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An Ohm's law analogy for the effective diffusivity of composite media

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HIGHLIGHTS

- An Ohm's law analogy for effective diffusivity in composite media is studied.
- Particles are seen as charges moving in an electrical resistance arrangement.
- Good agreement with Brownian particle simulations was found.

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ABSTRACT

The aim of this work is to obtain an equation for the effective diffusivity of permeable composite media based on an analogy with Ohm's law of electricity. Here, particles are transported across a composite medium, which is seen as an arrangement of series and parallel resistances. Comparison with simulations of Brownian particles traveling through the successive walls of the medium showed good agreement for moderate inclusion-to-continuous medium diffusivity ratio.

1. Introduction

Diffusion transport in inhomogeneous medium composed of different materials is found in a large diversity of applications, including biological tissues, filtration, oil recovery, chromatography, composite materials, etc. Commonly, the inhomogeneous material is composed of a continuous phase and inclusions of other materials that can be or not permeable to the transport of particles. Macroscopically, the diffusion transport can be described by a linear relationship between the macroscopic flux J and the average density gradient $\nabla\rho$; namely, $J = -D_{eff}\nabla\rho$, where D_{eff} is the effective (i.e., average) diffusivity of the medium. In general terms, the determination of the effective diffusivity requires knowledge of the interface geometry and the physical properties of the individual phases. It should be commented that a similar problem can be obtained in the description of other transport coefficients in a diversity of two-phase systems, like electrical conductivity [1], thermal conductivity [2], magnetic permeability [3], elastic modules [4], etc.

The prediction of the effective diffusivity of composite media where all phases are permeable to diffusion transport has a long history, starting with Maxwell-Garnett results [5]. For a composite medium with diffusivity D_I for inclusions and diffusivity D_C for the continuous medium, the Maxwell-Garnett expression for the effective diffusivity is given by

$$\frac{D_{eff}}{D_C} = 1 + \frac{d(D_I - D_C)\phi_I}{D_I + (d-1)D_C - (D_I - D_C)\phi_I} \tag{1}$$

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where ϕ_I is the inclusion volume fraction and d is the space dimension (either $d = 2$ or $d = 3$). Kalnin et al. [6,7] developed generalizations of the Maxwell-Garnet equation by considering the partial trapping of diffusing particles by an inclusion as well as the effects of energy barriers for the particle penetration in an inclusion:

$$\frac{D_{eff}}{D_C} = \frac{1}{1-\phi_I + k\phi_I}\left[1 + \frac{d(D_I k - D_C)\phi_I}{D_I k + (d-1)D_C - (D_I k - D_C)\phi_I}\right] \tag{2}$$

where k is a correction to the Maxwell-Garnet equation in order to account for a jump in concentration on the inclusion-continuous matrix boundary. It was shown that this correction factor can be taken as the density ratio $k = \rho_I/\rho_C$, where ρ_I and ρ_C are average particle densities (i.e., concentrations) in the inclusions and the continuous matrix, respectively. The main drawback of the Kalnin's correction given by Eq. (2) is that the correction factor k is, in general, not known in advance. If the composite is considered as a serial arrangement of grains and along the direction of the diffusion, it was found that the effective diffusivity can be expressed [8] as follows:

$$\frac{D_{eff}}{D_C} = \frac{D_I D_C}{\phi_I D_C + \phi_C D_I}. \tag{3}$$

Eq. (3) is quite simple, requiring only individual diffusivities and volume fractions. Hickey et al. [9] derived a mean-field expression for the effective diffusivity in a two-phase medium consisting of a hydrogel with large gel-free solvent inclusions, in terms of the homogeneous diffusivities in the gel and in the solvent. Upon comparing with exact numerical lattice calculations, it was found that the proposed expression provided accurate prediction for the effective diffusivity over a wide range of gel concentration and relative volume fraction of the two phases. Kingsburry and Slater [10] extend the Hickey et al.'s results by including local interactions between the gel and the analyte, interfacial effects between the main phase and the inclusions, and a possible incomplete separation between the two phases. Along the same line, Zhang and Liu [11] included the effect of partitioning between different phases and presented an approach to obtain the equations relating bulk diffusivity to individual-phase diffusivities in heterogeneous media. More recently, Kalnin and Kotomin [12] derived an expression for the effective diffusivity in one-dimensional discrete lattice model of random walks in matrix with inclusions and unequal hopping lengths. Indeed, the analytical results obtained were in good agreement with computer simulations of stochastic trajectories.

Brownian particles across a permeable composite medium can be seen as moving in the direction of a density gradient and constrained by the intrinsic resistance of the medium. Although Brownian particles move in several erratic directions, the imposition of a gradient at a given direction can provide a relative order to the bundle of trajectories into a composite medium. In this way, one can establish an analogy with the Ohm's law for the transport of electrical charges in a resistive circuit. This analogy is explored in this work to show that the effective diffusivity equation (3) can be derived from an analogy with the Ohm's law. Strict simulations of Brownian particles are used to assess the predictability of Eq. (3), finding good agreement for moderate inclusion-to-continuous medium diffusivity ratio.

2. Effective diffusivity from an analogy based upon Ohm's law

Consider the diffusion transport through a permeable composite formed of N parallel walls of different diffusivity, as shown in Fig. 1. For a given external density gradient $\delta\rho = \rho_a - \rho_b$ and by imposing continuity of density at interfaces, it can be shown that the steady-state particle flux, J, across the composite is given by

$$J = \frac{\delta\rho}{R_T} \tag{4}$$

where

$$R_T = \sum_{i=1}^{N} \frac{L_i}{D_i}. \tag{5}$$

Also, L_i and D_i are the width and the diffusivity of the ith wall. Note that Eq. (1) has the form of Ohm's law for electron transport. Here, R_T is seen as the total resistance obtained from a series circuit. The effective diffusivity, D_{eff}, of the composite is obtained by considering the flux J under the same external density gradient $\delta\rho = \rho_a - \rho_b$. That is,

$$\frac{L_T}{D_{eff}} = \sum_{i=1}^{N} \frac{L_i}{D_i} \tag{6}$$

where $L_T = \sum_{i=1}^{N} L_i$. Eq. (3) can be written as

$$D_{eff} = \frac{1}{\sum_{i=1}^{N} \frac{\phi_i}{D_i}} \tag{7}$$