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Asymmetrical diffusion across a porous medium-homogeneous fluid interface

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HIGHLIGHTS

- Fluid–porous medium interfaces exhibit sharp geometric and diffusion transitions.
- Brownian dynamics simulations were used for studying the diffusion.
- Asymmetrical diffusion across the interface was detected.
- Asymmetries are explained by the advection-like effects at the interface.

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ABSTRACT

Interfaces formed by a homogeneous fluid and a porous media are commonly found in nature and applications. This work uses Brownian motion simulations for exploring the effects of the interface in the diffusion transport of passive particles. The results revealed that the diffusion transport is asymmetric in the sense that particles migrate faster in the porous medium-to-homogeneous fluid interface than in the opposite direction. Besides, such asymmetry is stronger as the porosity decreases. Macroscopic model using volume averaging methods showed that the asymmetrical diffusion effect is induced by sharp transitions in porosity and effective diffusivity in a vicinity of the interface.

1. Introduction

Many natural and practical systems with diffusive mass transport are formed by a homogeneous fluid region and an adjacent porous medium saturated by the same fluid [1]. Examples of this class of configurations are filtration processes, ground water pollution, drying processes, separation membranes, transport in biological tissues, among many others. In general, the transport properties at the fluid bulk are well understood and diverse theoretical and experimental schemes are available nowadays. On the other hand, important efforts have been devoted to the experimental [2–4] and theoretical [5–8] determination of effective diffusivities for homogeneous porous media. However, the description of the diffusion of particles around the fluid–porous medium inter-region has received less attention due to the difficulty of understanding the geometrical effects of the transition region on the effective transport parameters. In particular, sharp variations of the porous medium properties (e.g., porosity) and transport parameters (e.g., diffusivity) around the fluid–porous medium inter-region hamper the derivation of models describing the macroscopic diffusion phenomenon.

Experimental results describing the diffusion transport across fluid–porous medium interfaces are scarce. Recent experimental results have shown evidence of asymmetrical dispersive transport of conservative tracers across interfaces

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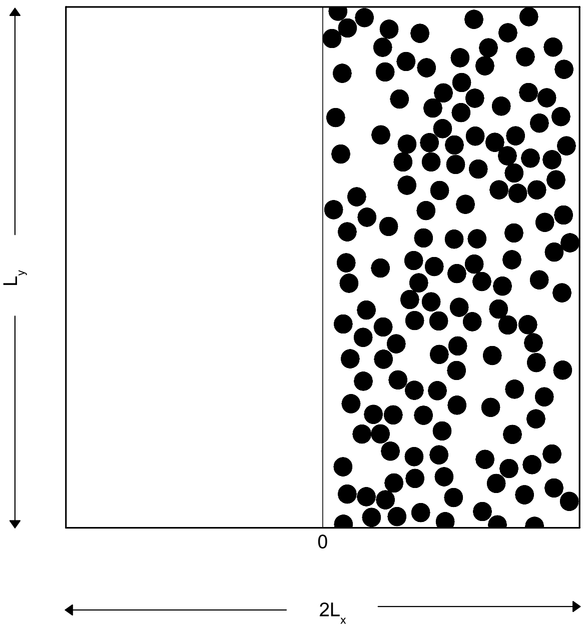

Fig. 1. Schematic diagram of the transport system. The porous medium is represented by circular obstacles with non-overlapping configuration.

between different porous materials [9,10]. Breakthrough curves showed that tracers migrating from fine medium to coarse medium arrive significantly faster than those in the opposite direction. On the other hand, some results regarding the macroscopic modeling have been reported in the recent years. The one-domain approach considers the porous medium as a continuum with effective transport coefficients, and the transition from the fluid to the porous medium is achieved through a continuous transition of properties, such as diffusivity and porosity [11]. In contrast, the two-domain approach describes the porous medium and the fluid according to the inherent properties of each region. Contrary to the one-domain approach, a model matching problem to couple the transport in both homogeneous regions needs to be addressed, resulting in the so-called jump boundary conditions [12]. These jump conditions often contain coefficients whose dependence of the local geometry of the inter-region is missing. To this end, some approximate approaches have been proposed [13]. In general, the derivation of macroscopic models for describing diffusion between a porous medium and a homogeneous fluid is made from volume averaging techniques [14], which leads to the formulation and solution of closure problems linked to effective transport parameters.

The region between a porous medium and a homogeneous fluid commonly involves sharp geometric (e.g., porosity) and transport (e.g., effective diffusivity) parameters. Despite the importance of such systems for natural and application systems, studies describing the effects of sharp transitions in the diffusion transport of passive particles are still lacking. Motivated by this, the aim of this work is two fold:

- To use Brownian random walk simulations for gaining insights in the effects of interfaces in the diffusion transport of passive particles. In analogy to recent experiments for packed columns [9], breakthrough curves show that tracers migrating from the porous medium to the homogeneous fluid arrive significantly faster than those in the opposite direction.
- To formulate a macroscopic diffusion model accounting for asymmetrical diffusion across porous medium-fluid interfaces. It is shown that asymmetrical transport can be modeled as an advection-like phenomenon induced by porosity and effective diffusivity transitions in the interface vicinity.

Overall, the results in this work indicate that transitions in the medium structure can lead to interesting transport effects that can be exploited for applications (e.g., mass transport rectification).

2. Methods

2.1. System description

The system under consideration consists of a two-dimensional saturated porous medium and a homogeneous fluid. The porous medium is composed by N_{obs} non-overlapping circular obstacles of radius R, randomly distributed in the right segment. Fig. 1 presents a schematic description of the porous medium system. Tracers are allowed to move either from the left to the right boundary or vice versa.