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Benchmark solutions

Lattice Boltzmann simulation of pressure-driven two-phase flows in capillary tube and porous medium

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ABSTRACT

In this study, we present lattice Boltzmann simulations of two-phase immiscible displacements driven by constant pressure differentials. The method to implement the pressure boundary condition is based on bounce-back of the total non-equilibrium distribution. Simulations show that phase and pressure distributions are consistent with the imposed pressure boundaries. The accuracy was verified by simulating flows in a capillary tube, a problem with a moving interface for which an analytical solution is available. Following the verification, we simulated two-phase immiscible displacements in a random sphere packing and characterized the effects of capillary number, viscosity ratio, and wettability on the dynamics of displacement and the relative permeability.

1. Introduction

Direct numerical simulation of multiphase flows through porous media is an important approach to obtain fundamental understanding of this complex problem central to many natural and engineering processes [1–5]. By directly solving the dynamics of fluid motion in the pore space, the effects of density, viscosity, capillarity, gravity, and pore geometry on multiphase flows can be directly evaluated.

Numerical methods developed to directly solve multiphase flows in porous media include the phase field (PF) method [6–9], the volume-of-fluid (VOF) method [10–13], the level-set (LS) method [14–17], the density functional method (DFM) [18] and the lattice Boltzmann (LB) method [19–27]. In the PF method, the interface is described as a transition layer where unstable mixtures are stabilized by non-local energy terms. This interface layer, however, must be thin compared to other hydrodynamic length scales to ensure accuracy [8]. The VOF method, as its name implies, tracks the volume of each fluid in cells that belong to the interface [13]. The VOF algorithms consist of three parts: interface reconstruction, advection and surface tension. The LS method defines the interface by a level-set function [14] and has been widely used due to its simplicity [16]. Re-initialization techniques can be employed to overcome interface smearing and enforce mass conservation [17]. For porous media flows, capillary forces often dominate over viscous forces, and both VOF and LS methods face challenges [28]. In LB methods, phase segregation is modeled by inter-particle interactions and interface tracking is not always needed [29,30]. Similar to PF, in LB methods interfaces are diffuse and high computational cost is usually needed to reduce the effect of a finite interface thickness on multiphase hydrodynamics. Owning to LB methods' simplicity and high computational efficiency [31], they are widely used in direct simulation of multiphase flows [32–38].

Several multiphase LB models have been developed for simulation of multiphase flows, such as the color gradient model [19–21,31], the pseudo-potential model [22,23], the free energy model [24] and the mean-field model [29]. The color gradient model uses the local gradient in the phase field to separate the phases. Although early color gradient model was criticized to be time-consuming and high spurious velocities can occur near the interface [39], a benefit of the color gradient model is that interfacial tension, contact angle, viscosity ratio and density ratio can be adjusted separately [40] and in a wide range. The pseudo-potential model introduces a pseudopotential to account for particle interactions and has been widely employed due to its conceptual simplicity and computational efficiency [37]. In the pseudo-potential model, however, interfacial tension, density ratio and viscosity ratio cannot be adjusted independently. The free energy model imposes a non-ideal pressure tensor on the equilibrium distribution function. This model is thermodynamically consistent and conserves local mass and momentum [24]. The original free energy approach lacks Galilean invariance for the viscous term in the Navier–Stocks equation and efforts have been made to propose a Galilean invariant model [41,42]. In the literature, comparisons of the above three multiphase LB models have been carried out and

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it was shown that the color gradient model and the free energy model have similar capabilities [43,44] and are superior to the pseudopotential model. The mean-field model proposed by He et al. [29] incorporates molecular interaction forces to model the interfacial dynamics and is more flexible for implementation of thermodynamic models [45].

As with other computational methods, boundary conditions are important for LB simulations. With properly implemented boundary conditions, one can drive and control flows for better simulation of real flows. For single-phase flows, both pressure and velocity boundary conditions have been developed [46–49]. Maier et al. [46] proposed an extrapolation scheme for the distribution function that achieved fixed pressures at inlet and outlet boundaries. Zou and He [47] built another pressure and velocity boundary condition by applying a bounce-back rule to the non-equilibrium distributions on the boundary nodes. Zero transverse velocities were assumed at inlet and outlet. Zhang and Kwok [48] proposed a modified periodic boundary condition to incorporate pressure difference for fully developed flows. Their model preserved system periodicity and no unphysical inlet/outlet flow disturbance was observed. Later, Kim and Pitsch [49] examined a boundary closure scheme for both compressible and incompressible flows that shows a higher accuracy than Zhang and Kwok's work.

