

Lattice Boltzmann simulations of liquid drop shape on an inclined surface

Hajar Ghannam*, Adil Chahboun, Mustapha Diani, Mohammed Addou
University Abdelmalek Essaadi, FST Tangier
Department of physics
Tangier, Morocco
Email*:ghannam11hajar@gmail.com

Abstract—A liquid drop has a property to be deformed due to weak bounds between the molecules. The shape of a liquid droplet can take several forms depending on the forces that are implemented. In this work, Lattice Boltzmann method was used to simulate the shape of water droplets on an inclined solid surface under gravity force and friction force. From the top views of the simulation results, the shape of the liquid droplet depends on the forces that are introduced. By combining the results of shape deformation on inclined surface with a theoretical model, we have introduced a coefficient called deformation factor. From theoretical model, deformation factor can take several values. Moreover, qualitative and qualitative properties are given through the deformation factor to classify and characterize the nature of liquid droplet shape deformation.

I. INTRODUCTION

The shape of liquid droplets are frequently encountered in a variety of industrial processes like ink-jet printing [1] where the print quality relies on the formation of small liquid drop-lets to deliver precise amounts of liquid to a substrate, spray cooling [2] etc, and in natural occurrences like falling rain drops, droplets impacting and sliding on surfaces. Many forms can take liquid drop when falling like spherical, curved disk, parachute. Deformation of falling droplets is determined as equilibrium between liquid surface tension which keep spherical form of the liquid drop and air resistance. The specific outcome of the deformation of falling drop depends mostly upon the air friction force and also upon the velocity of falling. Two phenomenons that we can observe when a liquid drop impacts a dry solid surface, spread followed by the retraction. The impact depends on the surface tension, viscosity, drop size, velocity, and on the surface roughness. The possible outcomes of drop impact are deposition, prompt splash and corona splash. Rein [3] and Yarin [4] have presented extensive reviews about the dynamic aspects of the impact phenomenon. When talking about deformation of liquid droplets shape on a solid, we think about contact angle (CA) which formed between liquid and solid surface. From (CA) we can characterize the nature of surface and their wettability property. A super-hydrophobic surface [5] causes liquid to bead upon and formed (CA) higher than 150° , while a super-hydrophilic surface allows a drop of liquid to spread out and formed (CA) approaches 0° . However, deformation of liquid droplets shape on a solid mainly depends on surface

tension of solid substrate and its roughness. The extreme water properties which are presented in super-hydrophobic surfaces such as lotus leaves [6] or animals skin are due to height surface roughness and low surface energy coating while super-hydrophilic surfaces are characterized by high surface energy coating. However, we have the dimensionless number bound number (Bo) [7] also called Eötvös number (Eu) [8] which uses surface tension forces and gravitational forces to get an idea about the droplet deformation. For a high bound number $Bo \gg 1$ the system is affected by gravitational forces and for a less bound number $Bo \ll 1$ the system is dominated by surface tension forces over the gravitational forces. In the case where the bound number equal to 1, we have a balance between two forces.

Several experimental studies of the liquid drop behavior on inclined surface have been reported. Pontus et al [9] have investigated the drop friction of super-hydrophobic inclined surface. In their work, they have introduced a frictional force where a new parameter b_{sh} named the super-hydrophobic sliding resistance. Also they are given a qualitative ranking of super-hydrophobic surfaces from b_{sh} . Nolwenn et al [10] have reported an experimental study of the shape and motion of drops sliding down an inclined plane, revealing qualitatively the different regimes observed of liquid drop on inclined surface and quantitative results of the drops motion. Ben Amar et al [11] have studied the transition of a moving contact line of a small droplet sliding under gravity down an inclined plane from smooth to angular.

