5th Multiphase Flow Journeys
May 17th-18th, 2019, Rio de Janeiro, RJ, Brazil

JEM-2019-0015
COMPARISON OF ENERGY MODELS BASED ON DISCRETE INTERFACE THEORY FOR MESOSCALE SIMULATION OF BOILING USING LATTICE BOLTZMANN METHOD

Matheus dos Santos Guzella
Universidade Federal dos Vales do Jequitinhonha e Mucurí – Rodovia MGT 367 nº 5000, Alto da Jacuba – Diamantina – MG, 39100-000, Brazil
matheusguzella@gmail.com

Luiz Eduardo Czelusniak
Escola de Engenharia de São Carlos – Universidade de São Paulo – Av. Trabalhador São-Carlense 400, Parque Arnold Schimidt, São Carlos - SP, 13566-590, Brazil
luizedu.cze@gmail.com

Vinícius Pessoa Mappeli
Escola de Engenharia de São Carlos – Universidade de São Paulo – Av. Trabalhador São-Carlense 400, Parque Arnold Schimidt, São Carlos - SP, 13566-590, Brazil
viniciusmapelli@gmail.com

Luben Cabezas-Gómez
Escola de Engenharia de São Carlos – Universidade de São Paulo – Av. Trabalhador São-Carlense 400, Parque Arnold Schimidt, São Carlos - SP, 13566-590, Brazil
lubencg@sc.usp.br

Abstract. *In this paper, mesoscopic simulations of boiling heat transfer are performed using a Hybrid Pseudopotential Lattice Boltzmann Method. In this model, the hydrodynamic equations are solved using the Pseudopotential Lattice Boltzmann Method (Shan-Chen Model) and the energy equation is solved by the 4th order Runge-Kutta Method. The collision operator is computed from the Bhatnagar-Gross-Krook model. Two-dimensional simulation results are presented first for the nucleation of a single bubble in the center of the heated surface. Results of a single bubble nucleation, growth and departure are presented for different energy equations considered in the literature. Results clearly show that some considerations performed during the derivation of these equations are questionable.*

Keywords: *Lattice Boltzmann Method, Boiling heat transfer, Pseudopotential*

1. INTRODUCTION

The LB method is a mesoscopic procedure based on the numerical solution of the Boltzmann transport equation. It can be seen as both a discrete special procedure for solving the Boltzmann equation and as a form of the Boltzmann equation in which the principles of microscopic kinetics are preserved in order to recover the hydrodynamic behavior on a macroscopic scale. The LB method is based on the concept simulate particles distribution in order to predict the macroscopic properties.

Boiling heat transfer is very important in many industrial applications. Among boiling heat transfer modes, nucleate boiling has been recognized as one of the most effective, been used in different cooling applications, such as nuclear reactors, computer chips and micro-electronic devices. From the phenomenon point of view, nucleate boiling is extremely complex, involving processes of nucleation, growth, departure and coalescence of vapor bubbles.

In this paper, an analysis and comparison of the energy models applied for the simulation of boiling heat transfer using LBM is presented. A hybrid pseudopotential Lattice Boltzmann Method with the BGK collision operator is used to simulate boiling heat transfer. The density and velocity fields are obtained from a distribution function and the temperature field is obtained from a traditional 4th order Runge-Kutta scheme. Results for the nucleation, growth and departure for a single bubble are presented for different energy equations. These results are confronted and some errors adopted in these energy equations are commented.

2. NUMERICAL MODEL

The Lattice Boltzmann Method is based on a mesoscopic approach for the simulation thermo-hydraulic problems. It is based on the collision of simulated particles and the evolution of a distribution function is used in order to obtain the macroscopic quantities. The discretized evolution equation for the density distribution function is given by Chen et al. (1992), considering the BGK operator:

$$f_i(\mathbf{x}+\mathbf{c}_i\Delta t, t+\Delta t) = f_i(\mathbf{x}+\mathbf{c}_i\Delta t, t+\Delta t) - \frac{1}{\tau}\left[f_i(\mathbf{x},t) - f^{eq}\right] + F_i \tag{1}$$

The local equilibrium distribution function is obtained from an expansion and discretization of the Maxwell-Boltzmann distribution function:

$$f^{eq} = w_i\rho\left[1+3(\mathbf{c}_i \bullet \mathbf{v}_i) - 1.5(\mathbf{v}_i \bullet \mathbf{v}_i) + 4.5(\mathbf{c}_i \bullet \mathbf{v}_i)^2\right] \tag{2}$$

The D2Q9 scheme is chosen for the two-dimensional numerical simulations. In this case, the lattice discrete velocities $\boldsymbol{c}_i$ and the weights w_i are given, respectively, by:

$$\mathbf{c}_i = \begin{cases} (0,0) \text{ for } i=1 \\ (\pm 1,0),(0,\pm 1) \text{ for } i=\{2...5\} \\ (\pm 1,\pm 1) \text{ for } i=\{6...9\} \end{cases} \tag{3}$$

$$w_i = \begin{cases} 4/9 \text{ for } i=1 \\ 1/9 \text{ for } i=\{2...5\} \\ 1/36 \text{ for } i=\{6...9\} \end{cases} \tag{4}$$

