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Investigation of two-phase flow in porous media using lattice Boltzmann method

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ABSTRACT

In this paper penetration of a liquid drop in a porous media is investigated by the lattice Boltzmann method (LBM). Two-phase flow has been simulated by the Lee method which is based on the Chan–Hilliard binary fluid theory. The contact angle between solid, liquid and gas phases has been considered in the simulations. The porous medium is generated by locating square obstacles randomly in a domain. The Reynolds number, the Froude number, the Weber number, viscosity and density ratios are numbered as the non-dimensional flow parameters which influence the domain. The porosity, the Darcy number and the pore to solid length ratio are the non-dimensional characteristics of the porous structures affecting the penetration of liquid inside the porous media. To ensure the validity of the code, the release of a square drop in the computational field was tested and the equilibrium contact angle between the droplet and solid surface was modeled according to Lee. Penetration and the non-absorbed coefficient have been presented to show penetration of the drop. Investigation of numerical results showed that increasing the Reynolds number, the Froude number, porosity and density ratio will increase the penetration rate while increasing the Weber number causes scattering of the drop.

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1. Introduction

Wide ranges of droplet penetration applications in porous substrates have led to myriad experimental and numerical investigations [1–3]. Any increase in the quality of inkjet printers depends directly on the droplet radius after impingement on a porous surface and its spreading rate. Environmental applications, such as hazard assessment of the accidental release of liquids onto the soil [4], are mainly concerned with the evaporation rate of the liquid droplet, which is a function of the wet spot area on the surface of the porous medium, exposed to the atmosphere, as well as the penetration depth. Most of the studies focus on the droplet impact on non-permeable and permeable surfaces based on CFD approaches [5–9]. Recently researchers have been trying to develop fluid flow modeling especially two-phase flows, using the lattice Boltzmann method (LBM) because of its exclusive features such as parallelism of computation, capture of the complex geometries and simple coding. In order to simulate two-phase flows, Shan and Chen [10] proposed a facile method which is executable in complex geometries. He et al. [11] developed the LBM two-phase modeling by introducing two distinct distribution functions for the evaluation of mass, momentum and pressure, but they did not distinguish between thermodynamic and dynamic pressures. In their work parasitic velocities at the interface area have been reduced, but they did not disappear completely. To simulate the contact angle in this method, Shiladitya Mukherjee and John Abraham [12] introduced an external force which acts on a wall and its strength controls the wettability of the surface. Recently Lee [13] suggested a two-distribution function LBE method in which the incompressibility is enforced by the pressure evolution equation. As long as the intermolecular force is

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expressed in the potential form, the incompressible LBE method for binary fluids is able to eliminate parasitic currents. His method can simulate two-phase flow in the wide ranges of density and viscosity ratios (up to 1000). To model the contact line dynamics on partially wetting surfaces T. Lee and L. Liu [14] developed Lee's method for incompressible binary fluids.

In the current work we have imposed Lee's method in a porous substrate and investigated droplet dynamics after impingement on the permeable surface. Then the effects of flow and substrate characteristics variations have been discussed comprehensively.

2. Simulation of two-phase flow

2.1. Two-phase flow models

Discretization of the force terms in the LBM is considered as a major factor causing the numerical instability and limitation in its use in practical cases as the Shan and Chen model. Using a method that uses the proper expression for the pressure term can be useful in stabilizing the simulations. Taehun Lee in 2005 [15] presented a stable LBM method to simulate the two-phase flow with high viscosity and density ratios by a low Mach number assumption and utilizing the stress and potential forms of the surface tension force. In the absence of external forces, errors resulting from the discretization appear as parasitic velocities near the interface area. Numerical instability will increase with increase in both surface tension and amount of parasitic velocities. Two mechanisms have been proposed to reduce parasitic velocities in the LBM. One is modification of the pressure gradients and surface tension terms formulations and the other one is using the sharp interface method [13]. Wagner [16] showed that using the potential form of surface tension instead of the pressure form could eliminate the parasitic velocities. Lee in 2009 [13] presented a method for simulating the binary fluid flow based on the Cahn–Hilliard diffuse interface theory.

2.2. Cahn–Hilliard model

By assuming a binary flow, using the continuity equation for each phase leads to evaluation of composition C as follows:

$$\frac{\partial \tilde{\rho}_i}{\partial t} + \nabla(\tilde{\rho}_i \mathbf{u}_i) = 0, \tag{1}$$

where $\tilde{\rho}_i$ is related to local density and $\mathbf{u}_i$ is the velocity of the i-th component ($i = 1, 2$). The total density $\rho = \sum_{i=1}^{2} \tilde{\rho}_i$ is also conserved. For convenience, one chooses the heavier fluid as species 1 and the lighter fluid as species 2. Volume diffusive flow rate $\mathbf{j}_i$ is related to local density and velocity of the i-th component by

$$\rho_i \mathbf{j}_i = \tilde{\rho}_i(\mathbf{u_i} - \mathbf{u}), \tag{2}$$

where $\mathbf{u}$ is the volume averaged velocity, and ρ_i is the constant bulk density.

By definition of $C = \tilde{\rho}_1/\rho_1$, Eq. (1) can be rewritten as

$$\frac{\partial C}{\partial t} + \nabla(\mathbf{u}C) = -\nabla \mathbf{j_1}. \tag{3}$$

If the diffusive flow rate does not relate to the densities but to the local compositions of two components, it yields $\mathbf{j}_1 = -\mathbf{j_2} = \mathbf{j}$ and from Eq. (3) $\nabla \mathbf{u} = 0$. This result is just satisfied in the LBM method at low Mach number. The diffusive flow rate is related to the gradient of the chemical potential μ by the Cahn–Hilliard advection equation:

$$\mathbf{j} = -M\nabla\mu, \tag{4}$$

where $M > 0$ is the constant mobility.

Cahn and Hilliard [17] asserted that the mixing energy density for an isothermal system takes the following form

$$E_{\text{mix}}(C, \nabla C) = E_0(C) + \frac{k}{2}|\nabla C|^2, \tag{5}$$

where k is the gradient parameter and E_0 denotes bulk energy by

$$E_0(C) \approx \beta C^2(C-1)^2, \tag{6}$$

where β is a constant. The classical part of the chemical potential is also derived by the derivative of E_0 with respect to C:

$$\mu_0 = \frac{\partial E_0}{\partial C}. \tag{7}$$

With the assumption of a short-range effect of liquid–gas interaction with a solid surface, the total free energy then takes the following form:

$$\Psi_b + \Psi_s = \int_V \left(E_0(C) + \frac{k}{2}|\nabla C|^2\right) dV + \int_S (\phi_0 - \phi_1 C_s + \phi_2 C_s^2 - \phi_3 C_s^3 + \cdots) dS. \tag{8}$$

The second term in Eq. (8) models the free energy associated with any interfaces in the system. The second integral in Eq. (8) is over the system's solid surface and is used to describe the interactions between the fluid and the solid surface. C_s is the composition at the solid surface and ϕ_i, $i = 0, 1, 2, 3, \ldots$ are constant coefficients.

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