Application of Lattice Boltzmann method (LBM) for simulating fluid behavior has become an established tool. In recent years, LBM has been developed as an alternative numerical approach in computational fluid dynamics. The fundamental idea of LBM is to construct simplified kinetic model that incorporates the essential physics of microscopic processes in which the macroscopic behavior of a fluid corresponds to many microscopic particle behaviors in the system. Investigations of deformation of liquid droplets shape using LBM have been carried out by several researchers. A. Fakhari and M. H. Rahimian [12] have used multiple-relaxation-time LBM to investigate deformation and breakup of a falling liquid drop under gravity forces. Lee and Lin [13] have been proposed a formulation to simulate the dynamics side of droplet impact

and coalescence using high density ratio multiphase LBM. Lee and liu [14] have employed a high-density ratio based on LBM to study the micro-scale droplets impact on dry surfaces. Recently, the study of dynamics of successive droplets impact on a solid surface using high-density ratio based on lattice Boltzmann model have reported by Kuppa et al [15]. In fact, LBM have been used to model droplets on super-hydrophobic surfaces [16], drop motion on surfaces [17], [18] and contact angel hysteresis [19], [20].

In this work, we have studied the deformation of the liquid drop shape on inclined surface using LBM through a parameter called deformation factor which we introduced in this study. The different deformation of the liquid drop shapes under gravity and friction forces of inclined surfaces is depicted. A numerical equation expressing the relationship between deformation of drop shape, inclination angle of the surface and friction coefficient of the substrate is given. Also qualitative and qualitative properties are classified thought the deformation factor of liquid drop shape.

II. NUMERICAL METHOD

LBM is based on microscopic models and mesoscopic kinetic equations to give the probability to find a swarm of particles $f_i(x, c_i, t)$ (distribution function) in a lattice at time t , positioned between x and $x + dx$, and velocities between c_i and $c_i + dc_i$. In the microscopic scale, swarm of particles tents to interact one with another. This interaction between particles with different velocities or trajectories called collision. The temporal evolutions of distribution function under two processes streaming and single relaxation time collision operator is expressed by following equation:

$$f_i(x + c_i, \delta t, t + \delta t) = f_i(x, t) - Q(f_i) \quad (1)$$

And

$$Q(f_i) = \frac{1}{\tau}(f_i(x, t) - f_i^{eq}(x, t)) \quad (2)$$

$Q(f_i)$ is collision operator proposed by Bhatnagar Gross and Krook (BGK) [21]. It expresses the collision as a relaxation of f_i to equilibrium f_i^{eq} . This relaxation is weighted by a time τ which is average time between two collisions. f_i^{eq} is equilibrium distribution function corresponding to Maxwell distribution. Boltzmann equation on a lattice is applied to distribution function of same velocity c_i . However, the lattice must conserve the basic quantity during the movement of f_i in the lattice. For (D_2Q_9) (Figure 1) Lattice Boltzmann model (two-dimensional and uses 9 velocities) the particle velocity vector e_i is given by:

$$[e_0, e_1, e_2, e_3, e_4, e_5, e_6, e_7, e_8] = \begin{bmatrix} 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \end{bmatrix} \quad (3)$$

Through the velocities discretization, we can associate the equilibrium distribution function for each velocity c_i . The discrete formula of f_i^{eq} is:

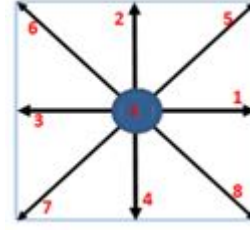


Fig. 1. Lattice arrangements for 2-D problems, D_2Q_9 .

$$f_i^{eq}(x) = w_i \rho(x) \left(1 + 3 \frac{e_i u}{c^2} + \frac{9}{2} \frac{(e_i u)^2}{c^2} - \frac{3}{2} \frac{u^2}{c^2} \right) \quad (4)$$

For each velocity c_i the equilibrium is expressed by w_i weight. The w_i depend on the velocities discretization that used. In other words it depends on the Lattice arrangements. For Lattice Boltzmann model D_2Q_9 $w_i (i = 0, 1, \dots, 8)$ is as following,

$$\begin{aligned} w_0 &= \frac{4}{9}, i = 0 \\ w_i &= \frac{1}{9}, i = 1 \dots 4 \\ w_i &= \frac{1}{36}, i = 5 \dots 8 \end{aligned} \quad (5)$$

