Numerical Simulation of Liquid-vapor Phase Change via a Two-phase Lattice Boltzmann Method

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Abstract. In this work a two-phase lattice Boltzmann model is adopted to simulate the liquid–vapor flows in this work. This lattice Boltzmann model is based on a pseudo-potential scheme, which is proved to be able to account for the liquid-vapor phase transition during the process of heat transfer. For the purpose of validation, the result of liquid-vapor coexistence curve is compared with the theoretical result. Then the problem of the formation of vapor bubble as well as its departure in pool boiling is examined.

Introduction

Two-phase flows are very common in many natural processes such as the weather as well as in industrial applications such as combustion engines, heat exchangers, boilers, dryers. For liquid–vapor two-phase flows, the phase change takes place under certain conditions, which is proved to be a useful and efficient process to transfer energy in numerous domestic and industrial applications. It is important to understand the phenomena and mechanism of the phase change between liquid and vapor to provide an insight into the behavior of heat transfer in liquid.

The lattice Boltzmann method (LBM), which is based on mesoscopic kinetic equations, has emerged as a powerful numerical scheme for the simulation of particle suspensions, multiphase flow, microfluidics, and turbulence due to its several remarkable advantages since it was originated. In particular, the LBM is proved to be a promising method for dealing with interfacial flows such as solid-liquid and liquid-vapor flows. So far several lattice Boltzmann (LB) models have been proposed to simulate the liquid-vapor flows, including the color-gradient LB model [1–3], the pseudo-potential LB model [4–7] and the free-energy LB model [8, 9]. The pseudo-potential model which was first proposed by Shan and Chen [4], has become very popular due to its conceptual simplicity and computational efficiency. On the basis of Shan and Chen [4], Gong and Cheng [5, 6] proposed an improved lattice Boltzmann model for liquid-vapor phase change. In their model, a new form of the source term in the energy equation was derived, which was demonstrated to improve the numerical stability. The reader is referred to a recent review [10] that detail the tremendous progress in the development of multiphase flow simulation methods.

The liquid-vapor phase change is omnipresent in science and technology, but, as far as basic understanding of the hydrodynamics, this phenomenon remains unclear. Much more attention should be paid to the effect of the boiling on the heat transfer. The objective of this work is to present a preliminary understanding of the fluid dynamics and heat transfer of the liquid-vapor phase transition. The improved LB model proposed by Gong and Cheng [6, 7] is used here.

Lattice Boltzmann Model

The lattice Boltzmann model proposed by Gong and Cheng [6, 7] is briefly introduced here. The discrete lattice Boltzmann equations of a single-relaxation-time model are expressed as,

\[ f_i(x + e_i \Delta t, t + \Delta t) - f_i(x, t) = -\frac{1}{\tau} (f_i(x, t) - f_i^{eq}(x, t)) + \Delta f_i(x, t) \] (1)
where \( f_i(x, t) \) is the distribution function for the microscopic velocity \( e_i \) in the \( i \)-th direction, \( \Delta t \) is the time step of the simulation, \( \tau \) is the relaxation time. \( f_i^{(eq)}(x, t) \) is the equilibrium distribution function which is given by,

\[
f_i^{(eq)} = w_i \rho \left[ 1 + \frac{e_i \cdot u}{c^2_i} + \frac{(e_i \cdot u)^2}{2c^4_i} - \frac{u^2}{2c^2_i} \right],
\]

where \( c_s \) is the speed of sound, and \( w_i \) are weights related to the lattice model. \( \Delta f_i(x, t) \) is the body force term, which accounts for the inter-particle interactions force \( F_{int} \), the gravitational force \( F_g \) and the interaction force between solid surface and fluid \( F_s \). According to Gong and Cheng [6], the inter-particle interactions force \( F_{int} \) has the following expression,

\[
F_{int}(x) = -\beta \psi(x) \sum G(x, x') \psi(x')(x' - x) - \frac{1}{2} \sum G(x, x') \psi'(x')(x' - x).
\]

where \( G(x, x') \) is given by,

\[
G(x, x') = \begin{cases} 
  g_1, & |x-x'| = 1 \\
  g_2, & |x-x'| = \sqrt{2} \\
  0, & \text{otherwise}
\end{cases}
\]

with \( g_1=2g, g_2=g/2 \) for D2Q9 model. \( \psi(x) \) is the “effective mass” which is defined by,

\[
\psi(\rho) = \frac{2(\rho - \rho c_s^2)}{c_0 g}.
\]

