Computers and Fluids 168 (2018) 130–143

Contents lists available at ScienceDirect

Computers and Fluids

journal homepage: www.elsevier.com/locate/compfluid

Benchmark solutions

3D lattice Boltzmann simulation for a saturated liquid droplet at low Ohnesorge numbers impact and breakup on a solid surface surrounded by a saturated vapor

Wei Xiong, Ping Cheng*

MOE Key Laboratory for Power Machinery and Engineering School of Mechanical Engineering, Shanghai Jiao Tong University, Shanghai 200240, PR China

ARTICLE INFO

Article history:
Received 10 October 2017
Revised 23 March 2018
Accepted 30 March 2018
Available online 31 March 2018

Keywords:
Droplet impact dynamics
3D LBM
High density ratios
Low viscosities

ABSTRACT

In this paper, new simulation results of a saturated liquid droplet impact dynamics on hydrophilic ($\theta = 80°$) and hydrophobic ($\theta = 170°$) solid surfaces surrounded by a saturated vapor are obtained based on a 3D lattice Boltzmann method (LBM). A novel piecewise relaxation time is proposed to overcome numerical instability at high liquid/vapor density ratios and low liquid droplet viscosities. Simulations are carried out for low Ohnesorge (*Oh*) numbers in the range from 0.01 to 0.05, corresponding to a water droplet diameter in the range of 1 μm to 130 μm. The impinging droplet deformation process including breakup phenomena is illustrated on hydrophilic and hydrophobic surfaces at different Weber (*We*) numbers. Droplet spread factors obtained from simulations match well with existing experimental data and theoretical values, validating the accuracy of the present 3D LBM. It is found that a water droplet, after reaching its maximum spread factor, breaks up into a toroid shape with a vapor cavity or a liquid film left at its center at large *We* numbers on a hydrophilic and a hydrophobic surface, respectively. A map in terms of *We* number versus *Oh* number is obtained for predicting the breakup occurrence. The critical *We* number is monotonically increasing with the increase of the *Oh* number, meaning that the smaller diameter water droplet requires a larger *We* number for breakup. Droplet breakup is more likely to occur on a hydrophobic surface than on a hydrophilic surface at larger *Oh* numbers, while the behavior is opposite at lower *Oh* numbers.

1. Introduction

Droplet impact dynamics on a solid surface has wide applications in technologies [1–4]. It is known [5] that the droplet impact dynamics is characterized by the following three dimensionless parameters: Weber (*We*) number, Reynolds (*Re*) number, and Ohnesorge (*Oh*) number, which are defined as

$$We = \rho V_i^2 D_d/\sigma, \tag{1a}$$

$$Re = \rho V_i D_d/\mu, \tag{1b}$$

$$Oh = \mu/(\rho\sigma D_d)^{0.5} = We^{0.5}/Re \tag{1c}$$

where ρ is the droplet density, V_i is the droplet impacting velocity, D_d is the droplet diameter, μ is the droplet dynamic viscosity, and σ is the droplet surface tension. Note that only two of the three dimensionless parameters are independent in a physical problem.

Previous experimental results indicated that a droplet impacting on a surface could break up into a toroid shape at large *We* numbers [6–11], causing defects in many practical applications. Understanding the breakup mechanism and finding the threshold separating breakup and non-breakup regions is important for practical applications. Due to the short time scale and the micro size of the impacting droplet, it is difficult to study its physical process in details experimentally. As a result, numerical studies provide an effective tool for the study of these behaviors. It is relevant to point out that most of the simulations for droplet impact dynamics in the past were based on the traditional continuum approach. Renardy et al. [10] studied 3D droplet impact dynamics by solving Navier-Stokes equations numerically, and obtained a *We*-*Re* map for droplet breakup or non-breakup. Caviezel et al. [12] developed a 2D axisymmetric model using the Level Set approach, where the toroid formation was reproduced in their simulations. Zhang et al. [13] used a phased field model, and the breakup droplets on hydrophilic and hydrophobic surfaces were simulated in their work. In the above numerical and experimental studies, the liquid droplet is surrounded by air, where a sharp liquid/air interface exists.

* Corresponding author.
E-mail addresses: pingcheng@sjtu.edu.cn, ijhmt.cn@sjtu.edu.cn (P. Cheng).

https://doi.org/10.1016/j.compfluid.2018.03.082
0045-7930/

Nomenclature

c	lattice speed (m/s)
c_s	lattice sound speed (m/s)
D	diameter (m)
$\mathbf{e}_i$	discrete lattice velocity vector (m/s)
EK	kinetic energy
ES	surface energy
f_i	density distribution function
$\mathbf{F}$	total force (N)
$\mathbf{F_{int}}$	inter-particle interaction force (N)
$\mathbf{F_s}$	fluid-solid interaction force (N)
$\mathbf{F_g}$	gravitational force (N)
$\mathbf{g}$	gravitational acceleration (m/s^2)
N	lattice number
Oh	Ohnesorge number
p	pressure (Pa)
Re	Reynolds number
T	temperature (K)
t	time (s)
t^*	dimensionless time (s)
$\mathbf{u}$, $\mathbf{U}$	velocity vector (m/s)
V	velocity (m/s)
W	viscous dissipation
We	Weber number
x, y, z	co-ordinates (m)

