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Investigation of Density Ratio Effects on Performance of Pseudo-Potential Model in Multiphase Flows Simulation

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ABSTRACT: In this research, performance and capability of the developed pseudo-potential Shan- Chen model for simulation of multiphase flows with large density ratios are evaluated. This model is applied in the Palabos open source software which simulates fluid flows by means of the Lattice Boltzmann method. For this reason, some well-known multiphase benchmarks are investigated such as the Laplace law, segregation, bubbles coalescence and droplet impact with solid and liquid surfaces. According to the Laplace law, this model is capable of determining a wide range of surface tensions in different density ratios. In addition, this model is able to predict interface shape and phase segregation automatically very well. However, convergence rate is reduced as the density ratio increases. The simulation of two bubbles coalescence reveals that large spurious current and large interface oscillation are two main drawbacks of the pseudo-potential model. In droplet impact with a solid surface simulation, effects of density ratio which leads to a difference in surface tension and the Weber number are considered. When the Weber number is increased (at a constant Reynolds number), maximum spread increases but its vacillation decreases. Ultimately, results of the splash process show that the Weber number has a remarkable influence on breaking of a part of crown layer.

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1- Introduction

Recently, the Lattice Boltzmann Model (LBM) has captured a growing interest for the simulation of complex flows. Multiphase flows are regarded as one of the most sophisticated phenomena and possess a wide range of applications such as those in the petroleum industry, water recourses, and liquid metals.

For the first time, Shan and Chen [1] suggested a method based on the intermolecular interaction potential to improve the surface tension related collision operator. In their method, phase separation occurs automatically and naturally. The prototype of the pseudo-potential model had some drawbacks such as large spurious currents and being limited to relatively small density ratios. Kupershtokh et al. [2] suggested an Exact Difference Method (EDM) to enhance the density ratio and accuracy of the model. Then Gong and Cheng [3] proposed a new parameter based on the EDM scheme to achieve more accurate results.

In this study, the Palabos open source software is developed to evaluate the ability of the pseudo-potential model in modeling flows with large density ratios. Therefore, it is focused on some popular benchmarks such as the Laplace law, the bubbles coalescence, and the droplet impact with a solid wall as well as the splashing of a droplet on a thin liquid film. The oscillation of the interface is a dominant effect in most simulations.

2- Pseudo-potential Model

In the LBM, the properties are described via the particle distribution functions. The LBM for an isothermal fluid with the most popular Bhatnagar-Gross-Krook (BGK) collision operator and the external force term can be expressed as:

$$f_i(x+e_i\delta t, t+\delta t)-f_i(x,t)=-\frac{1}{\tau}[f_i(x,t)-f_i^{eq}(x,t)]+\Delta F_i(x,t) \quad (1)$$

Where f_i is the particle distribution function, τ the relaxation time, ΔF_i the body force, and f_i^{eq} is the equilibrium distribution function that can be expressed as

$$f_i^{eq}(x,t)=w_i\rho(x,t)\left[1+\frac{e_i u^{eq}}{c_s^2}+\frac{(e_i u^{eq})^2}{2c_s^4}+\frac{u^{eq\,2}}{2c_s^2}\right] \quad (2)$$

Where c_s is the speed of sound, w_i are the weighting factors and e_i are the discrete velocities.

After each step, the density and velocity are given by

$$\rho=\sum_i f_i=\sum_i f_i^{eq} \quad (3)$$

$$\rho u^{eq}=\sum_i e_i f_i=\sum_i e_i f_i^{eq} \quad (4)$$

In the EDM forcing scheme the body force ΔF_i can be given by

$$\Delta F_i(x,t)=f_i^{eq}\left(\rho,u^{eq}+\frac{F_i(x,t)\delta t}{\rho}\right)-f_i^{eq}(\rho,u^{eq}) \quad (5)$$

Gong and Cheng [3] proposed another interaction force and they asserted that their model can be applied on various equations of state versus other models. Their model can be written as

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$$F_i(x,t) = -\beta\psi(x)c_s^2\sum_i w\left(|e_i|^2\right)G(x,x')\psi(x,x')e_i$$
$$-\frac{1-\beta}{2}\sum_i w\left(|e_i|^2\right)G(x,x')\psi^2(x,x')e_i \quad (6)$$

where β is the weighting factor determined from the simulation and differs for each EOS. The function $\psi(x)$ denotes the pseudo-potential function and $G(x,x')$ is the Green function that reflects intensity of the interaction strength between particles. The pseudo-potential function can be written as

$$\psi = \sqrt{\frac{2\left(p-\rho c_s^2\right)}{c_0 g}} \quad (7)$$

For D2Q9 lattice, c_0=6 and p is obtained from a given EOS. In this case, the temperature is defined explicitly by the EOS.

3- Results and Discussion

3- 1- Laplace Test

According to the Laplace law, pressure difference inside and outside of a drop is proportional to the radius and the surface tension by the following equation:

$$\Delta P = P_{in} - P_{out} = \frac{\sigma}{R} \quad (8)$$

where parameter σ refers to the surface tension. Hence, the surface tension was calculated by simulating a series of drops with different radii.

To validate our numerical code, we simulate a static liquid droplet in vapour. Simulation results show a plot of ΔP versus $1/r$ for different density ratios (110, 800, 8300), which is a straight line as predicted by the Laplace law. Furthermore, the lines slopes are related to the surface tension values.