Then the fluid density and velocity are obtained through,

\[
\rho = \sum f_i, \rho u = \sum e_i f_i.
\]

The real fluid velocity of fluid \( U \) should be modified,

\[
\rho U = \sum e_i f_i + \frac{\Delta t}{2} F.
\]

To solve the temperature, another lattice Boltzmann equations are proposed [6],

\[
g_i(x + e_i \Delta t, t + \Delta t) - g_i(x, t) = -\frac{1}{\tau_T} (g_i(x, t) - g_i^{(eq)}(x, t)) + \Delta t w_i \phi.
\]

where \( \tau_T \) is the relaxation time and \( g_i^{(eq)}(x, t) \) is the equilibrium distribution function for the temperature,

\[
g_i^{(eq)} = w_i T \left[ 1 + \frac{e_i \cdot U}{c^2_i} + \frac{(e_i \cdot U)^2}{2c^4_i} - \frac{U^2}{2c^2_i} \right].
\]

The source term \( \phi \) in is responsible for the phase change, which is determined through,

\[
\phi = T \left[ 1 - \frac{1}{\rho c_p} \frac{\partial \rho}{\partial T} \right] \nabla \cdot U.
\]

The temperature is obtained by,

\[
T = \sum g_i.
\]
Validation

The equation of state (EOS) relates the pressure $p$, volume $V$ and temperature $T$ of a physically homogeneous system in the state of thermodynamic equilibrium. So far, the Peng-Robinson (P-R) equation of state has become the most popular equation of state for natural gas systems in the petroleum industry, which is adopted in the present work.

In order to validate the present lattice Boltzmann model, the liquid-vapor coexistence curve obtained from the simulations is compared with the theoretical curve predicted by the Maxwell equal-area construction. This comparison is given in Figure 1. In thermodynamics, the coexistence curve, also known as binodal curve, denotes the condition at which two distinct phases may coexist. Equivalently, it is the boundary between the set of conditions in which it is thermodynamically favorable for the system to be fully mixed and the set of conditions in which it is thermodynamically favorable for it to phase separate.

As can be seen from Figure 1, the simulated coexistence curves fit well with the theoretical values. Note that $\rho/\rho_c < 1$ and $\rho/\rho_c > 1$ represent the vapor phase and liquid phase, respectively. Obviously, the present simulation results agree well with analytical solutions both in the liquid branch and vapor branch, as shown in Figure 1. Furthermore, the liquid/vapor density ratio can be higher than 1000 for the P-R EOS.

![Figure 1. Comparison of coexistence curves obtained from simulations with theoretical values for P-R EOS.](image)

Numerical Results

First of all, the effect of the saturated temperature $T_s$ on the liquid-vapor change is studied. The focus of this work is on the motion of gas bubble. Therefore, the density $\rho$ is initially set lower than the critical density $\rho_c$ at the central domain (with a radius of $R = 20$) and higher than $\rho_c$ elsewhere at a given saturated temperature $T_s$. For simplicity, an $80 \times 80$ computational domain is chosen and boundary conditions are set to be periodic on all directions. Each test was run for 20 000 time steps. At that point, the relative differences of the maximum magnitudes of the velocities at time step $t$ and $t-1000$ are on the order of $10^{-6}$, suggesting that a steady state is reached and a gas bubble ($\rho/\rho_c < 1$) surrounded by liquid ($\rho/\rho_c > 1$) is formed.
Figure 2. Instantaneous distribution of fluid density for different saturated temperature $T_s$ at different times: (a) $t=400$, (b) $t=800$, (c) $t=1600$, (d) $t=3200$ and (e) $t=6400$. The values of $T_s$ are $0.9T_c$ (top), $0.92T_c$ (middle) and $0.95T_c$ (bottom), respectively.

