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Application of a high density ratio lattice-Boltzmann model for the droplet impingement on flat and spherical surfaces

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ABSTRACT

In the current study, a 3-dimensional lattice Boltzmann model which can tolerate high density ratios is employed to simulate the impingement of a liquid droplet onto a flat and a spherical target. The four phases of droplet impact on a flat surface, namely, the kinematic, spreading, relaxation and equilibrium phase, have been obtained for a range of Weber and Reynolds numbers. The predicted maximum spread factor is in good agreement with experimental data published in the literature. For the impact of the liquid droplet onto a spherical target, the temporal variation of the film thickness on the target surface is investigated. The three different temporal phases of the film dynamics, namely, the initial drop deformation phase, the inertia dominated phase and the viscosity dominated phase are reproduced and studied. The effect of the droplet Reynolds number and the target-to-drop size ratio on the film flow dynamics is investigated.

1. Introduction

The droplet impingement on a solid surface is a common phenomenon, such as rain drops falling on the ground, ink-jet printing, spray cooling of hot surfaces, spray painting and coating, plasma spraying, fuel spray in combustion chamber, catalytic processing in fixed bed reactors and more recently in microfabrication and microchannels [1]. Therefore, research on droplets impacting on a solid surface attracts great interest from researchers. Rein [2] presented a comprehensive review on this phenomenon. Systematic studies have been carried out by Rioboo et al. [3], where six possible outcomes of drop impact on a dry wall were revealed, namely deposition, prompt splash, corona splash, receding break-up, partial rebound and complete rebound. The influence of the droplet size, impact velocity, droplet viscosity, interfacial surface tension, surface roughness amplitude and surface wettability characteristics on the impingement process have been investigated. To systematically study the dynamics of a spreading droplet, three major non-dimensional parameters are usually employed, specifically the Weber number (We), Reynolds number (Re) and the Ohnesorge number (Oh) which is also directly related to We and Re. They are defined as

$$We = \frac{\rho_L D_0 U_0^2}{\sigma}, \tag{1}$$

$$Re = \frac{\rho_L D_0 U_0}{\mu_L}, \tag{2}$$

$$Oh = \frac{\mu_L}{\sqrt{D_0 \sigma \rho_L}} = \frac{\sqrt{We}}{Re}, \tag{3}$$

where U_0 is the drop impaction speed, D_0 is the diameter of the spherical drop prior to impact, μ_L is the liquid viscosity, σ is surface tension of the interface between liquid and gas, and the ρ_L is liquid density. The spread factor, which is an effect of the impact process, is defined as the ratio of the total diameter of the spreading droplet (not the lamella diameter) and the initial droplet diameter:

$$D^* = \frac{D}{D_0}. \tag{4}$$

Experimental and analytical investigations have been performed to study the time evolution of the spread factor and to determine the correlation between the maximum spreading factor and the Weber, Reynolds and Ohnesorge numbers [4–9]. The maximum spreading factor is defined as $D^*_{\max} = D_{\max}/D_0$, where

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$D_{\max}$ is the maximum diameter of the contact area of the drop on the substrate. Asai et al. [4] examined the spreading of a micron size droplet from an inkjet printhead impacting on moving paper and obtained a simple correlation formula to predict the maximum spreading ratio. Scheller and Bousfield [5] showed that the contact angle effect on the spreading film diameter is negligible for droplet $Re > 10$, and that the maximum spread factor follows the correlation given by $D_{\max} = 0.61(Re^2Oh)^{0.166}$. Roisman et al. [9] modeled the drop impaction process to predict the evolution of the drop diameter. The model accounts for the capillary force, viscosity and inertial effects, as well as the dynamic contact angle. Micron drop impaction on smooth solid substrates was investigated by Dong [10] over a wide range of impaction speeds, surface contact angles and drop diameters. The experimental results were compared with several existing equations for predicting maximum spreading. The prediction equation of Roisman et al. [9] agrees well with the experimental results for both low and high *We* impactions. The empirical equation of Scheller and Bousfield [5] also gave a good fit even though the effect of the equilibrium contact angle was neglected.

Previously published work [11–13] has shown that the impaction of droplets onto curved surfaces (e.g. spheres), differs significantly from the impact of droplets on large substrates. The studies for the droplet impact onto curved surfaces will have enormous utility in several industrial applications, such as tablet coating, encapsulation processes and catalytic processing in fixed beds. Hung and Yao [11] have carried out experiments on the impaction of water droplets with diameters of 110, 350 and 680 μm on cylindrical wires. The effects of droplet velocity and wire sizes were studied parametrically to reveal the impaction characteristics. Bakshi et al. [13] have reported experimental data and theoretical investigations on the impact of a droplet onto a spherical target over a range of Reynolds numbers and target-to-drop size ratios. Three distinct temporal phases of the film dynamics were found, namely the initial drop deformation phase, the inertia dominated phase, and the viscosity dominated phase. The influence of the droplet Reynolds number and the target-to-drop size ratio on the dynamics of the film flow on the surface of the target were conducted.