Greek symbols

δx	lattice spacing (m)
δt	time step (s)
β	weighting factor
ρ	density (kg/m^3)
θ	static contact angle (°)
ψ	effective mass
ω_i	weight coefficient
τ	relaxation time
μ	dynamic viscosity (Pa•s)
υ	kinetic viscosity (m^2/s)
σ	surface tension (N/m)
ξ	droplet spread factor

Subscripts or superscripts

d	droplet
cr	critical
eq	equilibrium
i	impacting
ini	initial
l	liquid
max	maximum
sat	saturation
v	vapor

The impact dynamics of a saturated liquid droplet surrounded by saturated vapor is different from those surrounded by air. This is because the saturated liquid-saturated vapor interface does not have a sharp interface, and instead, it has a finite thickness. As a mesoscopic method, lattice Boltzmann method (LBM) [14] has been shown to be an effective method for simulating liquid/vapor flows due to its advantages that no interface capturing is required, and the dynamic contact angle needs not assumed to be constant. Gupta and Kumar [15] carried out a 2D LBM for studying droplet impacting and breakup behaviors. However, the deficiency of 2D simulations is that 3D toroid shape droplet cannot be reproduced. Some 3D LB simulations have been carried out [16–21], but the breakup phenomenon did not occur in these 3D LB simulations. As shown in Fig. 1, most of the previous LB simulations [15–20] were carried out for water droplets impacting at a large Oh number, which corresponds to a micron sized droplet. This diameter scale is much smaller than those used in industrial applications. Thus, simulations of droplets impacting on surfaces at low Oh numbers are needed for practical applications. It is relevant to point out that the LB simulations in [15–17] are based on Shan-Chen's pseudo-potential model [22] and the LB simulations in [18–21] are based on the free-energy model by Swift et al. [23].

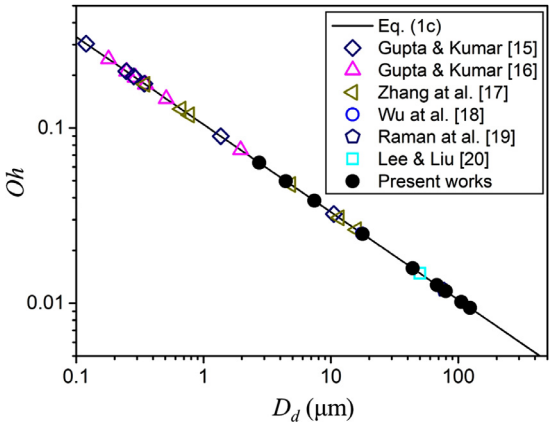

Fig. 1. Summary of LBM studies on water droplet impacting on a solid surface with different Oh numbers in previous work and present work.

In this paper, we first simulate a saturated liquid droplet at low Oh numbers impact a solid surface based on the Gong-Cheng's model [24], where the liquid/vapor density is determined by the equation of state of a real gas. A novel piecewise relaxation time is proposed to improve numerical instability at high liquid/vapor density ratios and low droplet viscosities. As shown in Fig. 1, the Oh number of water droplet in this paper ranges from 0.01 to 0.05, corresponding to the droplet diameter in the range from 1 to 130 μm. The breakup phenomena is illustrated on hydrophilic and hydrophobic surfaces at different We numbers. The good agreement of the present 3D LBM with the previous correlation equation and experimental data [25–28] validates the accuracy of the present 3D LBM for droplet impact dynamics. Finally, a map in terms of We number versus Oh number for the threshold dividing the region of breakup and non-breakup on a hydrophilic surface and a hydrophobic surface is obtained.

2. Description of the simulation model

In this section, we first describe the 3D pseudo-potential lattice Boltzmann method with the original BGK collision operator [29]. Then, we analyze the computational convergence and modify the original BGK collision operator to extend the numerical stability at small relaxation times.

2.1. The 3D pseudo-potential lattice Boltzmann model

The evolution equation of the density distribution function with the original BGK collision operator is written as:

$$f_i(\mathbf{x}+\mathbf{e}_i\delta t, t+\delta t) - f_i(\mathbf{x}, t) = -\frac{1}{\tau}\left(f_i(\mathbf{x}, t) - f_i^{eq}(\mathbf{x}, t)\right) + \Delta f_i(\mathbf{x}, t) \tag{2}$$

where $f_i(\mathbf{x}, t)$ is the particle distribution function with velocity $\mathbf{e}_i$ at position $\mathbf{x}$ and time t. τ is the relaxation time which is related to the kinematic viscosity of the liquid phase or vapor phase. $f_i^{eq}(\mathbf{x},$