The macroscopic quantities of particles density and velocity are related to the local distributions by following equations:

$$\rho(x, t) = \sum_{i=0}^8 f_i(x, t) \quad (6)$$

$$\rho(x, t) u(x, t) = \sum_{i=0}^8 c_i f_i(x, t) \quad (7)$$

For incorporating forces like gravitational force of inclined plane $F_g = mg \sin(\theta)$ and friction force $F_f = \mu mg \cos(\theta)$ into LBM. The second Newton's law $F = ma = mdu/dt$ provides a means to incorporate the forces via velocities. So, from discrete representation of relaxation time and velocity, and using density as mass per unit area basis, we have

$$u^{eq} = u + \tau \frac{F_1}{\rho} + \tau \frac{F_2}{\rho} \dots \quad (8)$$

The fluid-solid surface force given by (Equation (9)) [22] is incorporated to Lattice Boltzmann equation for describe the substrate wettability.

$$F_{ads} = -G_{ad} E(x, t) \sum_{i=0}^8 W_i s(x + e_i \delta t) e_i \quad (9)$$

G_{ad} is the interaction strength parameter, E is the interaction potential, where s is a switch that takes value one if the site at $x + e_i \delta t$ is a solid and is zero otherwise. The wettability of the substrate is given by adjusting the fluid interaction strength parameter G_{ad} .

In this work, to study deformation of the liquid drop shape using LBM we introduce a dimensionless parameter called

deformation factor. We define deformation factor as a ratio between liquid drop size along x axis (a) and liquid drop size along y axis (b) (Equation (10)) (Figure 2).

$$\zeta_{def} = \frac{a}{b} \quad (10)$$

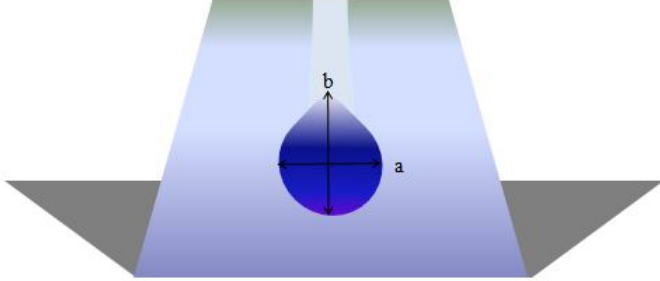


Fig. 2. Parameters of study.

III. RESULTS AND DISCUSSION

A liquid drop on a surface can take several forms depending on many parameters like surface tension, surface roughness and surface inclination angle also on the liquid properties such as density, viscosity. The results of the following sections are given for a liquid density of $1000\text{kg}/\text{m}^3$, viscosity 10^{-3}Pas.s , and for a partial wetting (contact angle formed between liquid and surface of 90°). The first section shows the effect of gravity force of inclined surface on the liquid shape where inclination angle θ varied between 0° and 54° , then a theoretical equation is extracted to express the liquid drop deformation as function of θ . The second section displays how the liquid varied as function of and friction coefficient, also a theoretical equation linking between ζ_{def} , μ and θ is given through the simulation results. Finally, deformation factor ζ_{def} used in two sections allows for qualitative and quantitative rankings of the liquid drop shape.

A. Deformation of liquid drop under gravity force of inclined solid substrate

In this part, LBM have been used to simulate liquid drop deformation under gravity force of inclined defect-free surface. An ideal periodic computational domain with 101×101 grids is considered. A drop is set at the center of the computational domain, and a D_2Q_9 lattice model is adopted.

Figure 3 displays the effect of inclination angles of the surface on droplet shape using D_2Q_9 model. From the top view, an oval shape of liquid drop appears for $\theta = 0^\circ$ (Figure (3.a)). Under gravity effect $\theta > 0^\circ$, a droplet of liquid tends to be deformed into a crescent shape. This deformation from oval shape to crescent one is due to the increases gravitational force which are incorporated to one direction of D_2Q_9 model also it due to different w_i weight which are presented in lattice arrangement of D_2Q_9 . Through the deformation factor defined in (Equation 10), we can quantify the liquid shapes deformation on inclined surface of figure 3. We find an

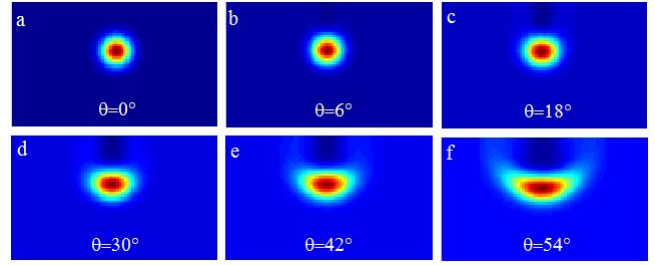


Fig. 3. Liquid drop shape on inclined surfaces.

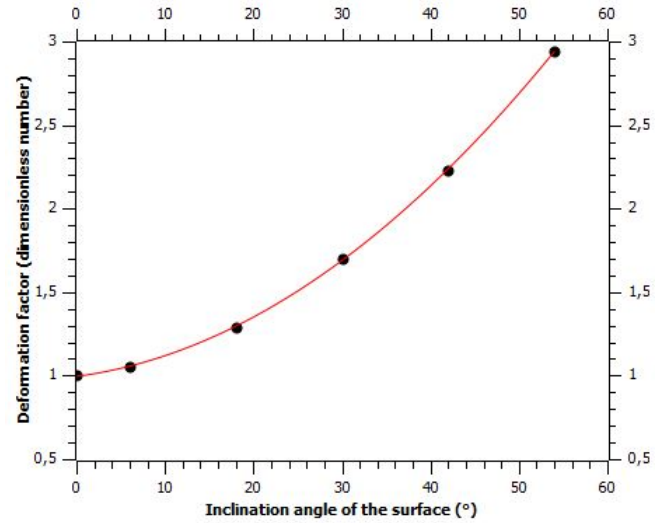


Fig. 4. Deformation factor as function of inclination angle.

increase of the liquid drop size along x axis when inclination angle of the surface increases. However, the liquid drop keeps its diameter size along y axis despite of inclination angle of the substrate (Figure 3).

The graph of Figure 4 shows the evolution of deformation factor as function of the inclination angle of the substrate (points are calculated from simulation results and continuous line is a fit using equation (11)).

$$\zeta_{def} = 1 + 7.10^{-3}\theta + 5.36.10^{-4}\theta^2 \quad (11)$$

As shown in figure 4, the deformation factors take the values higher than 1. As the deformation factor increases, the deformation of droplet shape becomes more significant forming a crescent shape. Equation 11 expresses the relationship between ζ_{def} and inclination angle. It fits perfectly the calculated deformation factors.

B. Deformation of liquid drop under gravity force and friction force

For no ideal surface which some defaults are presented as roughness, the liquid drop slid over this surface under-goes two principal forces, gravity and friction. In this part, we follow the evolution of droplet shape as a function of the friction coefficient for different inclination angles. Figure 5 shows the shape

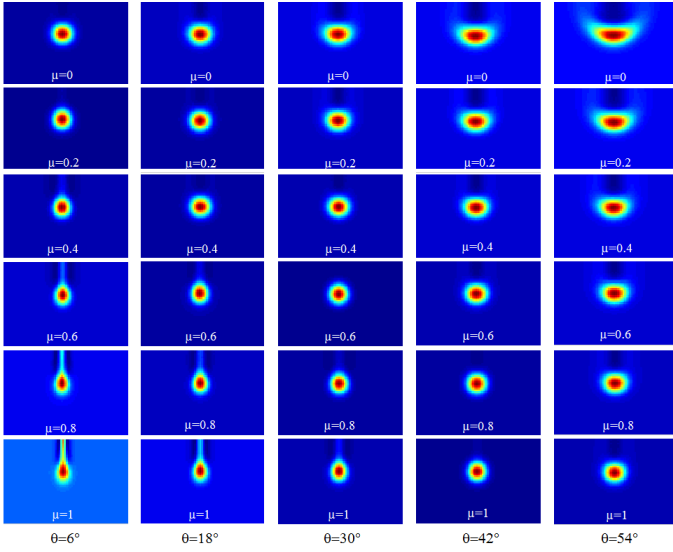


Fig. 5. Liquid drop shape undergoes friction force and gravity force.

