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Numerical Simulation of the Droplet Dynamics with an Improved Pseudopotential Lattice Boltzmann Model

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In this paper, we extend an improved multi-component pseudopotential lattice Boltzmann model to simulate the dynamics of droplets with large density ratio and relatively large kinematic viscosity ratio. This improved model is validated to be feasible to simulate multiphase flow via examples of the stationary droplet, the droplet oscillation process, and the droplets collision. The results indicated that the improved model is effective for simulating multi-component multiphase flow with small spurious current. The spurious current reduces to 0.0072, which is much smaller than the spurious current (0.033) of the same order of magnitude density ratio in literature. For the droplet oscillation process with large density ratio, the numerically predicted oscillation period by the improved model is 2400, which agrees well with the analytical result. Finally, the droplets collision process with different impact parameters are studied by this improved model. It shows good agreement between the simulated results and the existing experimental results.

1. Introduction

The dynamic of droplets is one of the most common multiphase flow phenomena, such as the inkjet printing and the separation process of oil-gas in aircraft lubrication systems (Eastwick et al., 2006). Numerical simulation of droplets involves the tracking of interface between the different phases with traditional computational fluid dynamics (CFD) such as Level-Set method and Volume of Fluid method (Sussman, 2002). These methods require complex technologies to tracking or capturing interface. For this reason, there is a need for an alternative method to consider the interactions in microscopic level and the computational efficiency for engineering application.

The lattice Boltzmann (LB) method has many unique advantages, and it's a powerful tool for simulating complex flows (Chen and Doolen, 1998). Over the last few decades, several multiphase LB models have been developed (Gunstensen et al., 1991; Shan and Doolen, 1995; Swift et al., 1995). Due to its simplicity and versatility (Chen et al., 2014), the pseudopotential LB model, devised by Shan and Chen, has received a wildspread attention. However, there are several limitations with the pseudopotential LB model, such as large spurious currents and low density ratio. However, there are many real-world multiphase flows related to large density ratio (O(1000)). To overcome those drawbacks, there are many previous studies related to the improvements about pseudopotential LB model. Yuan and Schaefer (2006) raised the density ratio to 1000 by introducing various equations of state (EOS) to the pseudopotential LB model. Shan (2006) reduced the spurious currents by using the interaction force with high-order isotropic. Hu et al, Stiles and Xue took a similar approach to modify the equations of state by including a coefficient k. Hu et al. (2013) indicated that a smaller value of k led to smaller spurious currents and better numerical stability, which provides a new approach to adjust the surface tension. Stiles and Xue (2016) pointed out that a smaller value of k led to smaller interface thicknesses and smaller spurious currents. It is important to note that the studies mentioned above are almost improvements about single-component pseudopotential LB model. The multi-component pseudopotential LB model is needed for some cases in practical problems, and some works have focused on multi-component pseudopotential LB model. Bao and Schaefer (2013) developed a new multi-component pseudopotential LB model with large density ratio (O(1000)) by including the Peng-Robinson (P-R) EOS. However, the multi-component pseudopotential LB models mentioned in the above studies also have the disadvantages of large spurious currents and numerical instability, and most studies focused on stationary multiphase problems.

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We have improved a pseudopotential LB model in the previous study (Zhu et al., 2017). However, the study is still focused on stationary problems. In this paper, numerical simulations of the stationary droplet will be carried out by this improved multi-component pseudopotential LB model firstly. Then, it will be validated to be effective on simulating large density ratio (O(1000)) multiphase flow (the droplet oscillation process) via comparing with literatures and analytical results. Finally, we will propose this improved model for the dynamic multiphase problems of droplets collisions with large density ratio and relatively large kinematic viscosity ratio.