Recently, numerical investigations have drawn increasing attention in simulating the impingement process, because experiments alone are not adequate enough to define the governing physics [14]. Trapaga and Szekely [15] used a commercial code (FLOW-3D) that incorporates the “volume of fluid”(VOF) method to study the impact of molten particles in the thermal spray process. Bussmann et al. [16] studied the dynamics of droplet impact on flat and inclined surfaces with a 3D VOF method. As a modern method, lattice Boltzmann method (LBM) has attracted considerable attention in simulating the droplet impingement on solid surfaces. Gupta and Kumar [17,18] studied the droplet impingement on a flat solid surface at low density ratios. Yan and Zu [19] reported a new numerical scheme for the lattice Boltzmann method, which combines the existing model of Inamuro et al. [20] and Briant et al. [21] for calculating the liquid droplet behavior on partial wetted surfaces, typical for large density ratios gas–liquid systems. However, Inamuro et al.'s model [20] involves the solution of Poisson equation, which decreases the simplicity of the usual LBM. Moreover, Fakhari and Rahimian [22] found that the free-energy-based model [23] is not capable of dealing with two-phase flows with different densities and is mostly suitable for binary fluids for which the Boussinesq approximation holds. Until now, most of the studies focus on flat and inclined solid surfaces. Few studies focus on the simulation of a droplet impact on a curved surfaces. Shen et al. [24] adopted the two-dimensional lattice Boltzmann pseudo-potential method to simulate the droplets impacting on curved solid surfaces. However, the gas–liquid density ratio is limited to unity.

In the current study, we apply a 3-dimensional lattice Boltzmann model based on the original Shan-Chen model [25] and the improvements in the single-component multiphase flow model reported by Yuan and Schaefer [26] to study the impaction of a liquid droplet on a dry flat surface and a curved surface for a liquid–gas system with large density ratio. The influence of Reynolds number, Weber number, Ohnesorge number and the target-to-drop size ratio on the impingement process is reported. The results are compared with experimental data reported in the literature.

2. Numerical method

In recent years, LBM has become a promising numerical technique for the simulation of multiphase flows due to its local nature of interactions. Unlike traditional CFD, it does not need to track or construct the vapor–liquid interface. Several models have been developed for multiphase and multi-component flows during the last twenty years, such as Rothman and Keller's color method [27], Shan et al.'s potential method [25], Swift et al.'s free energy method [23] and He et al.'s phase field method [28]. However, all of the above LBM models are limited to small density ratios, usually less than ten, due to numerical instabilities. To overcome this difficulty, Reis and Phillips [29] changed the forcing scheme of the perturbation operator based on the color method to induce the appropriate surface tension term in the macroscopic equations. Leclaire et al. [30] adapted the recoloring operator for the Reis and Phillips model in the case of variable density ratios and this model could be used to simulate flows with large density ratios in some test cases. Leclaire et al. [31] modified the original equilibrium distribution functions to capture the momentum discontinuity in the two-layered Couette flow with large density ratio. Inamuro et al. [20] proposed a model based on the free energy method for multiphase flows with large density ratio. However, in this model, the pressure correction is applied to enforce the continuity condition after every collision-streaming step, which is similar to the VOF method and the level set method. The projection step would reduce the efficiency of the method greatly [32]. Lee and Lin [33] achieved a high density ratio by improving Swift's free-energy model [23] and the model of He et al. [28], respectively. Zheng et al. [34] proposed a method for simulating multiphase flows with high density ratio based on the free-energy approach. Recently, Fakhari and Rahimian [22] found that this model is not capable of dealing with two-phase flows with different densities and is mostly suitable for binary fluids in which the Boussinesq approximation holds. Recently, Yuan and Schaefer [26] expressed that the equation of state (EOS) plays an important role in achieving high-density ratios. Thus, the incorporation of the Peng–Robinson equation of state into the Shan–Chen [25] multiphase lattice Boltzmann model is adopted in the present study.

2.1. Pseudo-potential model

The particle distribution function is governed by the discretized Boltzmann equation with single relaxation time for the collision term [35]:

$$f_\alpha(x + e_\alpha \delta t, t + \delta t) = f_\alpha(x,t) - \frac{1}{\tau}\left[f_\alpha(x,t) - f_\alpha^{\mathrm{eq}}(x,t)\right], \tag{5}$$

where f_α is the particle distribution function along the αth direction, f_α^{eq} is equilibrium distribution function, δt is the time step, e_α is the particle velocity in the αth direction, τ is the single relaxation time. The viscosity in the LBM model is given by