In Eq. (1), F_i is the term associated with the forces which arises in the simulation of a given problem with LBM. These forces will be presented in detailed below. The interparticle interaction force, which is responsible for phase separation, is given by Li et al. (2015):

$$\mathbf{F}_{\text{int}} = -\psi(\mathbf{x})\sum_i w_i^*\psi(\mathbf{x}+\mathbf{c}_i)\mathbf{c}_i \tag{5}$$

Where w_i^* are given by:

$$w_i^* = \begin{cases} 0 \text{ for } i=1 \\ 1/3 \text{ for } i=\{2,3\} \\ 1/12 \text{ for } i=\{4...9\} \end{cases} \tag{6}$$

The pseudopotential is obtained directly from the equation of state (EOS) used in the simulations:

$$\psi(\mathbf{x}) = \sqrt{\frac{2(p-\rho/3)}{|\mathbf{c}_i|G}} \tag{7}$$

The Peng-Robinson equation of state (P-R EOS) is applied to compute the pseudopotential and allow the separation of phases in this Lattice Boltzmann model:

$$p = \frac{\rho RT}{1-b\rho} - \frac{a\rho^2\left[1+\left(0.37464+1.54226\omega-0.26992\omega^2\right)\left(1-\sqrt{T/Tc}\right)\right]^2}{1+2b\rho-b^2\rho^2} \tag{8}$$

For the critical point, it can be shown that $a=0.45724R^2T_c^2/p_c$, $b=0.0778RT_c/p_c$. The parameter ω is the acentric factor is considered equal to 0.344, according to Li et al. (2015).
The gravity force is computed as:

$$\mathbf{F}_g = \mathbf{g}(\rho-\bar{\rho}) \tag{9}$$

Where $\boldsymbol{g}$ is the gravity acceleration and $\overline{\rho}$ is the average density. The forcing scheme developed by Li et al. (2015) is applied:

$$F_i = w_i\left(1-\frac{1}{2\tau}\right)\left\{\left[3\left(\mathbf{c}_i-\mathbf{v}_i+\frac{0.105\,\mathbf{F}_{\text{int}}}{(\tau-0.5)\psi^2}\right)+81\left(\mathbf{c}_i-\mathbf{v}_i+\frac{0.105\,\mathbf{F}_{\text{int}}}{(\tau-0.5)\psi^2}\right)\mathbf{c}_i\right]\mathbf{F}_{\text{int}}+\left[3(\mathbf{c}_i-\mathbf{v}_i)+81(\mathbf{c}_i-\mathbf{v}_i)\mathbf{c}_i\right]\mathbf{F}_g\right\} \quad (10)$$

From the density distribution function, the macroscopic density and velocity fields are obtained:

$$\rho=\sum_i f_i \quad (11)$$

$$\mathbf{u}_i=\frac{\sum_i \mathbf{c}_i f_i}{\rho}+\frac{(\mathbf{F}_{\text{int}}+\mathbf{F}_g)}{2\rho} \quad (12)$$

From Chapman-Enskog expansion, the relation between the mesoscopic scale and the macroscopic scale is expressed by the kinematic viscosity:

$$\nu=\frac{1}{3}(\tau-0.5) \quad (13)$$

From Anderson et al. (1998) the energy equation obtained from the discrete interface theory, considering the internal energy as the evolution variable, is given by:

$$\rho\left(\frac{\partial e}{\partial t}+\mathbf{v}\bullet\nabla e\right)=\nabla\bullet(k\nabla T)-p\nabla\bullet\mathbf{v} \quad (14)$$

In order to obtain a temperature-based energy equation, the following thermodynamic relation is considered:

$$de=c_v dT+\frac{1}{\rho^2}\left[p-T\left(\frac{\partial p}{\partial T}\right)_\rho\right]d\rho \quad (15)$$

Substituting Equation 15 in Equation 14, the energy equation considered by Li et al. (2015) is obtained:

$$\frac{\partial T}{\partial t}=-\mathbf{v}\bullet\nabla T+\frac{\nabla\bullet(k\nabla T)}{\rho c_v}-\frac{T}{\rho c_v}\left(\frac{\partial p}{\partial T}\right)_\rho\nabla\bullet\mathbf{v} \quad (16)$$

Other energy equations have been considered for the simulation of nucleate boiling using Lattice Boltzmann Method. Gong and Cheng (2012) used the following equation:

$$\frac{\partial T}{\partial t}=-\mathbf{v}\bullet\nabla T+\nabla\bullet(\alpha\nabla T)-\frac{T}{\rho c_v}\left(\frac{\partial p}{\partial T}\right)_\rho\nabla\bullet\mathbf{v} \quad (17)$$