3- 2- Segregation

The pseudo-potential model has the capability of prediction of the segregation automatically. Based on the results, convergence speed decreases when density ratio goes up. In addition, the final interface has a round shape due to the minimum surface tension.

3- 3- Bubbles coalescence

We consider two stationary bubbles without collision. Initially, two bubbles with the radius R are located horizontally with a gap of d. The periodic boundary condition is employed at all boundaries. For the two stationary bubbles without collision, it is found that the distance (gap) between the bubbles, the interface width (w), and the density ratio are the major factors to decide whether the two bubbles merge together or not. Table 1 demonstrates when the density ratio goes up, the minimum gap of the two bubbles for the lack of the coalescence increases. The spurious current has a dominant effect on this phenomenon. Because there is a much stronger velocity field in large density ratios, it is expected that we need a longer distance to prevent coalescence.

3- 4- Droplet impact with a solid surface

This section presents the results obtained for the simulation of a droplet impact with a solid surface. The no-slip and periodic boundary conditions are used in the bottom and x direction respectively to investigate the drop diameter during the spreading process. Two different density ratios

Table 1. Effect of Density Ratio on d_{min}

Number	Density ratio	d_{min}
1	110	$3w$
2	1000	$9w$
3	8300	$12w$

are considered. With increasing the density ratio from 110 to 1000 in water the surface tension rises. To investigate the surface tension effect on the spread rate, Re=69 is chosen for both cases and the Weber number is 505 and 409, respectively (Fig. 1).

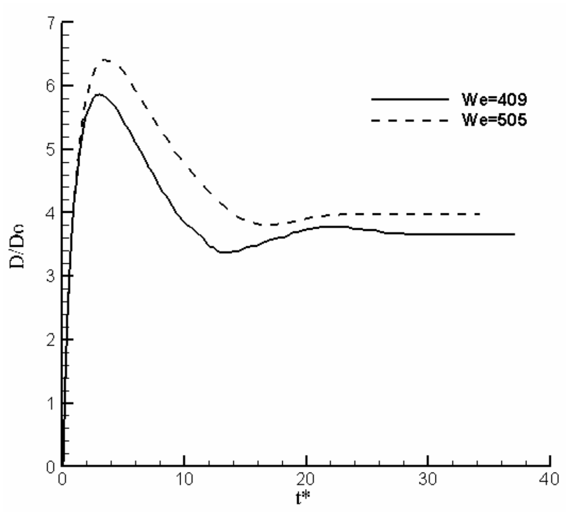


Figure 1. Time Evolution of Spread Factor

3- 5- Droplet impact on a thin liquid film

In this simulation, a droplet (with a diameter of D) falls down onto a thin liquid film with a thickness of $0.2D$. In order to investigate the effect of the Reynolds number (Re) and the Weber number (We), we simulate three cases with different Reynolds and Weber numbers. Fig. 2 shows the time evolution of the crown radius for these three cases. According to these cases, the Ohnesorge number can be used as a scaling factor for the prediction of the crown radius.

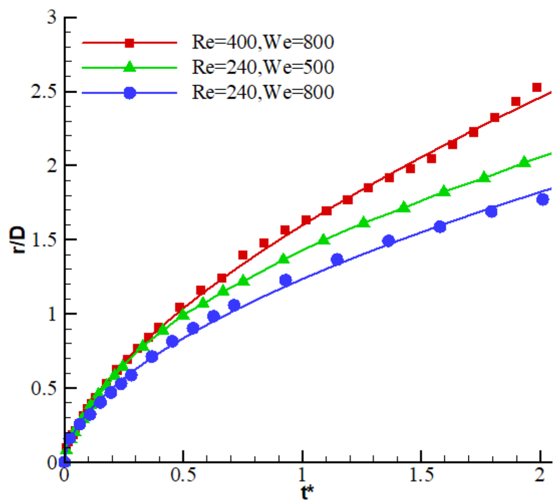
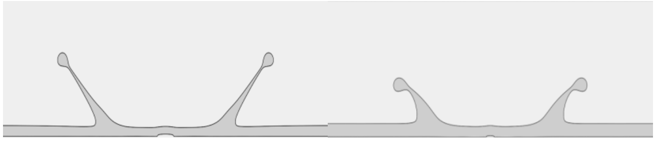


Figure 2. Time Evolution of Crown Radius in Different *Re* and *We* Numbers

Breaking a small drop is another important phenomenon of the splashing process. As it is clear from Fig. 3, an increase in the Weber number leads to a new regime in the droplet splashing.



a) t^*=3.3 b) t^*=2.3

Figure 3. A Droplet Splashing on a Thin Liquid Film in *Re*=240 and *We*=800 (Left), *We*=500 (Right)

4- Conclusions

In the present study, the developed Shan-Chen model is employed to simulate the static bubble (Laplace test), the segregation, the bubbles coalescence, the collision of a drop with a solid surface, and the droplet impact on a liquid film. The model capabilities are discussed in details and its drawbacks are discussed.

The interface behavior in most simulations is predicted with a good agreement compared to those of the other multiphase models. The bubbles coalescence process and the liquid drop and solid surface collision are captured in flows with large density ratios. The accuracy of the simulation of the drop splashing is very good compared with those of previous researches.

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