Numerical simulation of droplet evaporation on a hot surface near Leidenfrost regime using multiphase lattice Boltzmann method

Naser Karami, Mohammad Hassan Rahimian*, Mohsen Farhadzadeh

School of Mechanical Engineering, Faculty of Engineering, University of Tehran, Tehran, Iran

1. Introduction

Impinging of liquid drops into a hot surface is an important phenomenon in industrial applications. It plays significant role in internal combustion engines as well as metallurgical heat treatment and cooling of the electronic devices. When a drop of liquid is deposited on a hot surface with the temperature around liquid boiling point, the drop boils and quickly vanishes. But if the surface temperature is far greater than the boiling point, the drop is levitated above its own vapor, and not anymore in contact with the surface. In this case, the evaporation rate decreases due to the insulation properties of the vapor film. Furthermore, the absence of contact between the hot surface and the droplet prevents the nucleation of bubbles, so that the droplet doesn’t boil but just quietly evaporates. Such floating droplets are called Leidenfrost droplets, the name of the physician who first surveyed the phenomenon [1].

Numerous experimental works are found in the literature for understanding the different aspects of droplet evaporation in the above mentioned flow. David Quere has presented a good review on Leidenfrost regime [2]. Different numerical works can also be found in the literature. Most of them have employed Navier–Stokes equations for solving the flow field and used either level set or volume of fluid (VOF) methods to capture the liquid–gas interface. One of the first investigators, who used the solution of Navier–Stokes equations for vaporizing droplet, was Karl et al. [3]. They used VOF method to simulate an
evaporating and non-wetting droplet in contact with a hot surface. The effect of the vapor velocity was neglected in the fluid flow. Using VOF method, Harvie and Fletcher [4] developed an axisymmetric code to simulate droplet evaporation in contact with a hot plate. They used a one-dimensional model for heat transfer inside the vapor film between wall and liquid drop. Fan and Ge [5] used level set method to simulate impact of saturated liquid drop on a hot surface. They solved a sub-cooled droplet impact on a hot surface and found that by increasing the sub-cooled degree, the Leidenfrost degree decreases. Chatzikyriakou et al. [6] solved a full Navier–Stokes equations for vapor under the boiling drop. Pournaderi and Pishavar [7] used projection method to solve Navier–Stokes equations for impinging of a droplet to a superheated wall. They used level set method for capturing the interface.

All of the aforementioned numerical works used the Navier–Stokes equations for the flow field. Although the research on the preceding flows is growing, the direct simulation of multi-phase flows including dynamic interfaces is still a challenging duty. The dominant difficulties are caused by the coupling of many effects such as latent heat, interfacial mass transfer, and surface tension, likewise the relevant conservation laws include energy, momentum, and mass.

The lattice Boltzmann method which is based on mesoscopic kinetic equations sounds to be a promising approach for dealing with multiphase and interfacial flows. The mesoscopic nature of the lattice Boltzmann method uses only a minimum amount of microscopic details to reproduce interfacial physics and macroscopic flow hydrodynamics in a consistent manner. Therefore, it can address length scales between micro- and macro-scale and simulate interfacial flows from a more fundamental basis. The lattice Boltzmann method has privileged aspects like simple coding, capture of complicated geometries, parallelism of computation. Shan and Chen [8] proposed a facile method for simulation of multi-phase flows which is executable in complex geometries. He et al. [9] developed two phase modeling based on LBM by introducing two specific distribution functions for the evaluation of mass, momentum and pressure, but they did not distinguish between thermodynamic and dynamic pressures. In their simulation parasitic velocities at the interface region have been decreased, but did not perish completely. Mukherjee et al. [10] introduced an external force which exerts on a wall in order to simulate the contact angle in previous method, and this force strengthens controls the wettability of the surface. Recently, Lee [11] proposed a two distribution function LBE method in the pressure evolution equation enforced the incompressibility. As long as the intermolecular force is indicated in the potential mode, the incompressible LBE method for interfacial flows could eliminate parasitic currents. His method is capable of simulation of multi-phase flows with density and viscosity ratios up to 1:1000. To model the interface dynamics on partially wetting surfaces, Lee et al. [12] extend Lee’s method for incompressible binary fluids.

Safari et al. [13] extended the multi-phase model of Lee to simulate thermal phase-change phenomena by incorporating a proper source term at the phase interface. They modified Chan–Hilliard equation in the existence of phase change, which was employed in Lee’s LBM model. Begmohammadi et al. [14] evaluated the capability of the model to simulate two-dimensional pool boiling with different density ratios up to 1:1000 and shown the consistency of the model with experimental correlations.

In the current work, Safari’s model is used to simulate droplet evaporation on a horizontal hot surface. It’s the first time that the evaporation and deformation of the drop in Leidenfrost regime is simulated by the Lattice Boltzmann method. First, the extension of the Chan–Hilliard equation in the presence of phase-change phenomena is presented. Then the LB model of Lee based on the classical convective Chan–Hilliard is given. In the following, the effects of variation of flow and surface characteristics have been explained thoroughly.