For multiphase LB methods, schemes to recover pressure or velocity boundary conditions are more involved than for single-phase LB, because constraints need to be set on the *total* particle velocity distributions that are related to the prescribed hydrodynamic conditions. The velocity distributions of *individual* components at the boundary need to be reconstructed carefully to avoid overly or inadequately defining the degree of freedom of the system. In the class of *open flow* boundary problems, pressure or velocity or both are specified at the inlet, and the outlet is set free. McCracken and Abraham [50] simulated such multiphase flows in the context of gas-gas mixing layers, using extrapolation boundary conditions. Dong et al. [51] simulated displacements in a channel using a velocity inlet and a free-flow boundary condition at the outlet. Lou et al. [52] specified velocity at the inlet and studied systematically the performance of extrapolation, Neumann, and convective outflow boundaries. In the class of *rate-driven* multiphase flows, velocity is specified at the inlet, and pressure is specified at the outlet. Huang et al. [53] conducted a study of immiscible displacement using a velocity boundary condition for the invading fluid at the inlet and a constant-pressure boundary condition for the defending fluid at the outlet based on the non-equilibrium bounce back assumption. The pressure of the defending fluid at the inlet and that of the invading fluid at the outlet were forced to be zero. The limitation of this implementation is that the constraints were imposed on distributions of individual components and not the total pressure. Later, Liu et al. [54] correctly simulated liquid CO_2 displacement of water with a constant flow rate imposed at the inlet and a constant pressure specified at the outlet.

In *pressure-driven* multiphase flows, pressures are specified at both inlet and outlet boundaries. Velocity and phase distribution, on the other hand, are allowed to freely evolve. For such flows there has not been a focused LB study. In some LB studies, a uniform body force was used to replace a pressure difference. However, even for single-phase flows it is known that pressure boundaries cannot always be replaced by a body force [48,55].

In this work, we incorporated a two-phase extension of Zou and He's non-equilibrium bounce-back method [47] into a LB multiphase flow simulator that uses a color gradient model with Multi-Relaxation-Time (MRT) collisions. By bouncing back the non-equilibrium part of the *total* distribution, the *total* pressure at the boundaries can be set. The fractions of the two fluids at the inlet and the outlet, as well as the velocities at the inlet and the outlet, are not constrained. We simulated several cases of pressure-driven multiphase flows, including flows through a porous medium where we extracted pressure and saturation profiles and relative permeability for comparison and discussion.

The materials in this article are organized as follow. In Section 2, we briefly cover the two-phase color gradient lattice Boltzmann method used in this study. In Section 3, we present details of the pressure boundary condition. In Section 4, we first examine the phase distributions and pressure fields of two-phase flows driven by the pressure boundary condition. Then, the accuracy of the method is tested by simulations of displacements in a capillary tube. In the end, simulations of displacements with different capillary numbers, viscosity ratios, and wettability through a sphere packing are presented and analyzed. The density ratio was kept at unity in all simulations.

2. Two phase lattice Boltzmann method

In this study, we used a three-dimensional color gradient multiphase LB model with MRT collision. As MRT-color-gradient models have already been presented in detail in several references, e.g. [53], here we only provide a brief description. In the color gradient LB model, multiphase hydrodynamics is recovered from the evolution of two discrete velocity distribution functions f_i^k that represents the fraction of fluid particles of type k moving with lattice velocity $\boldsymbol{c_i}$. As with most color gradient models, we assigned values of R and B to k to represent *red* and *blue* components in the binary mixture, respectively. The lattice velocity $\boldsymbol{c_i}$ follow the three-dimensional 19-velocity (D3Q19) model

$$\boldsymbol{c}_i = \begin{cases} (0,0,0) \; i = 1 \\ (\pm 1,0,0),\;\; (0,\pm 1,0), (0,0,\pm 1) \; i = 2 \sim 7 \\ (\pm 1,\pm 1,0),\;\; (\pm 1,0,\pm 1), (0,\pm 1,\pm 1) \; i = 8 \sim 19 \end{cases} \tag{1}$$

Density ρ_k and hydrodynamic velocity $\boldsymbol{u}$ are calculated from the distribution functions using:

$$\rho_k = \sum_i f_i^k \tag{2}$$

$$\rho \boldsymbol{u} = \sum_i \sum_k f_i^k \boldsymbol{c_i} \tag{3}$$

$\rho = \rho_R + \rho_B$ is the total density.

In each time step, distribution functions f_i^k are updated by collision and propagation

$$f_i^k(\boldsymbol{x} + \boldsymbol{c}_i \Delta t,\; t + \Delta t) = f_i^k(\boldsymbol{x},\; t) + \Omega_i^k(\boldsymbol{x}, t) \tag{4}$$

$f_i^k(\boldsymbol{x},\; t)$ is the distribution function at position $\boldsymbol{x}$ and time t and $\Delta t = 1$ is the time step. Ω_i^k is the collision operator. For the color gradient model, Ω_i^k includes three parts [56]:

$$\Omega_i^k = \left(\Omega_i^k\right)^3 \left[\left(\Omega_i^k\right)^1 + \left(\Omega_i^k\right)^2\right] \tag{5}$$

$(\Omega_i^k)^1$ is the single-component collision operator that simulates viscous relaxation of stress within the binary mixture, $(\Omega_i^k)^2$ is the inter-component collision operator that provides a means to simulate interfacial tension, and $(\Omega_i^k)^3$ is the recoloring operator that forces the separation of the two components.

In this study, we only considered components of equal densities, and adopted MRT collision due to its superiority over BGK in numerical instability [57], suppression of spurious velocities [58,59] and minimization of the viscosity-dependence of permeability [35]. When two components have equal densities, it is not necessary to perform separate single-component and inter-component collisions [53,54]. The total distribution function $f_i = f_i^R + f_i^B$ was instead used in the single-component and inter-component collisions. It should be mentioned here that the MRT-color-gradient procedures presented in this section only apply to