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LATTICE BOLTZMANN METHOD SIMULATION ON THE FLOW OF TWO IMMISCIBLE FLUIDS IN COMPLEX GEOMETRY*

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The multicomponent nonideal gas lattice Boltzmann model by Shan and Chen (S-C) can be used to simulate the immiscible fluid flow. In this paper, we show that the relaxation constant $\tau \leq 1$ is a necessary condition for the immiscible fluid flow in the S-C model. In a system with very complex boundary geometry, for $0.8 \leq \tau \leq 1$, the S-C model describes the immiscible flow quite well, and $\tau = 1$ is the best.

Keywords: lattice boltzmann method, immiscible fluid flow
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I. INTRODUCTION

The lattice Boltzmann method (LBM)[1,2] has become a promising tool to study the flow in very complex geometry.[3] Based on the lattice gas automata (LGA),[4] the LBM inherited most of the advantage of the LGA and eliminated the excessive statistical noise and the lattice artifacts such as the lack of the Galilean invariance. The LBM is ideally suited for computation on parallel computers since most algorithms only depend on nearest-neighbor information. It has shown great potential for the modeling of multicomponent fluid flow or flow in complexity geometry. The LBM can naturally incorporate interactions between different fluids and between fluids and solids.

There are several approaches to extend LBM for the study of immiscible fluids and flow in porous media. Rothman *et al.*[5] modeled immiscible fluids by introducing a mechanism that, according to information at neighboring lattice cells, alters the particle distributions at each lattice cell, enabling the pressure tensor to become anisotropic near the fluid-fluid interface. This approach has been applied to the study of multicomponent flow in porous media.[6] More recently, an alternative LB approach to modeling immiscible fluids has been developed by Shan and Chen.[7−10] Their approach (S-C model) involves the introduction of an external force at each cell as a function of neighboring cell properties. This force, assumed proportional to a parameter g_{12}, is used to modify the momentum values in the equilibrium distribution at the cell. A distinct feature of this formalism is that, although at each local cell there is a gain or loss of momentum, the global momentum conservation of the system is still exactly satisfied when boundary effects are excluded. However, the possibility of the application of the S-C model to the two-immiscible-fluid flow in the system with complex geometry is not clear. In this paper we will show that $\tau \leq 1$ is a necessary condition for the immiscible flow. For $0.8 \leq \tau \leq 1$, the S-C model can simulate the immiscible flow quite well, and $\tau = 1$ is the best. Moreover, the upper limit of g_{12} has to be lowered due to the boundary. We found that the upper limit of g_{12} depends on the complexity of the boundary condition.

This paper is organized in the following way. In Sec. II, a brief review of the LBM and the concept for dealing with fluid interaction is given. In Sec. III, we show that $\tau < 1$ is a necessary condition for the immiscible fluid flow in the S-C model. The effect of the boundary layer on the upper limit of g_{12} is discussed in Sec. IV. We give the conclusion in Sec. V.

II. THE MULTICOMPONENT LATTICE BOLTZMANN METHOD

In the multicomponent lattice Boltzmann model proposed by Shan and Chen,[7−10] the lattice Boltzmann equations for the kth component can be written in the form

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$$f_i^k(\boldsymbol{x}+\boldsymbol{e}_i,t+1)-f_i^k(\boldsymbol{x},t)=\Omega_i^k(\boldsymbol{x},t) \quad i=0,1,\cdots,8, \tag{1}$$

where $f_i^k(\boldsymbol{x},t)$ is the particle distribution in the ith velocity direction for the kth fluid at position $\boldsymbol{x}$ and time t. The index k runs from 1 to s, the total number of components. The collision term is

$$\Omega_i^k(\boldsymbol{x},t)=-\frac{1}{\tau_k}[f_i^k(\boldsymbol{x},t)-f_i^{k(eq)}(\boldsymbol{v}_k^{(eq)}(\boldsymbol{x},t))], \tag{2}$$

where τ_k is the dimensionless collision relaxation time for the kth component, and the equilibrium distribution of the species k as a function of $\boldsymbol{x}$, and t is given as