2. Mathematical modeling

Considering a binary flow including two incompressible fluids of different bulk density, the continuity equation for each phase without phase change could be written as:

$$\frac{\partial \bar{\rho}_i}{\partial t} + \nabla \cdot \bar{n}_i = 0 \quad (i = L, G)$$

(1)

where \(\bar{\rho}_i\) and \(\bar{n}_i\) are local density and the mass flow rate (per unit volume) of the component \(i\), and \(\rho_L\) and \(\rho_G\) denote liquid and gas phase density, respectively. In the bulk region, the mass flow is only attribute to advection, thus \(\bar{n}_i = \bar{\rho}_i \bar{u}_i\) where \(\bar{u}_i\) is the volume averaged velocity of the flow. When phase change occurs, \(m_{m}^\star\), the volumetric source due to phase change, should be added to the continuity equation for each phase as:

$$\frac{\partial \bar{\rho}_i}{\partial t} + \nabla \cdot \bar{n}_i = \pm m_{m}^\star \quad (i = L, G)$$

(2)

The two phases can be distinguished by their composition (C) in a volume element of the computational domain. By definition of \(C = \bar{\rho}_L / \rho_L\) the composition takes a value of 1 in the liquid phase and a value between 0 and 1 in the gas phase. So \(\bar{\rho}_i\) is related to \(\rho_i\) by \(\bar{\rho}_i = C \rho_L \rho_G = (1 - C) \rho_G\). In the interfacial region, a diffusive flow may exist as a result of mild transition of the interface. This diffusive mass flow is expressed by \(-\rho_{m} j_i\), where \(j_i\) is the volume diffusive flow rate. Thus the component \(i\)’s total mass flow rate can be denoted as \(\bar{n}_i = \bar{\rho}_i \bar{u}_i - \rho_{m} j_i\). The continuity equation can be written in the form of C as:

$$\frac{\partial C}{\partial t} + \nabla \cdot (\bar{u}C) - \nabla \cdot \bar{j}_i = -\frac{m_{m}^\star}{\rho_L}$$

(3)

$$\frac{\partial C}{\partial t} + \nabla \cdot (\bar{u}C) - \nabla \cdot \bar{j}_i = -\frac{m_{m}^\star}{\rho_L}$$

(3)
for the liquid phase and
\[
\frac{\partial (1 - C)}{\partial t} + \nabla \cdot (\mathbf{u}(1 - C)) - \nabla \cdot \mathbf{j}_g = - \frac{\dot{m}''}{\rho_g}
\] (4)
for the gas phase. Combining these two equations, the divergence of velocity field in the existence of phase change phenomena can be computed as:
\[
\nabla \cdot \mathbf{u} = \dot{m}'' \left( \frac{1}{\rho_g} - \frac{1}{\rho_l} \right)
\] (5)
while the diffusive flow rate is only related to \( C \) [15]. \( \mathbf{j}_g = - \mathbf{j}_c = \mathbf{j} \). Cahn and Hilliard stated that the diffusion flow rate is related to \( \mu \) as chemical potential by \( \mathbf{j} = \text{M} \nabla \mu \) where \( \text{M} \) is the mobility factor \((M > 0)\) [11]. Then the behavior of the multiphase system is govern by the transport equation of composition parameter \( (C) \) as:
\[
\frac{\partial C}{\partial t} + \nabla \cdot (\mathbf{u}C) = \nabla \cdot (\text{M} \nabla \mu) - \frac{\dot{m}''}{\rho_l}
\] (6)
For detailed explanation of the mobility factor and the chemical potential, refer to Safari et al. [13].

