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# Studying of Droplet Impingement on Hydrophilic and Hydrophobic Curved Surfaces by Lattice Boltzmann Method Based on Allen-Cahn Equation

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ABSTRACT: In this paper, an efficient lattice Boltzmann method is applied for the simulation of two-

phase flow problems at high density and viscosity ratios. The present lattice Boltzmann method employs

the Allen-Cahn equation to model the interfacial dynamics between two phases and an appropriate

collision operator is implemented to ensure the stability of the numerical solutions. The performance

of the numerical algorithm is examined by studying droplet dynamics at different flow conditions. Herein, the equilibrium state of a droplet on the flat and curved walls is verified by considering the wetting properties, namely the hydrophilic and hydrophobic characteristics, for solid surfaces. The

multiphase flow pattern and interfacial dynamics of an impinging droplet on a cylinder surface and a

semicircular cavity are also investigated and the obtained results are compared with the available data.

The present study demonstrates that the curved wall considering the wettability effects significantly

affects the droplet dynamics, depending on the properties of the liquid phase and the flow conditions.

This work also shows that the lattice Boltzmann method with the Allen-Cahn equation is more stable for simulation of liquid-gas systems at density ratio 1000 and viscosity ratio 100 which makes this method

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#### 1. Introduction

Recently, the importance of multi-phase flows is evident in a wide range of industrial applications. Investigation of the dynamic behavior of the impacting droplet on surfaces is one of the most important topics in this field which can be seen in the aerospace industry (liquid fuel propulsion systems), the pharmaceutical industry (microfluidics), and oil and energy (water droplet separation). Therefore, the study of this type of multiphase flow problem is crucial, and many researchers are interested in studying in this area to precisely predict the dynamics of the interface between the two phases of the liquid and gas after the droplet hits the surface. The Lattice Boltzmann Method (LBM), due to its mesoscopic nature, is known as an effective and efficient numerical method for simulation of multi-phase flows [1]. Among the multi-phase LBM models, one based on the Allen-Cahn (A-C) equation is employed in the present paper to solve the droplet dynamics at high-density and high-viscosity ratios [2].

more suitable for predicting practical flow characteristics.

Studying the effect of the physical parameters such as hydrophilicity and geometry characteristics (convexity or concavity) on the dynamics of the droplet collision on the surface are considered in this work.

## 2. Governing Equations

The LBM with the A-C equation can be defined in the discretized form as follows which recovers the order parameter  $\phi$  [2]:

$$h_{\alpha}(\mathbf{x} + \boldsymbol{e}_{\alpha}\delta t, t + \delta t) = h_{\alpha}(\mathbf{x}, t)$$

$$-\frac{h_{\alpha}(\mathbf{x}, t) - \overline{h}_{\alpha}^{eq}(\mathbf{x}, t)}{\tau + 0.5} + F_{\alpha}^{\phi}(\mathbf{x}, t)$$
<sup>(1)</sup>

Herein,  $h_{\alpha}$  is the distribution function,  $e_{\alpha}$  is the particle velocity,  $\tau$  is the relaxation time, and  $c_s = 1/\sqrt{3}$  indicates the speed of sound in the present LBM. The forcing term  $F_{\alpha}^{\phi}$  and the equilibrium phase-field distribution function  $\bar{h}_{\alpha}^{eq}$  are given by

$$F_{\alpha}^{\phi}(\boldsymbol{x},t) = \partial t \, \frac{\left[1 - 4(\phi - \phi_0)^2\right]}{\xi} \omega_{\alpha} \boldsymbol{e}_{\alpha} \cdot \frac{\nabla \phi}{\left|\nabla \phi\right|} \tag{2}$$

$$\bar{h}_{\alpha}^{eq} = h_{\alpha}^{eq} - 0.5 F_{\alpha}^{\phi} \tag{3}$$

in which  $h_{\alpha}^{eq} = \phi \Gamma_{\alpha}$  and  $\Gamma_{\alpha}$  is defined by

$$\Gamma_{\alpha} = \omega_{\alpha} \left[ 1 + \frac{\boldsymbol{e}_{\alpha} \boldsymbol{u}}{c_{s}^{2}} + \frac{(\boldsymbol{e}_{\alpha} \boldsymbol{u})^{2}}{2c_{s}^{4}} - \frac{(\boldsymbol{u} \boldsymbol{u})}{2c_{s}^{2}} \right]$$
(4)