$$\begin{aligned}
f_0^{k(eq)} &= \frac{4}{9}\rho_k[1-\frac{3}{2}\boldsymbol{v}_k^{(eq)}\cdot\boldsymbol{v}_k^{(eq)}],\\
f_i^{k(eq)} &= \frac{1}{9}\rho_k[1+3(\boldsymbol{e}_i\cdot\boldsymbol{v}_k^{(eq)})+\frac{9}{2}(\boldsymbol{e}_i\cdot\boldsymbol{v}_k^{(eq)})^2\\
&\quad -\frac{3}{2}\boldsymbol{v}_k^{(eq)}\cdot\boldsymbol{v}_k^{(eq)}] \quad i=1,\cdots,4,\\
f_i^{k(eq)} &= \frac{1}{36}\rho_k[1+3(\boldsymbol{e}_i\cdot\boldsymbol{v}_k^{(eq)})+\frac{9}{2}(\boldsymbol{e}_i\cdot\boldsymbol{v}_k^{(eq)})^2\\
&\quad -\frac{3}{2}\boldsymbol{v}_k^{(eq)}\cdot\boldsymbol{v}_k^{(eq)}] \quad i=5,\cdots,8.
\end{aligned} \tag{3}$$

The (macroscopic) density of the kth fluid is calculated from $f_i^k(\boldsymbol{x},t)$ for $\rho_k(\boldsymbol{x},t)=\sum_{i=0}^8 f_i^k(\boldsymbol{x},t)$. The total density is $\rho(\boldsymbol{x},t)=\sum_k\rho_k(\boldsymbol{x},t)$. The (macroscopic) local velocity $\boldsymbol{v}$ is defined as $\rho(\boldsymbol{x},t)\boldsymbol{v}(\boldsymbol{x},t)=\sum_k\sum_{i=1}^8\boldsymbol{e}_i f_i^k(\boldsymbol{x},t)$. The equilibrium velocity $\boldsymbol{v}_k^{(eq)}$ is given by the relation

$$\rho_k\boldsymbol{v}_k^{(eq)}=\rho_k\boldsymbol{v}'+\tau_k\boldsymbol{F}_k, \tag{4}$$

where $\boldsymbol{v}'$ is a common velocity. $\boldsymbol{F}_k$ (to be given below) is the total interparticle force acting on the kth component. Thus, in this model, interaction of particles is through the equilibrium distribution. To conserve momentum at each collision in the absence of interaction (i.e., in the case of $\boldsymbol{F}_k$=0), $\boldsymbol{v}'$ has to satisfy the relation

$$\boldsymbol{v}'=(\sum_{k=1}^S\frac{\rho_k\boldsymbol{v}_k}{\tau_k})/(\sum_{k=1}^S\frac{\rho_k}{\tau_k}). \tag{5}$$

Hence, given f_i^k, ρ_k and $\boldsymbol{v}_k$ can be calculated, and then the $\boldsymbol{v}'$, $\boldsymbol{v}_k^{(eq)}$, and $f_i^{(eq)}$. The interaction force between particles of the kth component at site $\boldsymbol{x}$ and the k' component at site $\boldsymbol{x}'$ is assumed to be proportional to the product of their "effective mass" $\psi_i(\rho_k)$, defined as a function of local density. The total interaction force on the kth component at site $\boldsymbol{x}$ is

$$\boldsymbol{F}_k(\boldsymbol{x})=-\psi_k(\boldsymbol{x})\sum_{\boldsymbol{x}'}\sum_{\bar{k}=1}^S G_{k\bar{k}}(\boldsymbol{x},\boldsymbol{x}')\psi_{\bar{k}}(\boldsymbol{x}')(\boldsymbol{x}'-x), \tag{6}$$

where $G_{k\bar{k}}(\boldsymbol{x},\boldsymbol{x}')$ is a Green's function and satisfies $G_{k\bar{k}}(\boldsymbol{x},\boldsymbol{x}')$=$G_{k\bar{k}}(\boldsymbol{x}',\boldsymbol{x})$; $\psi_k(\boldsymbol{x})$ is a function of $\boldsymbol{x}$ through its dependence of ρ_k. If only homogeneous isotropic interation between the nearest neighbours are considered, $G_{k\bar{k}}(\boldsymbol{x},\boldsymbol{x}')$ can be reduced to the following symmetric matrix with constant elements,

$$G_{k\bar{k}}(\boldsymbol{x},\boldsymbol{x}')=\begin{cases}0, & |\boldsymbol{x}-\boldsymbol{x}'|>c,\\ g_{k\bar{k}} & |\boldsymbol{x}-\boldsymbol{x}'|\le c.\end{cases} \tag{7}$$