The Boltzmann equation for the mass and momentum equations for an incompressible binary fluids system can be written as:
\[
\frac{Df_{\alpha}}{Dt} = \frac{\partial f_{\alpha}}{\partial t} + \mathbf{e}_\alpha \cdot \nabla f_{\alpha} = -\frac{1}{\chi} \left( f_{\alpha} - f_{\alpha}^{eq} \right) + \frac{1}{\rho_c^2} \left( \mathbf{e}_\alpha - \mathbf{u} \right) \cdot \mathbf{F}_{\alpha}^{eq}
\] (7)
where \( f_{\alpha} \) is the distribution function, \( \rho \) is the density, \( \mathbf{e}_\alpha \)is the microscopic directional velocity of particles, \( \mathbf{u} \) is the volume averaged velocity, \( c_s^2 \) is the speed of sound, \( \lambda \) is the relaxation time, and \( f_{\alpha}^{eq} \) is equilibrium distribution function calculated according to the following equation:
\[
f_{\alpha}^{eq} = \omega_{\alpha} \rho \left[ 1 + \frac{\mathbf{e}_\alpha \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_\alpha \cdot \mathbf{u})^2}{2c_s^4} - \frac{(\mathbf{u} \cdot \mathbf{u})}{2c_s^2} \right]
\] (8)
where \( \omega_{\alpha} \) is the weight factor and its value depends on lattice structure. \( \mathbf{F} \) as intermolecular forces can be calculated by:
\[
\mathbf{F} = \nabla \rho c_s^2 - \nabla p_h + C \nabla \mu
\] (9)
where \( p_h \) is related to the hydrodynamic pressure. The body forces can be applied to Eq. (9) to consider its effects as [16]:
\[
\mathbf{F}_{\text{ext}} = \begin{cases} 
\mathbf{g}(\rho_l - \rho_c) & \rho_l \neq 0 \\
0 & \rho_l = 0 
\end{cases}
\] (10)
where \( \mathbf{g} \) indicate the gravitational acceleration. The discrete form of Eq. (7) evolves the density and momentum. One can evolve the pressure instead of the density by introducing a new distribution function as:
\[
g_{\alpha} = f_{\alpha} c_s^2 + (p_h - \rho_c c_s^2) \Gamma_{\alpha}(0)
\] (11)
where \( \Gamma_{\alpha} = \Gamma_{\alpha}(\mathbf{u}) = f_{\alpha}^{eq} / \rho \). The discrete Boltzmann equation (DBE) for the evolution of the hydrodynamic pressure and momentum is as follows:
\[
\frac{\partial g_{\alpha}}{\partial t} + \mathbf{e}_\alpha \cdot \nabla g_{\alpha} = -\frac{1}{\chi}(g_{\alpha} - g_{\alpha}^{eq}) + (\mathbf{e}_\alpha - \mathbf{u}) \cdot \left[ \nabla \rho c_s^2 (\Gamma_{\alpha} - \Gamma_{\alpha}(0)) - (\nabla \mu + \mathbf{F}_{\text{ext}}) \Gamma_{\alpha} \right] + \rho_c c_s^2 \dot{m}'' \left( \frac{1}{\rho_c} - \frac{1}{\rho_l} \right) \Gamma_{\alpha}(0)
\] (12)
where the equilibrium distribution function is stated as:
\[
g_{\alpha}^{eq} = f_{\alpha}^{eq} c_s^2 + (p_h - \rho_c c_s^2) \Gamma_{\alpha}(0) = \omega_{\alpha} \left[ p_h + \rho_c c_s^2 \left( \frac{\mathbf{e}_\alpha \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_\alpha \cdot \mathbf{u})^2}{2c_s^4} - \frac{(\mathbf{u} \cdot \mathbf{u})}{2c_s^2} \right) \right]
\] (13)
A new distribution function is needed for evolution of the composition \( C \). One of the simplest choices for particle and equilibrium distribution functions are \( h_{\alpha} = (C_{\rho}) f_{\alpha} \) and \( h_{\alpha}^{eq} = (C_{\rho}) f_{\alpha}^{eq} \) respectively. Taking the total derivative of \( h_{\alpha} \) and combining it with continuity equation for the composition leads to:
\[
\frac{\partial h_{\alpha}}{\partial t} + \mathbf{e}_\alpha \cdot \nabla h_{\alpha} = -\frac{1}{\chi}(h_{\alpha} - h_{\alpha}^{eq}) + (\mathbf{e}_\alpha - \mathbf{u}) \cdot \left[ \nabla C - \frac{C}{\rho c_s^2} (\nabla p_h + C \nabla \mu + \mathbf{F}_{\text{ext}}) \right] \Gamma_{\alpha} + \left( \text{M} \nabla^2 \mu - \frac{\dot{m}''}{\rho_l} \right) \Gamma_{\alpha}
\] (14)
The discrete form of Eqs. (12) and (14) along characteristics over the time step $\delta t$ is summarized as follows:

$$
\tilde{g}_\alpha (x + e_\alpha \delta t, t + \delta t) - \tilde{g}_\alpha (x, t) = -\frac{1}{\tau + 0.5} \left[ (\tilde{g}_\alpha - \tilde{g}_{\alpha}^eq) \right]_{(x,t)} + \frac{\delta t}{2} \left[ \nabla \cdot \left( \rho \tilde{c}_\alpha^2 (\Gamma_\alpha - \Gamma_\alpha (0)) - (C \nabla \mu + F_{ext}) \right) \Gamma_\alpha \right]_{(x,t)} + \frac{\delta t}{2} \rho \tilde{c}_\alpha^2 \tilde{m}'' \left( \frac{1}{\rho_c} - \frac{1}{\rho_L} \right) \Gamma_\alpha (0) \left|_{(x, t + \delta t)} \right.
$$

(15)

where $\tilde{g}_\alpha$ is introduced to summarize equations as

$$
\tilde{g}_\alpha = g_\alpha + \frac{\left( g_\alpha - g_{\alpha}^eq \right)}{2\tau} - \frac{\delta t}{2} (e_\alpha - u) \cdot \left[ \nabla \rho \tilde{c}_\alpha^2 (\Gamma_\alpha - \Gamma_\alpha (0)) - C \nabla \mu G_\alpha \right]
$$

and the equilibrium distribution function ($g_{\alpha}^{eq}$) as:

$$
\tilde{g}_{\alpha}^{eq} = g_{\alpha}^{eq} - \frac{\delta t}{2} (e_\alpha - u) \cdot \left[ \nabla \rho \tilde{c}_\alpha^2 (\Gamma_\alpha - \Gamma_\alpha (0)) - C \nabla \mu G_\alpha \right]
$$

