Eqs. (1) and (2) yields the following boundary-value problems: