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Study of immiscible displacements in porous media using a color-gradient-based multiphase lattice Boltzmann method

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ABSTRACT

A multiple-relaxation-time (MRT) Rothman and Keller (R–K) lattice Boltzmann model is presented for two phase flows with kinematic viscosity contrast. For two-phase flows in porous media, the numerical stability may be reduced due to the presence of complex wall boundaries. The MRT R–K model is shown to be able to ensure better numerical stability and reduce spurious currents significantly. The non-equilibrium bounce back scheme is extended to handle the pressure and velocity boundary condition in two-phase flow simulations. Immiscible displacement in complex heterogeneous media is investigated and three typical flow patterns are obtained, stable displacement, viscous fingering and capillary fingering. Cases with both capillary number Ca and viscosity ratio M ranging from 10^{-3} to 10^{3} are simulated. The three typical flow patterns correspond to the three domains in the M–Ca phase-diagram. The boundaries that separate the three domains in the model results are qualitatively consistent with previous experimental studies. The MRT R–K model coupled with the developed boundary condition is a good tool for the study of two-phase flows in porous media.

1. Introduction

Numerous macroscopic numerical methods have been developed for solving the two-phase Navier–Stokes (N–S) equations [1], such as the front-tracking method, volume-of-fluid (VOF) method, level set method, and so on. The former three methods are the most popular ones. However, the front-tracking method is usually not able to simulate interface coalescence or break-up [1,2]. In the VOF and level set methods, usually the interface reconstruction step or interface reinitialization is required, which may be non-physical or complex to implement [2]. Besides, numerical instability may appear when the VOF and level set methods are applied to simulate surface-tension-dominated flows in complex geometries [1].

In the last twenty years, the Lattice Boltzmann method (LBM) has been developed into a good tool to solve two-phase flow in porous media [3–8]. The LBM is a mesoscopic method and easily handles complex wall geometries. It is also an explicit method, which makes the code easy to parallelize. In the LBM, solving the Poisson equation is not required, hence it is more efficient than common macroscopic schemes.

There are many multiphase LBMs available in the literature, such as the Shan–Chen model [9], free energy model [10], Rothman–Keller model [11], and so on. The Shan–Chen multiphase model is the simplest one [4]. However, quantitative numerical study shows the existing model is not accurate [12] due to the inaccurate forcing term used in the model [13].

The first multi-component lattice gas model was proposed by Rothman and Keller [11]. The model was further developed by Gunstensen et al. [14] and an extra binary fluid collision was introduced into the Lattice Boltzmann equation. Latva-Kokko and Rothman [15] improved the recoloring step in the R–K model, reduced the lattice pinning effect and decreased the spurious currents [2,16]. Now that recoloring step is widely used in applications of the R–K model [2,12,17]. Recently, Reis and Phillips developed a two-dimensional nine-velocity R–K model [18]. In the model, a revised binary fluid collision is proposed and is shown to be able to recover the additional term which accounts for surface tension in the N–S equations [18].

Swift et al. analyzed the possible similarity between the free energy model and the R–K model [10]. However, the recoloring step in the R–K model prevented further theoretical comparative analysis between the two models. Numerical study shows that the numerical accuracy and efficiency of the free energy model and the R–K model are comparable [12], which suggests some potential similarity between the models.

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On the other hand, the ways of imposing wetting boundary conditions for the two models are very different [12]. For the free-energy model, the gradient of the density near the wall should be imposed and the normal derivative has to be calculated. To apply the condition, the densities of the surrounding lattice nodes near the wall are involved [19]. For example, using the free-energy model, Liu et al. achieved density ratio as high as $O(100)$ in their simulations [19], and they identified three typical flow patterns in the immiscible displacements in porous media. However, in their simulations, to get the surface normal derivative in an arbitrary inclined direction is not easy and hence, only simple squares are used to represent the solid grains [19].

For the R–K model, specifying the wetting condition is much simpler because only the densities of the two fluids in the solid nodes should be specified. Due to this simplicity, the R–K model has advantages over the free-energy model for two-phase flows in porous media. Hence, this model has been applied to simulations of multiphase flows in porous media [5,20]. However, most previous LBM studies are confined to only a narrow range of parameters [5,20,21]; for example, the maximum viscosity ratio in Ref. [5] is approximately 10.

Later, by introducing two free parameters in the rest equilibrium distribution function (DF), Grunau et al. [22] claimed the improved R–K model was able to simulate flows with different densities. However, it has been proved theoretically and numerically that this is not true for general two-phase flows [23,24]. The improvement proposed by Huang et al. [24] for the model is valid for cases with lower density ratios. Here, we focus on the model with identical densities but different viscosities.

Applying a more sophisticated finite difference method could make the color gradient more isotropic and eliminate the spurious currents around the bubble or droplet [25]. However, the more sophisticated finite difference has to include many surrounding points. For example, usually the color gradient can be obtained from the information on the surrounding 8 points in 2D simulations when the D2Q9 velocity model is used. However, the sophisticated finite difference requires information of the surrounding 25 points. Hence, it is not convenient to perform this sophisticated finite difference on the simulations of flow in porous media because the densities of the solid nodes inside the first layer of the wall, which may be used in the computation, are not specified and unknown.

As we know, reducing spurious currents is an important issue for multiphase models. In almost all of the lattice Boltzmann multiphase models, when surface tension increases, the magnitude of spurious current would increase to some extent [12,13]. In simulations of two phase flows with low capillary number ($Ca = \frac{\mu u}{\sigma}$, where μ, u, σ are fluid dynamic viscosity, characteristic flow velocity, and surface tension, respectively) in porous media, a large surface tension coupled with small spurious currents is preferred, otherwise the spurious current would affect the main flow (velocity is small) in the pore space.