(17)

Similarly for $\tilde{h}_\alpha$ we have

$$
\tilde{h}_\alpha (x + e_\alpha \delta t, t + \delta t) - \tilde{h}_\alpha (x, t) = -\frac{1}{\tau + 0.5} \left[ (\tilde{h}_\alpha - \tilde{h}_{\alpha}^{eq}) \right]_{(x,t)} + \delta t (e_\alpha - u) \cdot \left[ \nabla C - \frac{C}{\rho_c} (\nabla p_h + C \nabla \mu + F_{ext}) \right] \Gamma_\alpha \left|_{(x,t)} \right.
$$

$$
+ \frac{\delta t}{2} \left( \nabla \rho \tilde{c}_\alpha^2 \Gamma_\alpha \right) \left|_{(x,t)} \right.
$$

(18)

Where

$$
\tilde{h}_{\alpha} = h_{\alpha} + \frac{\left( h_{\alpha} - h_{\alpha}^{eq} \right)}{2\tau} - \frac{\delta t}{2} (e_\alpha - u) \cdot \left[ \nabla C - \frac{C}{\rho_c} (\nabla p_h + C \nabla \mu) \right] \Gamma_\alpha
$$

(19)

and the equilibrium distribution function ($h_{\alpha}^{eq}$) is expressed as:

$$
\tilde{h}_{\alpha}^{eq} = h_{\alpha}^{eq} - \frac{\delta t}{2} (e_\alpha - u) \cdot \left[ \nabla C - \frac{C}{\rho_c} (\nabla p_h + C \nabla \mu) \right] \Gamma_\alpha
$$

(20)

Finally the value of density, velocity and pressure is calculated by taking the zeroth and first moments of the modified particle distribution function as follows:

$$
C = \sum_\alpha \tilde{h}_\alpha
$$

(21)

$$
\rho = C \rho_0 + (1 - C) \rho_L
$$

(22)

$$
\rho u = \frac{1}{c_s^2} \sum_\alpha e_\alpha \tilde{g}_\alpha - \frac{\delta t}{2} C \nabla \mu
$$

(23)

$$
p_h = \sum_\alpha \tilde{g}_\alpha + \frac{\delta t}{2} u \cdot \nabla C
$$

(24)

Cahn and Cahn-Hilliard wetting theory is used to obtain the equilibrium contact angle between the solid, liquid and the gas interfaces. No mass flux boundary necessitates zero chemical potential gradients in the direction normal to the solid boundary:

$$
n \cdot \nabla \mu |_s = 0
$$

(25)

where $n$ is the unit vector normal to the surface. Another boundary condition is obtained by minimizing the total free energy with respect to $C$, yields [12]

$$
n \cdot \nabla C |_s = \frac{\partial \phi}{\partial C} (C_\mu - C_s^2)
$$

(26)

where $\phi$ is constant coefficient, known as wetting potential. The passive scalar method with low Mach number limit is used to simulate heat transfer. The pressure work and dissipation of energy are neglected due to low Mach number limit and an
advection-diffusion energy equation is solved, using a separate distribution function \( s_\alpha \) in the LB framework. The DBE for the new distribution function is written as:

\[
\frac{\partial s_\alpha}{\partial t} + \mathbf{e}_\alpha \cdot \nabla s_\alpha = -\frac{1}{\lambda T} \left( s_\alpha - s_\alpha^{eq} \right) \tag{27}
\]

with equilibrium distribution in the form of:

\[
s_\alpha^{eq} = \omega_\alpha T \left( 1 + \frac{\mathbf{e}_\alpha \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_\alpha \cdot \mathbf{u})^2}{2c_s^4} - \frac{(\mathbf{u} \cdot \mathbf{u})}{2c_s^4} \right) \tag{28}
\]

The DBE of Eq. (27) is integrated along characteristics to achieve LBE for the temperature. Applying the trapezoidal integration leads to

\[
s_\alpha(\mathbf{x} + \mathbf{e}_\alpha \delta t, t + \delta t) - s_\alpha(\mathbf{x}, t) = -\frac{s_\alpha - s_\alpha^{eq}}{2\tau_T} \bigg|_{\mathbf{x} + \mathbf{e}_\alpha \delta t, t + \delta t} - \frac{s_\alpha - s_\alpha^{eq}}{2\tau_T} \bigg|_{\mathbf{x}, t} \tag{29}
\]

where \( \tau_T = \lambda T/\delta t \) is the nondimensional relaxation time. Since Eq. (29) is implicit in time, the modified distribution function is introduced as follows to make the scheme explicit with second-order accuracy:

\[
\tilde{s}_\alpha(\mathbf{x}, t) = s_\alpha(\mathbf{x}, t) + \frac{s_\alpha(\mathbf{x}, t) - s_\alpha^{eq}(\mathbf{x}, t)}{2\tau_T} \tag{30}
\]