Here $g_{k\bar{k}}$ is the strength of the interaction potential between components k and $\bar{k}$; c is the lattice spacing (=1 in lattice unit). The effective mass $\psi_k(\rho_k)$ is taken to be ρ_k in this study; other choices will give a different equation of state. The total mass density of the whole fluid is defined as $\rho=\sum_k\rho_k$, and the whole fluid velocity $\boldsymbol{v}$ is defined by $\rho\boldsymbol{v}=\sum_k\rho_k\boldsymbol{v}_k+\frac{1}{2}\sum_k\boldsymbol{F}_k$.

The Chapman-Enskog method has been applied to the above lattice Boltzmann equation to derive a set of macroscopic equations for each component, which is very similar to the Navier-Stokes equations.[9,10]

Ⅲ. PARAMETER SETTING

Consider the case for two immiscible fluids. Let us rewrite the equations (1) and (2) as

$$\begin{aligned}
f_i^k(\boldsymbol{x}+\boldsymbol{e}_i,t+1) &= (1-\frac{1}{\tau_k})f_i^k(\boldsymbol{x},t)\\
&+\frac{1}{\tau_k}f_i^{k(eq)}(\boldsymbol{v}_k^{(eq)}(\boldsymbol{x},t)).
\end{aligned} \tag{8}$$

If the scheme is for the immiscible fluids, $f_i^k(\boldsymbol{x}+\boldsymbol{e}_i,t+1)$ in some velocity direction, say $i=N$, should be close to zero. Since $f_N^{k(eq)}(\boldsymbol{v}_k^{(eq)}(\boldsymbol{x},t))$ is non-negative, the only possibility for $f_N^k(\boldsymbol{x}+\boldsymbol{e}_i,t+1)=0$ is

$$\begin{cases}(1-\frac{1}{\tau_k})f_N^k(\boldsymbol{x},t)\le 0,\\ f_N^{k(eq)}(\boldsymbol{v}_k^{(eq)}(\boldsymbol{x},t))=0.\end{cases} \tag{9}$$

Consider that $f_i^k(\boldsymbol{x},t)$ is also non-negative, we get

$$\tau_k \leq 1. \tag{10}$$

In the S-C model, that the two fluids are immiscible is only an extreme case. If the tolerant error is 10^{-8}, numerically we find that $g_{12} = 0.64$ for $\tau_1 = \tau_2 = 1$ to get the best approach for the immiscible fluid domain. Simulations for larger g_{12} causes some distribution functions negative. Since the boundary condition adds additional perturbation on the interface, the value of g_{12} will be limited. In practical simulation, g_{12} has to be taken a smaller value (see below and Table 1).

Table 1. The upper limit of g_{12} in fluid domain and for different boundaries

τ	0.6	0.7	0.8	0.9	1.0
The upper limit of g_{12} in the fluid domain	0.1	0.19	0.29	0.42	0.64
The upper limit of g_{12} for plane boundaries	0.06	0.13	0.22	0.34	0.50
The upper limit of g_{12} for sinusoidal boundaries			0.18	0.28	0.38

IV. THE EFFECT OF THE BOUNDARY CONDITION ON THE UPPER LIMIT OF g_{12}

For the S-C model, it is well known that there must be a small amount of one phase fluid inside the other phase fluid, and the amount of each phase fluid is determined by the simulation process, otherwise there might be negative distribution functions. On the other hand, the distribution function at the boundary is determined by an appropriate boundary condition, which is quite different from that in the fluid domain. We find that the distribution function might be negative for sufficient large g_{12} even all the distribution functions are non-negative in the fluid domain. Consequently, in order to make all the distribution functions be non-negative, the upper limit of g_{12} has to be lowered for a definite tolerant error. For different boundary, the upper limit of g_{12} is different. For $\tau_1 = \tau_2 = 1$, the upper limit of g_{12} is 0.65 in fluid domain, 0.5 for the plane boundary, and 0.38 for the systems with complex boundary geometry. In Fig.1(a), we show the density profile for g_{12}=0.38, 0.5, 0.64. We find that even for $g_{12} = 0.38$, the thickness of the interface is of three layers, which can be a good approach to the immiscible fluid flow. When $\tau_1 = \tau_2 = 0.8$, the upper limit is 0.18 for the system with complex geometry. We show the density profile in Fig.1(b) for this case. It is clear that the interface is rather thick in this case. In fact, for $\tau_1 = \tau_2 = 0.6, 0.7$, the upper limit of g_{12} is so small that the fluids are not immiscible. In Table 1, we show the upper limit of g_{12} in the fluid domain, for plane boundaries and sinusoidal boundaries, as shown in Fig.2, under simple bounce-back rule boundary condition.

