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Estimation of thermal and mass diffusivity in a porous medium of complex structure using a lattice Boltzmann method

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Abstract

The thermal and mass diffusivity in a porous medium of complex structure is studied by using the lattice Boltzmann method. The media under consideration include two-dimensional medium with an array of periodically distributed circular and square cylinders, three-dimensional granular medium of overlapping or non-overlapping spherical and cubical inclusions of different size, and randomly generated fibrous medium. The calculated effective diffusivities are in good agreement with existing analytical and numerical results when the inclusions, regardless of their shapes, are not overlapped. For the medium of overlapping inclusions, the effective diffusivity deviates from existing correlations as the inclusion fraction increases. In particular, the deviation increases dramatically if the thermal diffusivity of the inclusion is greater than that of the fluid in the medium for enhanced thermal conduction. A new empirical correlation between the effective diffusivity and the volume fraction for the medium of overlapping inclusions is proposed.

Keywords: Lattice Boltzmann method; Porous medium; Granular/fibrous inclusions; Effective thermal/mass diffusivity

1. Introduction

The macroscopic effective transport properties of a porous medium, such as permeability and diffusivity, are of great practical importance in applications of heat exchangers, filtration systems, or any engineering device that utilizes a porous medium. It is because that the microscopic flow analysis in the pore region of a porous medium is neither computationally feasible nor cost-effective when only the macroscopic behavior of the transport phenomenon is of interest.

For permeability, Jeong et al. [1] carried out a series of calculations using the lattice Boltzmann method (LBM) and obtained the drag characteristics of the porous medium of various structures at different flow conditions. As for the subject of effective diffusivity and conductivity, it also has been treated by numerous researchers. Among theoretical approaches, Maxwell [2] calculated the effective electrical resistance of a compound medium consisting of scattered non-overlapping small spheres. Weissberg [3] estimated the upper bound of the effective diffusion coefficient in a porous medium in terms of simplified statistical parameters by considering idealized spheres whose centers are randomly placed. The results can be applied to randomly overlapped spheres of either uniform or non-uniform sizes. For the fibrous medium, Koch and Brady [4] developed a theory based on ensemble averages to determine the effective diffusivity. They also examined the effects of the Peclet number, $Pe = Ua/D_C$, where U is the average velocity through the bed, a is the fiber radius, and D_C is the molecular diffusivity of the solute in the fluid. Using the weighted geometric mean, Nield [5] proposed a formula for the effective thermal conductivity for a porous medium whose constituents have moderately different conductivities.

For numerical approaches, Monte Carlo simulations have been carried out to investigate the Knudsen diffusion

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Nomenclature

C	macroscopic mean concentration
c_Q	lattice dependent coefficient
D,D_{eff}	diffusivity, effective diffusivity
D_P	local molecular or thermal diffusivity
D_C,D_I	molecular or thermal diffusivity of the fluid and the solid
d	diameter of a fiber
e_α,$e_{\alpha i}$	discrete velocity, microscopic velocity
f_α,$\tilde{f}_\alpha$	pre- and post-collision state of the particle distribution function
f_α^{eq}	equilibrium particle distribution function
J_α,K_α	specially chosen constants for heat or mass-transfer simulation, Eq. (2)
L	side length of the calculation domain
u_i	macroscopic velocity

Greek symbols

ε	porosity
ϕ	solid volume fraction
τ	non-dimensional relaxation times
ξ	concentration of species or temperature

of gases and the effective diffusivities in the porous medium of various structures. Riley et al. [6] applied Monte Carlo simulations to obtain the effective diffusivities in porous media whose inclusions have different diffusivity from that of bulk phase. They considered two-dimensional (2D) rounded inclusions or three-dimensional (3D) spherical inclusions of uniform size and three types of structure: uniformly placed non-overlapping inclusion, inclusion clustered in groups of 50, and arbitrarily overlapping inclusion. Trinh et al. [7] determined the effective diffusion coefficients in a porous medium by using Monte Carlo simulations of point-like molecules in random and structured media. For the structured media, uniformly distributed inclusions of circular or square cylinders in 2D and spheres or cubes in 3D were considered with staggered, in-line and face-centered arrangements. All the inclusions were impermeable. Sahimi and Stauffer [8] used the lattice gas automata model to calculate the permeability and effective diffusivity of 2D stratified and heterogeneous porous media. Alvarez-Ramirez et al. [9] calculated the effective diffusivity of a 2D heterogeneous medium of irregular shape for various inclusion fractions using the LBM. Their results were in good agreement with Monte Carlo simulations of tracer diffusion as well as Maxwell's equation when the inclusion fraction is small.

The LBM is computationally more efficient than the direct simulation Monte Carlo method and the lattice gas automata model. Therefore it is adopted in the current study. The objectives of this research are twofold. The first objective is to examine thermal conductivity and mass diffusivity in both 2D and 3D porous media of various structures by using the LBM, and compare the results with existing analytical and numerical studies. The second objective aims to improve the empirical correlation between the effective diffusivity and the volume fraction for some porous media. The structure of the porous medium depends on the way how it is made, and on the type or purpose of experiment. For example, for solid oxide fuel cells (SOFC), some inclusions are overlapped, but some are non-overlapped. Thus, both overlapped and non-overlapped cases are considered here. The media under consideration include the granular medium made up of 2D circular and square cylinders, 3D spheres and cubes in staggered and in-line arrangements, and 3D fibrous media of cylindrical shape. Because the effective mass diffusivity and the effective thermal conductivity of a medium are governed by the equations of the same form, no distinction between them is made in estimation of these properties.

2. Numerical method

The discretized Boltzmann equation without an external forcing term reads

$$f_\alpha(\vec{x}+\vec{e}_\alpha\delta t, t+\delta t) - f_\alpha(\vec{x}, t) = -\frac{1}{\tau}(f_\alpha - f_\alpha^{\text{eq}})|_{(\vec{x},t)} \tag{1}$$

where f_α is the particle distribution function, $e_{\alpha i}$ is the microscopic velocity, and τ is the non-dimensional relaxation time.

For thermal or mass transport, the equilibrium distribution function is expressed as [10]

$$f_\alpha^{\text{eq}} = \xi(J_\alpha + K_\alpha e_{\alpha i}\cdot u_i) \tag{2}$$

Here the concentration ξ is given by

$$\xi = \sum_\alpha f_\alpha \tag{3}$$

and J_α and K_α are constants, where J_α is determined from $\sum_\alpha f_\alpha^{\text{eq}} = \sum_\alpha f_\alpha$ and $K_\alpha = 1/2$.

Usually, the D2Q9 square lattice and the D3Q15 15-velocity LBM models shown in Fig. 1 are used for 2D and 3D simulations [11]. However, it has been known that, for the mass transport simulation, the lattice directions may be reduced from 9 to 5 and 15 to 7 for 2D and 3D cases, respectively, without degrading the accuracy [12].