The LBE for the modified distribution function of temperature can be derived as:

\[
\tilde{s}_\alpha(\mathbf{x} + \mathbf{e}_\alpha \delta t, t + \delta t) - \tilde{s}_\alpha(\mathbf{x}, t) = -\frac{1}{\tau_T + 0.5 \left( \tilde{s}_\alpha - \tilde{s}_\alpha^{eq} \right)} \bigg|_{\mathbf{x}, t} \tag{31}
\]

The temperature is calculated by taking the zero-order moment of the above distribution function as

\[
T = \sum_\alpha s_\alpha = \sum_\alpha \tilde{s}_\alpha \tag{32}
\]

And the thermal diffusion is related to relaxation time by \( \alpha = c_s^2 \tau_T \delta t \).

In the present paper the liquid phase temperature is assumed at saturation temperature and the driving force for evaporation is the amount of heat which is transferred to the interface. So by applying the energy balance for the interface regions the local vaporization mass flow rate per unit surface \((\dot{m}_v)\) may be written as

\[
\dot{m}_v'' = \frac{K \nabla T}{\rho_\ell} \cdot \hat{n} \tag{33}
\]

where \( \rho_\ell \) is the latent heat of vaporization, \( K \) is the thermal conductivity, and \( \hat{n} \) is the unit vector normal to the phase interface. The above vaporization rate is computed per unit surface, so it should be converted to the volumetric form in order to be employed in the convective Cahn–Hilliard equation. So by multiplying \( \dot{m}_v'' \) with the local interface content \((|\nabla \mathbf{c}|)\) and recalling \( \hat{n} = \frac{\mathbf{V}_C}{|\nabla \mathbf{C}|} \), the volumetric mass source of evaporation can be obtained as

\[
\dot{m}_v''' = \frac{K \nabla T}{\rho_\ell} \cdot \nabla C \tag{34}
\]

In the problem of drop spreading on a surface and its evaporation several non-dimensional parameters are considered including: the Archimedes number \( Ar = \frac{\rho_v \sqrt{\rho_\ell g}}{\mu} \); the Bond number \( Bo = \frac{\rho_v g D_\ell^2}{\mu^2} \); the Stefan number \( St = \frac{C_p(T_{wall} - T_{sat})}{h_\ell} \); the Prandtl number \( Pr = \frac{c_p \kappa}{\mu} \); the equilibrium contact angle \( \theta_{eq} \); the dimensionless time \( t^* = \frac{t}{\sqrt{\frac{D_\ell}{\rho_\ell}}} \). In order evaluate the evaporation rate, it is needed to define a new non-dimensional parameter. For this reason non-dimensional mass of liquid phase \( m_l/m_{eq} \) is considered. Where \( m_{eq} \) stands for droplet initial mass.

3. Result and discussion

3.1. Model validation

3.1.1. 1D evaporation

The one-dimensional Stefan problem, for which an analytical solution is available, is a well-known benchmark to test two-phase flow phase-change simulations. In the problem, the vapor and liquid phases are initially at stationary state with saturation temperature. As shown in Fig. 1, the vapor phase is in contact with an isothermal wall.

Once the wall experiences an increase in the temperature, heat is transferred to the interface leading the liquid to evaporate. In this flow, the vapor will be motionless while the interface and liquid would be driven away from the wall. Fig. 2 shows the comparison between D1Q3 Lattice Boltzmann model results and solution of one dimensional equation of Stefan flow for density ratio equal to 10, 100 and 1000. As it is shown they agreed well with analytical solution. The interested readers can refer to [13].
3.1.2. 2D evaporation

In this section, a 2D droplet is initialized at the center of the computational domain, and the gravitational acceleration is set to 0. The outflow boundary condition is considered by assuming \( \frac{\partial n}{\partial n} = 0 \), where \( n \) is the normal direction to the boundary. At the initial time step, the uniform temperature of \( T_{\text{gas}} \) is set for the gas phase, while the droplet temperature is fixed to \( T_{\text{sat}} \). The existence of temperature gradient at the phase interface leads to the vaporization of the droplet to the gaseous ambient. As a result of evaporation, a radial velocity profile called Stefan flow should be generated around the droplet in the gas phase, while the droplet remains stationary. The droplet radius is 20 LU. The liquid and the vapor density are fixed at 1.0 and 0.001 respectively.

It can be seen that the spherical shape of the 2D droplet is preserved during the evaporation process. The velocity vectors are presented in Fig. 3 for time step 40,000. The vector’s radial direction normal to the interface and rotational symmetry with respect to the center of the droplet are consistently reproduced as expected.