It is also noted in the study of Liu et al. [19], the kinematic viscosity ratio of liquid and gas is kept unity and the dynamic viscosity ratio is equal to the density ratio. The minimum viscosity ratio seems limited to 10^{-2}. Here in the R–K method, the multiple-relaxation-time (MRT) collision model [26] is adopted. The present method is able to reduce spurious currents and improve numerical stability significantly. The multiphase flows with viscosity ratios ranging from 10^{-3} to 10^3 can be simulated. Those are good ranges for reproducing the capillary fingering phenomena for two phase flows in porous media. That will be discussed in Section 5 in detail.

The paper is arranged in the following way. First the present MRT R–K model is introduced. Then the properties of surface tension calculation, isotropy, spurious currents, and contact angle of this model are investigated. The MRT R–K LBM is shown to be more stable and able to reduce the spurious current further than the BGK model. Two dynamic multiphase flow problems are simulated to validate our numerical method. Finally, displacements in porous media with capillary numbers and viscosity ratios ranging from 10^{-3} to 10^3 are simulated. The simulated flow patterns are consistent with experimental studies [27].

2. Method

2.1. R–K model

In the R–K model, the particle distribution function (PDF) for fluid k is defined to be f_i^k. For two-phase flows, two distribution functions are defined, i.e., f_i^b, and f_i^r, where b and r denote 'blue' or 'red' component. The total PDF at $(\mathbf{x}, t)$ is $f_i(\mathbf{x}, t) = \sum_k f_i^k(\mathbf{x}, t)$.

Usually there are two steps implemented in the LBM, collision and streaming. In the R–K model, there are three steps for each component: streaming, collision, and recoloring. Suppose an iteration begins from the streaming step. We illustrate how the three steps construct a loop. The streaming step is [18]

$$f_i^k(\mathbf{x} + \mathbf{e}_i\delta t, t + \delta t) = f_i^{k+}(\mathbf{x}, t), \tag{1}$$

where f_i^{k+} is the PDF after the recoloring step. In the above equation, $\mathbf{e}_i$, $i = 0, 1, \ldots, b$ are the discrete velocities of the velocity models. For the D2Q9 velocity model ($b = 8$), $\frac{e_{ix}}{c}$, $\frac{e_{iy}}{c}$ are illustrated in the 4th and 6th row vectors, respectively in Appendix. Here c is the lattice speed defined to be $c = \frac{\delta x}{\delta t}$. We use the lattice units of 1 l.u. = 1δx, 1 t.s. = 1δt, and the mass unit is m.u. in our study.

The collision step can be written as [15]

$$f_i^{k*}(\mathbf{x}, t) = f_i^k(\mathbf{x}, t) + (\Omega_i^k)^1 + (\Omega_i^k)^2, \tag{2}$$

where $f_i^{k*}(\mathbf{x}, t)$ is the post-collision state. There are two collision terms in the equation, i.e., $(\Omega_i^k)^1$ and $(\Omega_i^k)^2$. If the lattice BGK scheme is adopted, the first collision term is

$$(\Omega_i^k)^1 = -\frac{\delta t}{\tau}\left(f_i^k(\mathbf{x}, t) - f_i^{k,eq}(\mathbf{x}, t)\right), \tag{3}$$

where τ is the relaxation time.

The equilibrium distribution function $f_i^{k,eq}(\mathbf{x}, t)$ can be calculated using [18]

$$f_i^{k,eq}(\mathbf{x}, t) = \rho_k\left(C_i + w_i\left[\frac{\mathbf{e}_i \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_i \cdot \mathbf{u})^2}{2c_s^4} - \frac{(\mathbf{u})^2}{2c_s^2}\right]\right), \tag{4}$$

where the density of the kth component is

$$\rho_k = \sum_i f_i^k, \tag{5}$$

and the total density is $\rho = \sum_k \rho_k$. The momentum is

$$\rho\mathbf{u} = \sum_k \sum_i f_i^k \mathbf{e}_i. \tag{6}$$

In the above formula, the coefficients are [18] $C_0 = \alpha_k$, $C_i = \frac{1-\alpha_k}{5}$, $i = 1, 2, 3, 4$ and $C_i = \frac{1-\alpha_k}{20}$, $i = 5, 6, 7, 8$, where α_k is a parameter that is assumed able to adjust the density of fluids [18,22] but this is not true [24]. The other parameters are $w_0 = \frac{4}{9}$, $w_i = \frac{1}{9}$, $i = 1, 2, 3, 4$, and $w_i = \frac{1}{36}$, $i = 5, 6, 7, 8$.

When the relaxation time parameters for the two fluids are very different, for example, $\tau_r = 0.501$ and $\tau_b = 1.0$, $\tau(\mathbf{x})$ at the interface can be determined by a simple way: $\psi(\mathbf{x}) = \frac{\rho_r(\mathbf{x}) - \rho_b(\mathbf{x})}{\rho_r(\mathbf{x}) + \rho_b(\mathbf{x})} > 0$, $\tau(\mathbf{x}) = \tau_r$ and otherwise $\tau(\mathbf{x}) = \tau_b$. To make the relaxation parameter ($\tau(\mathbf{x})$) change smoothly at the interfaces between two fluids, here we adopt the interpolation scheme constructed by Grunau et al. [18,22].