Figure 2 shows the instantaneous distribution of fluid density for different saturated temperature $T_s$ at different times. In this case the influence of gravity is not considered. Three values of $T_s$ are taken into account in the simulations: $T_s=0.9T_c$, $0.92T_c$ and $0.95T_c$. The effect of $T_s$ is significant, as can be seen in Figure 2. For all cases a steady bubble is observed in the central domain. However, the liquid/vapor density ratio decreases fast as $T_s$ increases (note the color map). The size of bubble increases as $T_s$ increases. In addition, the interface thickness is very small for $T_s=0.9T_c$. It has been known that the sharp interface between liquid and vapor plays an important role in the process of heat transfer.

Figure 3. Instantaneous distribution of fluid density for $T_s=0.9T_c$ and $T_w=0.92T_c$ at different times: (a) $t=5000$, (b) $t=8000$, (c) $t=10000$, (d) $t=11000$, (e) $t=12000$, (f) $t=13000$, (g) $t=15000$, and (h) $t=16000$.

Now the influence of gravity is taken into account in the simulations of pool boiling resulted from a heated spot. A computation domain of $200 \times 400$ is chosen in this case. Initially, the whole domain is occupied by the saturated liquid with a temperature of $0.9T_c$. In order to make the phase change happen, a hot spot with a width of $6\Delta x$ is placed at the center of the bottom wall. The temperature of the hot spot is set to be $T_w=0.92T_c$, which is a little higher than that of the surrounding liquid. For simplicity, constant temperature ($T_s$) boundary condition is imposed on all the walls. Figure 3 shows the process of phase transition during which one can observe the growth and departure of a gas bubble from the heated spot. As shown in Figure 3, due to the heated spot the density of the liquid close to
the center of the bottom wall decreases with time. The phase change is clearly seen at $t=12000$, as plotted in Figure 3(e), which shows a vapor bubble ascending slowly in the liquid under the influence of buoyancy force. Then, a circular bubble is forming, whose volume is increasing quickly at the same time, as one can see in Figure 3(f-g).

![Figure 4. Instantaneous flow velocity as well as distribution of temperature for $T_s=0.9T_c$ and $T_w=0.92T_c$ at different times: (a) $t=5000$, (b) $t=10000$, (c) $t=13000$ and (d) $t=15000$.](image)

Corresponding to Figure 3, Figure 4 shows the instantaneous flow velocity as well as distribution of temperature. It is observed that one pair of counter-rotating circulations are generating above the center of the bottom wall due to the heating boundary, as shown in Figure 4(a) and (b). Furthermore, it’s found that the temperature is not the same everywhere inside the vapor bubble. The temperature is inhomogeneous, instead, which can be observed in Figure 4(d). It is also interesting to point out that two symmetric vortices are found inside the bubble, which is consistent with observation made by Gong and Cheng [5]. If there are two heated spots on the bottom wall, one can observe two vapor bubbles generating from the wall at the same time, which is illustrated in Figure 5 for. The parameters are set to be $T_s=0.9T_c$ and $T_w=0.92T_c$. As shown in Figure 5, the two bubbles are approaching to each other when ascending in the liquid. This may lead to bubble mergence, which is not observed in the present work because of limited computational domain. However, the effect of bubble mergence on the drag force of bubbles as well as the boiling heat transfer is remarkable, which will be our next future work.

![Figure 5. Instantaneous distribution of fluid density for $T_s=0.92T_c$ and $T_w=0.94T_c$ at different times: (a) $t=30000$, (b) $t=40000$, (c) $t=50000$ and (d) $t=60000$.](image)

**Conclusion**

In this work a two-phase lattice Boltzmann model based on a pseudo-potential scheme is adopted to simulate the liquid–vapor flows in this work. This lattice Boltzmann model is able to account for the liquid-vapor phase transition during the process of heat transfer. First of all, the result of liquid-vapor coexistence curve is compared with the theoretical result to validate the present code. Then the effect of saturated temperature $T_s$ is tested. It has been found that the liquid/vapor density ratio increases quickly as $T_s$ decreases. Instead, the interface thickness between the liquid and vapor decreases as $T_s$ decreases. Finally the simulations are carried out to illustrate the process of a vapor bubble growth and departure from a heated spot in pool boiling.
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References