One of the most effective parameter on evaporation is dimensionless Stefan number which is defined as the ratio of sensible heat to the latent heat. The decrease of latent heat or increase of the temperature difference causes the Stefan number to increase and vice versa. The reduced square diameter is plotted against time for various Stefan numbers in Fig. 4. As expected, the increase of Stefan number accelerates the evaporation, and the reduced square diameter is linearly proportional to time, which is consistent with the well-known \( d^2 \) law.

3.1.3. Laplace law

The Laplace law is the basic test to evaluate correct surface tension effects of multiphase models. According to Laplace law for spherical droplet (Eq. 35), the pressure difference between the inside and outside of the droplet (\( \Delta P \)) is proportional to \( \frac{1}{R} \), where \( R \) is the droplet radius.

\[
\Delta P = P_{\text{in}} - P_{\text{out}} = \frac{\sigma}{R}
\]  

(35)

In Fig. 5, it can be seen that the linear relationship between \( \Delta P \) and \( \frac{1}{R} \) agrees well with theory.

3.1.4. Contact angle

When a liquid-vapor interface meets a solid wall and goes in to equilibrium state, the angle between wall and interface is called contact angle. Briant et al. [17] investigated the contact angle using the free energy lattice Boltzmann method.
According to Young’s law, the contact angle is measured as

$$\cos \theta^\text{eq} = \frac{\sigma_{SG} - \sigma_{SL}}{\sigma_{GL}} = \Omega_c$$  \hspace{1cm} (36)

$$\Omega_c = \phi_c / \sqrt{2k\beta}$$  \hspace{1cm} (37)
Fig. 5. Laplace low validation.

Fig. 6. Final shape of a droplet with radius of 20 LU for different contact angles.

Fig. 7. Comparison between the numerical and analytical calculated contact angle versus wetting potential.

Where \( \theta_{\text{eq}} \) is the contact angle measured from liquid side, \( \Omega_c \) is wetting potential and \( \sigma_{SG} \), \( \sigma_{GL} \) and \( \sigma_{SL} \) are the solid–gas, liquid–gas and solid–liquid surface tension, respectively.

To verify the contact angle between the liquid–gas and solid surface, a droplet with a radius of 20 LU is initiated in the 150 × 100 computational field, tangent to the surface and after obtaining the equilibrium state, located at the solid wall. For the case of \( \theta_{\text{eq}} = 20 \), \( \theta_{\text{eq}} = 90 \) and \( \theta_{\text{eq}} = 150 \), the final shape of the droplet is presented in Fig. 6. Static contact angles as a function of wetting potential are presented in Fig. 7. From Fig. 7 it is clear that the calculated contact angles are consistent with analytical solution.
3.2. Droplet impingement on a hot surface

In order to validate the thermal behavior of the droplet, the influence of the Reynolds number on heat transfer during single drop impingement will be investigated. To isolate the influence of the Reynolds number, all the other dimensionless groups should be kept constant for all simulations. Therefore, all thermo-physical properties of the liquid, vapor and solid are kept constant. Thereby the Prandtl number equals 9.54 and all dimensionless quantities relevant to the micro region model remain unchanged. The initial wall super-heat is kept at $T_{wall} - T_{sat} = 10\,K$ and the heat input to the heater is 4400 W/m$^2$. To change only the Reynolds number, the ratio of the droplet diameter and its initial velocity is varied such that the Weber number stays at a constant value of 15. Due to the change in droplet diameter the gravitational acceleration has to be adapted to keep the Bond number at a constant value of 0.5. To be able to study the heat transfer, a dimensionless heat is defined as the ratio of $Q$, the heat transferred till a given time instant to the heat necessary to evaporate the droplet completely:

$$E^* = \frac{6Q}{\pi \rho_l D_0^2 h_l}$$  \hspace{1cm} (38)

Analogously, a dimensionless evaporative heat is defined as the ratio of the evaporated mass to the initial mass of the droplet

$$E_{evap}^* = \frac{6M_{evap}}{\pi \rho_l D_0^2}$$  \hspace{1cm} (39)

The overall impact process is subdivided into two distinct phases. In phase A, the droplet starts to spread and the fluid motion is dominated by inertia and the contact line is moving radially outwards. In this phase a part of the kinetic energy is dissipated while the residual energy is stored in the enlargement of the liquid–vapor interface. After reaching its maximal radius phase B starts to happen and the contact line starts to recede. The driving force is the surface tension which tries to minimize the surface area. Thereby the kinetic energy again rises causing a decrease of the contact line radius to a minimal value smaller than the one corresponding to the equilibrium shape.

Fig. 8 shows the evolution of dimensionless evaporative rate at different Reynolds number for the Herbert et al. [18] results and present simulation. It can be seen that the present results are in good agreement with Herbert et al. results. It can be concluded that most of the evaporation takes place during the receding phase B. Again, for a smaller droplet with a faster moving contact line the micro convection heat transfer close to the contact line is much more intense. Hence, the dimensionless evaporative heat is increasing with decreasing Reynolds numbers.