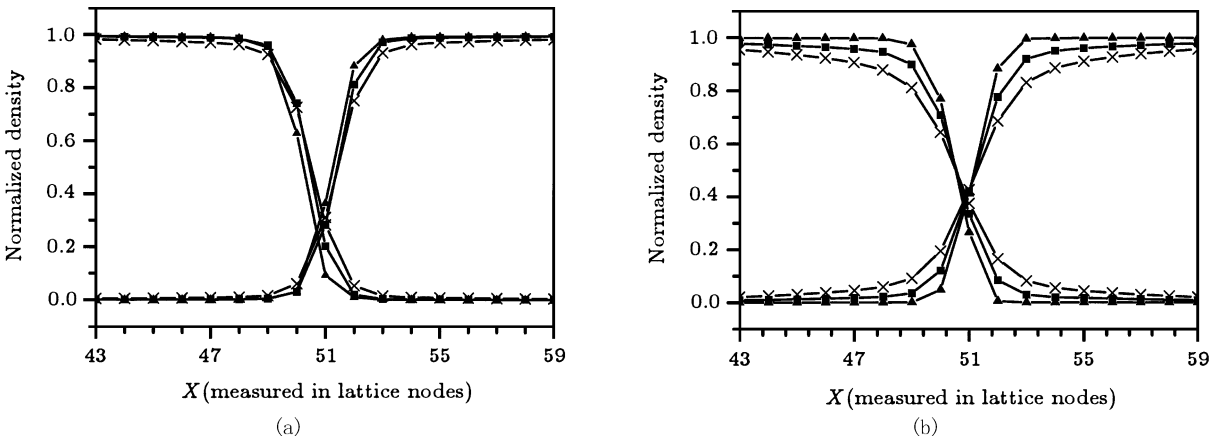

Fig.1. The normalized density profile. The triangles, diamonds and crosses are the calculated densities of phase one (or two) for (a) $\tau = 1$ and $g_{12} = 0.64, 0.5, 0.38$, respectively, (b) $\tau = 0.8$ and $g_{12} = 0.29$, $0.22, 0.18$, respectively. The solid, dashed, and dotted lines connect the calculated densities.

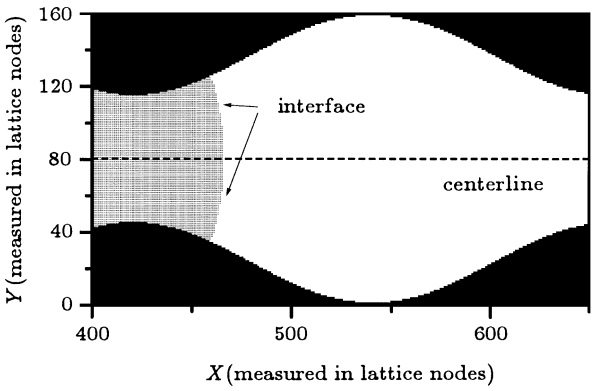

Fig.2. The sinusoidal tube considered in this paper. The shadowed area corresponds to phase one fluid and the empty part corresponds to phase two fluid.

V. CONCLUSION AND DISCUSSION

In this paper, we have shown that $\tau \leq 1$ is a necessary condition for the immiscible fluid flow in the S-C model. In a system with very complex boundary geometry, for $0.8 \leq \tau \leq 1$, the S-C model describes the immiscible flow quite well, and $\tau = 1$ is the best. Moreover, in the S-C model the viscosity is $(2\tau_k - 1)/6$ in a region of pure kth component. If we want to compare our simulation results with the experimental data, the viscosity has to be scaled according to the mesh and time scale. The limit of the selection of τ gives the constrain of the mesh and time scale.

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