2. Improvements of the multi-component pseudopotential LB model

Our investigation adopts the MRT model for the collision operator, the LB-MRT equation with a force term can be expressed as the following form

$$\boldsymbol{f}_\sigma\left(\boldsymbol{x}+\boldsymbol{e}_i\delta_t,t+\delta_t\right)-\boldsymbol{f}_\sigma\left(\boldsymbol{x},t\right)=-\boldsymbol{M}^{-1}\boldsymbol{S}_\sigma\left[\boldsymbol{m}_\sigma\left(\boldsymbol{x},t\right)-\boldsymbol{m}_\sigma^{eq}\left(\boldsymbol{x},t\right)\right]+\boldsymbol{F}_\sigma\left(\boldsymbol{x},t\right) \tag{1}$$

where $f_\sigma(x,t)$ is the density distribution function of the component σ, x is the position, t is the time, M is the transform matrix, and M^{-1} is the inverse matrix of M. For D2Q9 model, the discrete velocities $\boldsymbol{e}_i$ are defined as

$$\boldsymbol{e}_i=c\begin{bmatrix}0&1&0&-1&0&1&-1&-1&1\\0&0&1&0&-1&1&1&-1&-1\end{bmatrix} \tag{2}$$

where $c=\delta_x/\delta_t$ is the lattice velocity. m and m^{eq} are the distribution function and the equilibrium distribution function, respectively.

The exact difference method force scheme, derived from the Boltzmann equation, is incorporated into the LB equation in this paper, and the force term is given as (Kupershtokh et al., 2009)

$$F_{\sigma,i}=f_{\sigma,i}^{eq}\left(\rho_\sigma,\boldsymbol{u}^{eq}+\Delta\boldsymbol{u}_\sigma\right)-f_{\sigma,i}^{eq}\left(\rho_\sigma,\boldsymbol{u}^{eq}\right) \tag{3}$$

where $\Delta\boldsymbol{u}_\sigma=\boldsymbol{F}_{\sigma,total}\delta t/\rho_\sigma$, and the total force $\boldsymbol{F}_{\sigma,total}$ acts on σ component. The equilibrium velocity $\boldsymbol{u}^{eq}$ is defined as

$$\boldsymbol{u}^{eq}=\sum_\sigma\rho_\sigma\boldsymbol{u}_\sigma\Big/\sum_\sigma\rho_\sigma \tag{4}$$

In the LB-MRT method, we can rewrite Eq. (3) as follows

$$\boldsymbol{F}_\sigma=\boldsymbol{M}^{-1}\left[\boldsymbol{m}_\sigma^{eq}\left(\rho_\sigma,\boldsymbol{u}^{eq}+\Delta\boldsymbol{u}_\sigma\right)-\boldsymbol{m}_\sigma^{eq}\left(\rho_\sigma,\boldsymbol{u}^{eq}\right)\right] \tag{5}$$

The average velocity before and after the collision is the actual physical velocity of the fluid mixture $\boldsymbol{u}_p$, which is calculated as

$$\rho\boldsymbol{u}_p=\sum_\sigma\rho_\sigma\boldsymbol{u}_\sigma+\frac{\delta_t}{2}\sum_\sigma F_{\sigma,total} \tag{6}$$

where $\rho=\sum_\sigma\rho_\sigma$ is the density of fluid mixtures.

With the intra molecule force and inter molecule force, the multiphase flow can be separated into the gas phase and the liquid phase. The intra molecule force is defined as

$$\boldsymbol{F}_{\sigma\sigma}=-g_{\sigma\sigma}\psi_\sigma\left(\boldsymbol{x}\right)c_s^2\sum_{i=1}^{N}w(\left|\boldsymbol{e}_i\right|^2)\psi_\sigma\left(\boldsymbol{x}+\boldsymbol{e}_i\right)\boldsymbol{e}_i \tag{7}$$

where $g_{\sigma\sigma}$ and ψ_σ are the intra molecule interaction strength and the effective mass, respectively. We consider N=8. $W(|e_i|^2)$ are the weights, w(1)=1/3, w(2)=1/12.