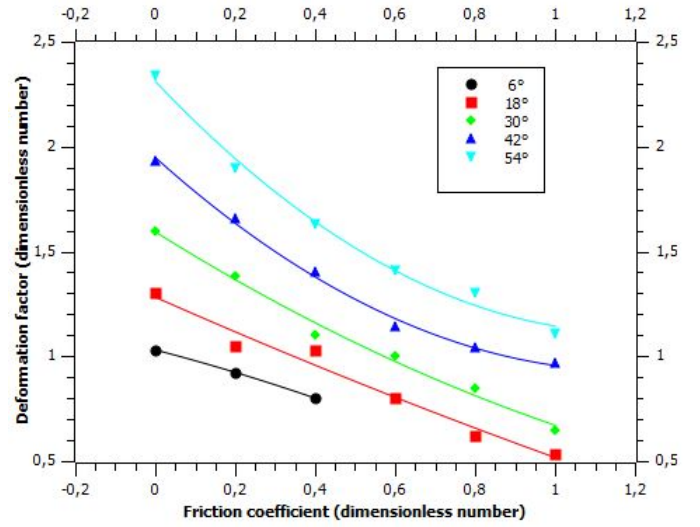


Fig. 6. Liquid drop shape undergoes friction force and gravity force.

of liquid drop on inclined surface $\theta = 6^\circ, 18^\circ, 30^\circ, 42^\circ, 54^\circ$ for a friction coefficient μ ranging between 0 and 1. To have a sliding of liquid drop on an inclined surface under action of friction force, some conditions and thresholds must be discussed: Gravitational force must be superior than frictional force, consequently μ must not exceed the threshold of $\tan(\theta)$.

The simulation results of figure 5 shows that the shape of liquid drop tends to be oval under friction force which is due to additional the friction force in opposite direction of gravity force. Deformation factor takes a value of 1 even if the surface is not plane. In this case, the value of 1 explains the equilibrium existing between gravity force and friction one. Other than oval and crescent, a pearling shape can appear on an inclined surface. This shape is obtained when μ exceeds $\tan(\theta)$ and is characterized by a $\zeta_{def} < 1$.

Figure 6 shows the evolution of the liquid shape as a function of friction coefficient. As it is displayed, deformation factor increases when μ decreases.

Equation 12 shows the relation that rely ζ_{def} with θ and μ .

$$\zeta_{def} = (1 + 7.10^{-3}\theta + 5.36.10^{-4}\theta^2) + (-0.03\theta - 0.19)\mu + (0.02\theta - 0.39)\mu^2 \quad (12)$$

Also through equation (12), we can predict the friction coefficient of the surface by the shape of the water drop on the surface.

We can generalize the deformation of liquid drop on inclined surface under friction force by following. In the case where the drop shape is crescent, the shape tends to be oval when friction coefficient increases. In this state, the deformation is governed by gravity force $\zeta_{def} > 1$. And in the case where the shape deforms from the oval shape to pearling shape under friction coefficient, the deformation is affected by friction force $\zeta_{def} < 1$. An oval shape appears as an intermediate shape between crescent shape and pearling

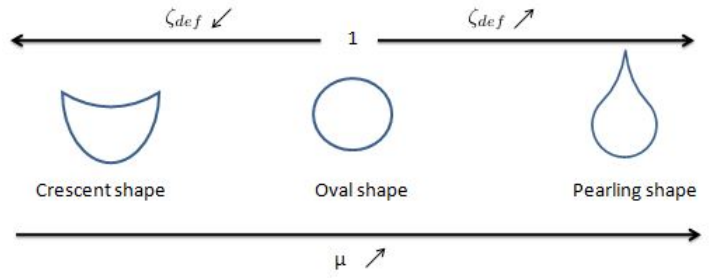


Fig. 7. Liquid drop shapes.

one. For the oval shape, the drop is balanced between gravity and friction forces $\zeta_{def} = 1$ (Figure.7).

IV. CONCLUSION

We report simulations on the liquid drop shape down an inclined surface in a situation of partial wetting using LBM. Two principal forces take into account during this study, which are gravity force of inclined surface and friction force. To describe the shape deformation under these two forces, we defined the deformation factor as the ratio between the drop size along x axis and the drop size along y axis. From simulation results, three main shapes can take a liquid drop on an inclined surface. (i) The oval shape appears when we have equilibrium between gravity force and friction one. This shape is observed for a deformation factor equal to 1. (ii) The crescent shape arising by the important of the gravity force and is characterized by a deformation factor higher than 1. (iii) The pearling shape occurrences when friction force is influenced than gravitational force and this shape appears for a deformation factor less than 1. Also in this paper, we have extracted an equation which express the relationship that rely the deformation factor with inclination angle of substrate and friction coefficient of the surface to predict the water drop shape on inclined surface.

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