As another test, the spreading ratio ($S$) is employed to compare the wetting characteristics.

$$S = \frac{D_{cl}}{D_0}$$  \hspace{1cm} (40)

$D_{cl}$ denotes the diameter of the wetted region. The spreading ratio is plotted against time in Fig. 9. There are three different stages of the impingement process visible. In the initial spreading phase the contact line is moving outwards until it reaches a maximum. Thereafter the fluid motion is reversed and the contact line contracts again (receding). If the receding is fast enough, a small undershoot in the contact line radius can be detected before the droplet reaches its equilibrium shape.
corresponding to that of a sessile droplet. As can be seen, good agreement between the simulation results and Herbert et al. [19] results can be found.

3.3. Computation domain

The simulation is carried out on the 225 × 150 computational domain with an initial droplet which is placed tangent to the surface and D2Q9 scheme is used for modeling. At the initial time step, the uniform temperature $T_{\text{gas}}$ is set for the gas phase, while the droplet temperature is fixed to saturated temperature ($T_{\text{sat}}$) and the horizontal surface remains at the superheated boundary condition. As shown in Fig. 10, the outflow boundary condition is considered by assuming $\frac{\partial p_h}{\partial n} = 0$, where $n$ is the normal direction to the boundary.

3.4. Grid independency

In order to show grid independency, four domains as 100 × 66, 150 × 100, 225 × 150 and 300 × 200 lattices are used. A droplet is located on the surface and starts to evaporate with $\frac{\rho_L}{\rho_g} = 1000$, $Bo=0.016$, $Ar_g=3.394$, $Ar_L=3.394$, $St_g=0.12$, $Pr_g=0.71$ and $\theta=60^\circ$. The dimensionless liquid mass at $t^*=3.7$ is calculated in Table 1. According to Table 1, grid resolution more than 225 × 150 has no effect on the dimensionless liquid mass, so it is concluded that the grid resolution has no substantial effect on the results.

3.5. Effects of Bond number

The Bond number shows the ratio of the gravitational force to the surface tension force. To show the effects of bond number, other non-dimensional parameters are held fixed and the Bond number varies from 0.00533 to 0.08. As illustrated in Fig. 11, by decreasing surface tension force, the Bond number increases and causes the droplet spreads out. In this situation, the droplet breaks up into 2 and 4 pieces at $Bo=0.016$ and $Bo=0.08$, respectively.
Table 1
Dimensionless liquid mass at different domain division.

<table>
<thead>
<tr>
<th>Domain</th>
<th>$t^*$</th>
<th>$\frac{m}{m_0}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>100 × 66</td>
<td></td>
<td>0.811</td>
</tr>
<tr>
<td>150 × 100</td>
<td>3.7</td>
<td>0.904</td>
</tr>
<tr>
<td>225 × 150</td>
<td></td>
<td>0.939</td>
</tr>
<tr>
<td>300 × 200</td>
<td></td>
<td>0.941</td>
</tr>
</tbody>
</table>

Fig. 11. Simulation of the droplet evaporation on the hot surface at different Bond numbers.

Dimensionless liquid mass is plotted against time for various Bond number in Fig. 12. As shows the significant deviations occur in ranging from $t^* = 7$ to $t^* = 9$, which is due to droplet breaks up. Thus, droplet breaks up leads to the augment of the drops’ surface and causes higher evaporation rate.

3.6. Effects of liquid Archimedes number

Liquid Archimedes number is the ratio of the gravitational force to the viscous force. To evaluate the effects of liquid Archimedes number, $Bo = 0.016$, $Ar_g = 3.394$, $St_g = 0.12$ and $Pr_g = 0.71$, while the liquid Archimedes number varies from 2.424 to 4.242. The results are plotted in Fig. 13. As shown in Fig. 13, the drop is detached from the heated wall due to the velocity of the vaporized gas under the drop. Reducing the liquid Archimedes number, by increasing the liquid viscosity, causes less elongation of the droplet and makes the droplet’s breakup to be postponed. From Fig. 14, it can be seen that the liquid Archimedes number has no substantial effect on the evaporation rate.
Fig. 12. Dimensionless liquid mass versus dimensionless time at different Bond numbers.

Fig. 13. Simulation of the droplet evaporation on the hot surface at different Archimedes numbers.
3.7. Effects of density ratio

Decreasing of the density ratio is obtained by reducing the density of liquid. When the density of the liquid decreases, the weight of the droplet decreases consequently and the degree of its deformation is reduced as well. In this case, the contact surface between the heated wall and the liquid part is reduced which leads to the reduction of the evaporation rate. The smaller density ratios, cause the bigger remained droplets as seen in Fig. 15a–d.

Fig. 16 shows that increase in the density ratio causes the evaporation to accelerate. The significant deviations occur in ranging from $t^* = 7$ to $t^* = 12$, which is due to droplet’s breakup.