In this paper, σ=1 and σ=2 represent the liquid phase and the gas phase, respectively. The gas phase is regarded as an ideal gas, hence g_{22}=0. For the non-ideal liquid phase, we introduce the non-ideal EOS, and the effective mass ψ_1 is written as

$$\psi_1=\sqrt{\frac{2\left(p-c_s^2\rho\right)}{c_s^2g_{11}}} \tag{8}$$

It is found that g_{11} can be cancelled out when Eq. (8) is taken into Eq. (7). So g_{11}=-1 is given to ensure the value inside the square root of Eq. (8) is positive. We adopt the C-S EOS for liquid as follows

$$p=\rho RT\frac{1+b\rho/4+\left(b\rho/4\right)^2-\left(b\rho/4\right)^3}{\left(1-b\rho/4\right)^3}-a\rho^2 \tag{9}$$

where $a=0.4963(RT_c)^2/P_c$, $b=0.18727RT_c/P_c$, a=1, b=4, R=1, T_c=0.094, ρ_c=0.13044. We include a coefficient k in our multiphase pseudopotential LB model, then the modified EOS is given as

$$p' = kp = k\left(\rho RT\frac{1+b\rho/4+(b\rho/4)^2-(b\rho/4)^3}{(1-b\rho/4)^3}-a\rho^2\right) \tag{10}$$

To increase the rate to the equilibrium state, the inter molecule force is given by

$$\boldsymbol{F}_{12} = -g_{12}\varphi_1(\boldsymbol{x})c_s^2\sum_{i=1}^{N}w\left(|\boldsymbol{e}_i|^2\right)\varphi_2(\boldsymbol{x}+\boldsymbol{e}_i)\boldsymbol{e}_i \tag{11}$$

$$\boldsymbol{F}_{21} = -g_{21}\varphi_2(\boldsymbol{x})c_s^2\sum_{i=1}^{N}w\left(|\boldsymbol{e}_i|^2\right)\varphi_1(\boldsymbol{x}+\boldsymbol{e}_i)\boldsymbol{e}_i \tag{12}$$

where g_{12}=g_{21}=0.0005, which represents the inter molecule interaction strength. φ_1 and φ_2 are expressed as follows

$$\varphi_1(\rho_2) = 1-\exp(-\rho_2/\rho_{20}) \tag{13}$$

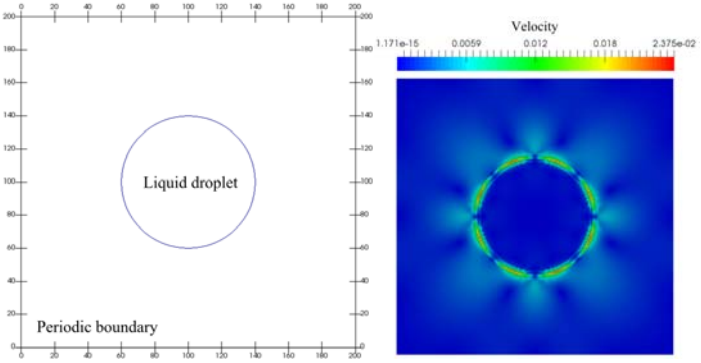
$$\varphi_2(\rho_1) = a_0-\exp(-\rho_1/\rho_{10}) \tag{14}$$

where a_0=0.005, ρ_{10}=-0.0008/log(a_0), ρ_{20}=0.0003.

3. Numerical results and discussion

3.1 A stationary droplet

In this section, we numerically investigate a stationary droplet with the improved multi-component pseudopotential LB model. A circular droplet of the initial radius of 40 lattice units (the follow units are all in lattice) is initially placed in a 201×201 square domain without body forces. As shown in Figure 1(a), we imposed periodical boundary conditions on the four boundaries. The temperature is set as 0.58T_c, and the initial density of liquid and gas is 0.42 and 0.0003 respectively. The simulation reached the steady state after a simulation time of 50000 time steps. It can be seen that the spurious currents exist around the gas-liquid interface from Figure1(b).