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To recover the hydrodynamic properties of a multiphase system, including the pressure and velocity components, a new distribution function  $g_{\alpha}$  is used in the LBM based on the A-C equation that reads

$$g_{\alpha}(\boldsymbol{x} + \boldsymbol{e}_{\alpha}\delta t, t + \delta t) = g_{\alpha}(\boldsymbol{x}, t) + \Omega_{\alpha}(\boldsymbol{x}, t) + F_{\alpha}(\boldsymbol{x}, t)$$
<sup>(5)</sup>

where  $\Omega_{\alpha}$  is the collision operator. Herein, a weighted multiple-relaxation-time collision model [2] is employed that is numerically stable and more accurate than the conventional single-relaxation-time collision operator:

$$\Omega_{\alpha} = -\boldsymbol{M}^{-1} \hat{\boldsymbol{S}} \boldsymbol{M} \left( \boldsymbol{g}_{\alpha} - \boldsymbol{\overline{g}}_{\alpha}^{eq} \right) \tag{6}$$

where M is an orthogonal transformation matrix and  $\hat{S}$  is the diagonal relaxation matrix. Finally, the order parameter  $\phi$ , normalized pressure  $p^*$ , and velocity u can be obtained by

$$\phi = \sum_{\alpha} h_{\alpha} \tag{7}$$

$$p^* = \sum_{\alpha} g_{\alpha} \tag{8}$$

$$\boldsymbol{u} = \sum_{\alpha} \boldsymbol{g}_{\alpha} \boldsymbol{e}_{\alpha} + \frac{\boldsymbol{F}}{2\rho} \delta t \tag{9}$$

#### 3. Results and Discussions

Fig. 1 shows the equilibrium state of the droplet on a circular cylinder obtained with the present A-C LBM at three different contact angles imposed on the solid wall. The density ratio and viscosity ratio of the multiphase system are set to be  $\rho_H / \rho_L = 1000$  and  $\mu_H / \mu_L = 100$ , respectively. It can be seen that at the equilibrium condition, the interfacial tension forces tend to minimize the free energy in the system by minimizing the peripheral area. Therefore, an arc is formed by the droplet on the top of the cylinder which contacts the solid surface with a contact angle imposed by the numerical algorithm. At the hydrophilic contact angle, the liquid spreads on the cylinder surface and the height of drop decreases. When the surface is hydrophilic, the droplet almost keeps its circular shape on the cylinder after reaching the equilibrium state. It should be noted that the shape of the equilibrated droplet also depends on the drop diameter and cylinder diameter which are considered constant in the

present work.

Fig. 2 demonstrates a sequence of results obtained for the droplet collision on the circular cylinder with hydrophobic solid wall. In this case, the intensity of the collision created by the gravity acceleration overcomes the surface tension of the liquid and causes the rupture of the joint between the drop and the surrounding gas. The breaking of the droplet into smaller drops is well captured by the present A-C LBM employed which demonstrates its performance and capability for predicting such complex multiphase flow structures. It should be noted that studying this flow problem at different wetting conditions is provided in the full paper.

The efficiency and stability of the A-C LBM are evaluated by simulation of the dynamics of droplet collision into a semicircular cavity in high-density and high-viscosity ratios. Fig. 3 shows a sequence of the obtained results for this test case with two wetting conditions. Due to the strong adhesion force between the liquid phase with the hydrophilic solid surface, the bubbles are trapped inside the droplet after impacting the surface. However, this phenomenon is not seen when the solid wall is hydrophobic. The present study shows that the splashing of the liquid phase to the out of the hole after the droplet collision is more related to the impaction intensity than the wetting condition of the wall. As seen in Fig. 3, the splashing dynamics of the droplet for both the hydrophobic and hydrophilic surfaces are the same at a certain flow condition.

### 4. Conclusions

In the present work, the A-C LBM is employed for simulation of the dynamics of droplet collision on different flat and curved surfaces with various wetting conditions. This study shows that with specific physical parameters for the liquid phase, the droplet dynamics at the equilibrium state is affected by the hydrophilicity of the solid surface. However, the wetting condition has no significant effect on the interfacial dynamics of an impacting droplet. Instead, the impaction intensity is more dominant at this condition and the droplet dynamics significantly depend on the collision parameters, e.g. the velocity and surface geometry. The present study also demonstrates that the A-C LBM is an accurate and efficient numerical technique for the simulation of the droplet dynamics at the high-density and high-viscosity ratios which introduces this algorithm as an appropriate one for the predicting of the applied multiphase flow characteristics.



Fig. 1. Equilibrium state of a drop with density ratio 1000 and viscosity ratio 100 on a circular cylinder at three different contact angles



Fig. 2. Impact of a drop with a density ratio 1000 and viscosity ratio 100 on a circular cylinder with hydrophobic surface at contact angle of 170 and Bo = 6.6



Fig. 3. Results obtained for sequence of droplet collision into a semicircular cavity with density ratio 1000, viscosity ratio 100, Re = 80 and Bo = 5000 at contact angle of 40 (top row) and 170 (bottom row).

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