3.8. Effects of gas Stephan number

To estimate the effects of Stefan number, the simulation parameters are fixed at $Bo = 0.008$, $Ar_g = 3.394$, $Ar_l = 4.242$, $Pr_g = 0.71$, $\theta = 60^\circ$. At low Stefan number, the rate of droplet evaporation is so weak that it’s unable to keep the droplet from touching the surface. It can be seen that the Leidenfrost regime is reached where the Stefan number is higher than 0.094. From Fig. 17, it is obvious that increase in the evaporation rate also effects the droplet deformation, it forms the drop more concave on lateral sides and Makes the droplet reach more aerodynamic efficient shape.

To investigate the effects of latent heat and temperature difference on the evaporation, the liquid dimensionless mass is plotted against time for various Stefan numbers in Fig. 18. The decrease of latent heat or increase of the temperature difference causes the Stefan number to increase and vice versa. As expected, the increase of Stefan number accelerates the evaporation.

It should be noted that, attachment of the liquid phase to the wall is also a function of equilibrium contact angle. To show this phenomenon, Fig. 19 presents the results for two different contact angles. It can be concluded that increasing the contact angle helps the generated vapor to detach the droplet from the surface.

3.9. Effects of gas Prandtl number

In this section, behavior of a droplet on a hot surface is investigated in different gas Prandtl number. Gas Prandtl number is the ratio of the thermal diffusivity coefficient to the momentum diffusivity coefficient. Increasing the Prandtl number causes the decreasing of heat transfer rate and vice versa. Fig. 20 shows the droplet interface variation with the time for different Prandtl number. The non-dimensional parameters are set to: $\frac{Pr_l}{Pr_g} = 1000$, $Bo = 0.008$, $Ar_g = 3.394$, $Ar_l = 4.242$ and $St_g = 0.12$. It is observed that decreasing the gas Prandtl number causes the increasing in heat transfer and accelerates the evaporation (Fig. 21). Thus, as expected, increasing the mass flux will substantially increase the distance between the surface and the droplet which due to thrust force resulting from the vapor evaporation.

3.10. Flow field

Flow field and temperature field during drop evaporation and spreading on a hot surface are indicated in Fig. 22. As shown, two symmetric counter-rotating vortices are generated during the evaporation. Fig. 22c obviously demonstrates the generation of gas phase. As shown the evaporative mass flux reaches its maximum at the bottom of the drop where it meet
Fig. 15. Simulation of the droplet evaporation on the hot surface at different density ratios.

Fig. 16. Dimensionless liquid mass versus dimensionless time in different density ratios.
the hot surface. As time passes, the gravitational acceleration makes the drop spread along side of the surface and the vapor generation is big enough to avoid direct contact with the hot surface.

### 4. Conclusion

In this paper, the evaporation of a liquid drop in contact with a heated wall was investigated. The flow field was solved by incompressible two phase flow lattice Boltzmann method. Cahn–Hilliard equation was employed to capture the interface between the gas and liquid phases. Passive scalar method was used to solve the energy equation. Volume of gas generated
at the interface due to the liquid vaporization, is calculated by the balance of energy transferred to the liquid phase and latent heat of the liquid. The effects of several non-dimensional numbers including the Bond number, liquid Archimedes number, gas Stefan number, the Prandtl number, density ratio and equilibrium contact angle on behavior of liquid droplet are investigated. The simulation results in this paper can be summarized as follows:

- By decreasing surface tension force, the Bond number increases and causes the droplet spreads out. In this situation, the droplet breaks up and leads to the augment of the drop surface and causes higher evaporation rate.
- Reducing the liquid Archimedes number, by increasing the liquid viscosity, causes less elongation of the droplet and makes the droplet's breakup to be postponed. It's also shown that the liquid Archimedes number has no substantial effect on the evaporation rate.
- At low Stefan number, the rate of droplet evaporation is so weak that it's unable to keep the droplet from touching the surface. It's shown that the Leidenfrost regime is reached where the Stefan number is higher than 0.094.
- Decreasing the gas Prandtl number causes the increase in heat transfer and accelerates the evaporation. Increasing the mass flux will substantially increase the distance between the surface and the droplet which due to thrust force resulting from the vapor evaporation.
Fig. 21. Dimensionless liquid mass versus dimensionless time in different gas Prandtl number.

Fig. 22. Temperature, velocity and mass source contours at two different dimensionless time (\( \frac{\rho_L}{\rho_g} = 1000 \), Bo = 0.08, \( \text{Ar}_g = 3.394 \), \( \text{Ar}_L = 4.242 \), St\(_g\) = 0.12, Pr\(_g\) = 0.71, \( \theta = 60^\circ \)).
• When the density of the liquid decreases, the weight of the droplet decreases consequently and the degree of its deformation is reduced as well. In this case, the contact surface between the heated wall and the liquid part is reduced which leads to the reduction of the evaporation rate.
• Decreasing the equilibrium contact angle causes the lagging of the Leidenfrost regime in the domain.

Considering the 2D simulation results, it can be shown that the used method is feasible for simulation of near Leidenfrost regime. Furthermore, it is straightforward to extend into 3D cases and study more challenging real world problems such as droplet impingment onto a hot porous media.

References