(a) liquid drop (b) spurious current

Figure 1: The position of the liquid drop and the distributions of spurious current

As shown in Table 1, five values of *k* are considered: 0.05, 0.08, 0.1, 0.5, 1.0, the gas-liquid interface thickness *D* decreases as the value of *k* increases. The density ratios are almost the same, which shows that the effect of *k* on the density ratio is slight. The spurious current reduces as the interface thickness increases, and the optimal value of *D* should be around 4~5 for multiphase LB model. Figure 2 shows the spurious current has an obvious decrease from *D*=3 to 5, then has slight decrease from *D*= 5 to 7. It agrees well with the previous studies that *D*=5 is the best choice for multiphase LB model. It should be noted that the maximum spurious current reduces to 0.0072 in this case, which is much smaller than 0.033 (density ratio of 971) achieved by Bao and Schaefer (2013) and 0.05 (density ratio of 152) achieved by Chen et al (2015). To verify the improved multi-component pseudopotential LB model by the Laplace law, we numerically investigate stationary droplets with the radius r_0 from 20 to 60. It can be observed from Figure 3 that a linear relationship is obtained between Δp and 1/*r*, which shows that the Laplace law is accurately satisfied.

Table 1: The relationship between k and D and density ratio

k	0.05	0.08	0.1	0.5	1.0
D	7	6	5	4	3
ρ_l/ρ_g	1285	1301	1300	1316	1264

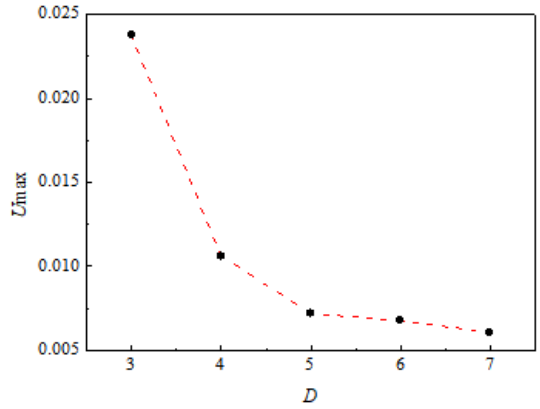


Figure 2: The effect of interface thickness on spurious current

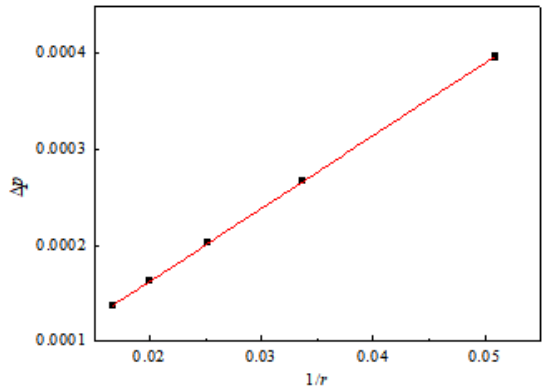


Figure 3: The verification of Laplace law

3. 2 Droplet oscillation

With the major radius *a*=55, the minor radius *b*=11, an elliptic droplet is initially placed in a 301×201 square domain without body forces. In simulations, we imposed periodical boundary conditions on the four boundaries. The density ratio ρ_l/ρ_g≈1000, the kinematic viscosity ratio v_l/v_g=1/15, v_l=0.1, and the surface tension σ=0.00752. In Figure4, the droplet exhibits the periodic oscillation process between oblate and prolate spheroid shapes. The simulated results agree well with the experiment in literature. For 2-D droplet, the oscillation period is defined as $T=2\pi\left[n\left(n^2-1\right)\frac{\sigma}{\rho_l R_0^3}\right]^{-1/2}$, where the equilibrium radius $R_0=\sqrt{ab}$ and *n*=2 (for an initial elliptic shape in this paper). Our simulated result (*T*=2400) agrees well with the analytical oscillation period of 2346.7.

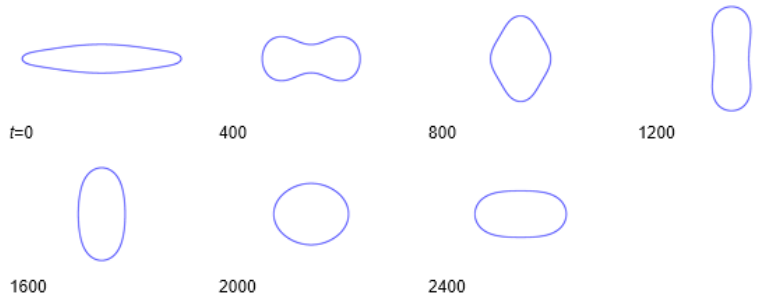


Figure 4: The periodic oscillation process of a droplet

3.3 Droplets collision

In this section, two 2-D circular droplets of the same radius of 40 are positioned at a 301×201 domain without body forces. As mentioned above, we impose periodical boundary conditions on the four boundaries. In this case, the liquid kinematic viscosity v_l=0.1, the surface tension σ=0.00752, the density ratio ρ_l/ρ_g≈1000, and the kinematic viscosity ratio v_l/v_g=1/15.

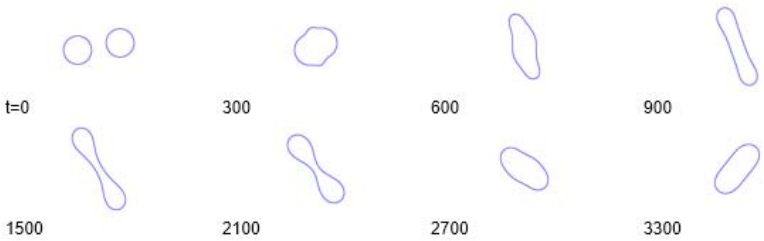


Figure 5: We=32.6, B=0.25

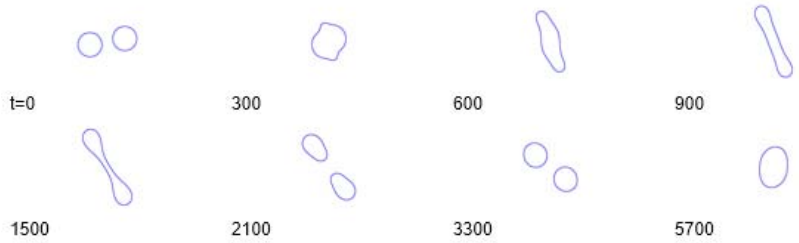


Figure 6: We=50.5, B=0.25

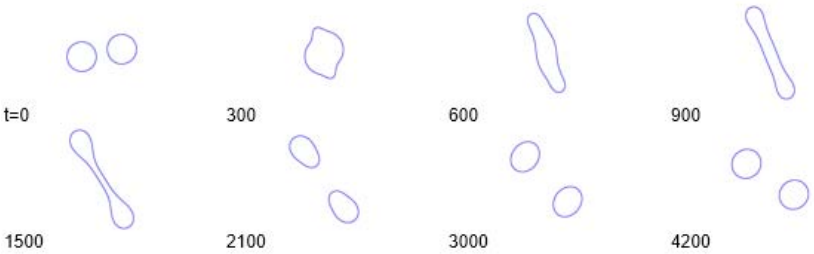


Figure 7: We=57.5, B=0.25

Figure 5-7 show the typical regimes of the droplets collisions by the improved multi-component pseudopotential LB model. With *B*=0.25, three different values of *We* are considered: 44.0, 50.5, 57.5. For a small value of *We*=44.0, we can see that a regime of droplets coalescence from Figure 5. As the value of *We* increases to 50.5, an intermediate regime will be observed, where the droplets separate briefly, but then re-coalesce, as shown in Figure 6. Moreover, it can be seen that the regime of droplets separation appears in Figure7 when *We*=57.5. The simulated results agree well with the experiment results by Qian (1997).

4. Conclusions

We have provided an improved multi-component pseudopotential LB model to investigate the dynamics of droplets. Through comparing the simulated spurious currents of the stationary droplet with the results in literature, it shows that the improved LB model is effective for simulating multi-component multiphase flow with small spurious current. The maximum spurious current reduces to 0.0072 with *D*=5, which is much smaller than the spurious current (0.033) of the same order of magnitude density ratio in literature. Furthermore, we have investigated the oscillation of droplet with large density ratio (O(1000)). The numerically predicted oscillation period by the improved model is 2400, which agrees well with the analytical result. Finally, the

droplets collision processes with different impact parameters are studied by this improved model. It has shown good agreement with the existing experimental results. According to the simulations, this improved multi-component pseudopotential LB model can be effective on simulating the problems of dynamic multiphase flow which are involved in large density ratio and relatively large kinematic viscosity ratio.

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