From Equation 17, it can be seen that Gong and Cheng (2012) wrongly ignore the density variation across the interface, since the authors considered a different second term on the right hand side.
In another publication, Gong et al. (2018) considered the following energy equation:

$$\frac{\partial T}{\partial t}=-\mathbf{v}\bullet\nabla T+\frac{\nabla\bullet(k\nabla T)}{\rho c_v}-\frac{p\nabla\bullet\mathbf{v}}{\rho c_v} \quad (18)$$

A close analysis of Equation 18 reveals that the relation between the internal energy and temperature is linear ($de=c_v dT$). This means that the authors neglected the second term on the right hand side of the thermodynamic relation presented in Equation 15. A close analysis of this term, reveals that the authors considered as equation of state the ideal gas relation ($p=\rho RT$) for the energy equation while they considered the Peng-Robinson equation (Equation 8) of state to compute the pseudopotencial (Equation 7). This can be seen as an inconsistency of this energy equation.

3. RESULTS AND DISCUSSION

A 151x300 computational mesh is chosen for the simulations. As initial conditions, the domain is initialized as a liquid-vapor distribution at saturation temperature, with half of the domain occupied by the vapor phase and the other half occupied by the liquid phase as shown in Figure (1).

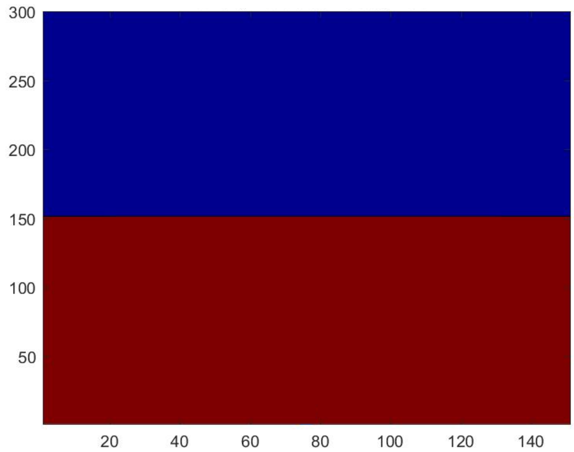

Figure 1. Schematic representation of the domain at $t=0$.

The initial distribution function (at $t=0$) is assumed to be the equilibrium distribution function. For the first 2000 timesteps, only the density and velocity fields are solved in order to improve the numerical instability. Then the energy model is solved coupled with the hydrodynamic model. Then, the gravity force is included after 100 timesteps. These numerical approaches were also considered by Gong and Cheng (2012) and Li et al. (2015).

As hydrodynamic boundary conditions for the simulations, a no-slip condition is applied into the bottom and upper surfaces using Zou and He (1997) scheme. For the lateral boundaries, periodic conditions are applied. The heat surface is the center node and its immediate neighbor nodes of the bottom surface and with constant temperature of $T_b=1.50T_c$. The other nodes of the bottom surface are assumed to be at saturation temperature ($T_{sat}=0.86T_c$). The upper surface is assumed to be at saturation temperature. Using Maxwell construction, the equilibrium liquid and vapor densities for the Peng-Robinson EOS are obtained as $\rho_v=0.38$ and $\rho_l=6.5$. The parameters for the P-R EOS (Equation 8) are given by: $a=3/49$, $b=2/21$ and $R=1$. Considering these values, the critical temperature is obtained: $T_c=0.109383$. Gravity acceleration is set to 2.5×10^{-5}. The liquid kinematic viscosity is 0.1 and this value is considered to compute the relaxation time (Equation 13). Hence, a constant relaxation time is considered for the simulations. The specific heat at constant volume is taken as 5. It should be pointed that all parameters are presented in lattice units.

Figure (2) presents results of boiling simulations considering the energy models previously presented. These results reveal the influence of the energy equation into the simulation of the nucleation of a bubble in a heated surface. Clearly, Gong and Cheng (2012) does not capture the correct physics regarding the nucleation, growth and departure in a nucleation site. The energy equation considered by Gong et al. (2018) gave similar results when compared with the presented model although the considerations to obtain the energy equation considered by the authors may be questionable.

An analysis considering a variable relaxation time is performed. Following Li et al. (2015), the vapor kinematic viscosity is 0.5/3. In order to take into account a variable kinematic viscosity, Gong and Cheng (2017) considered the following relation:

$$\nu = \nu_l \frac{\rho - \rho_v}{\rho_l - \rho_v} + \nu_v \frac{\rho_l - \rho}{\rho_l - \rho_v} \tag{19}$$

From Equation 19, a smooth transition for the kinematic viscosity is obtained through the interface. From Equations 13 and 19, a variable relaxation time is obtained. In Figure (3) results are presented considering the same parameters used before. The results revealed that, when a variable relaxation time is considered, the bubble cycle is smaller. It should be noticed that, by using Equation (19), the relaxation time changes only near the interface. The results confirmed that the presented model, which is coherent with the discrete interface theory, could capture all the effects associated with bubble nucleation, growth and departure from the heated surface. Is interesting to note that, the energy model used by Gong et al. (2018) presented similar results when compared with the presented model.

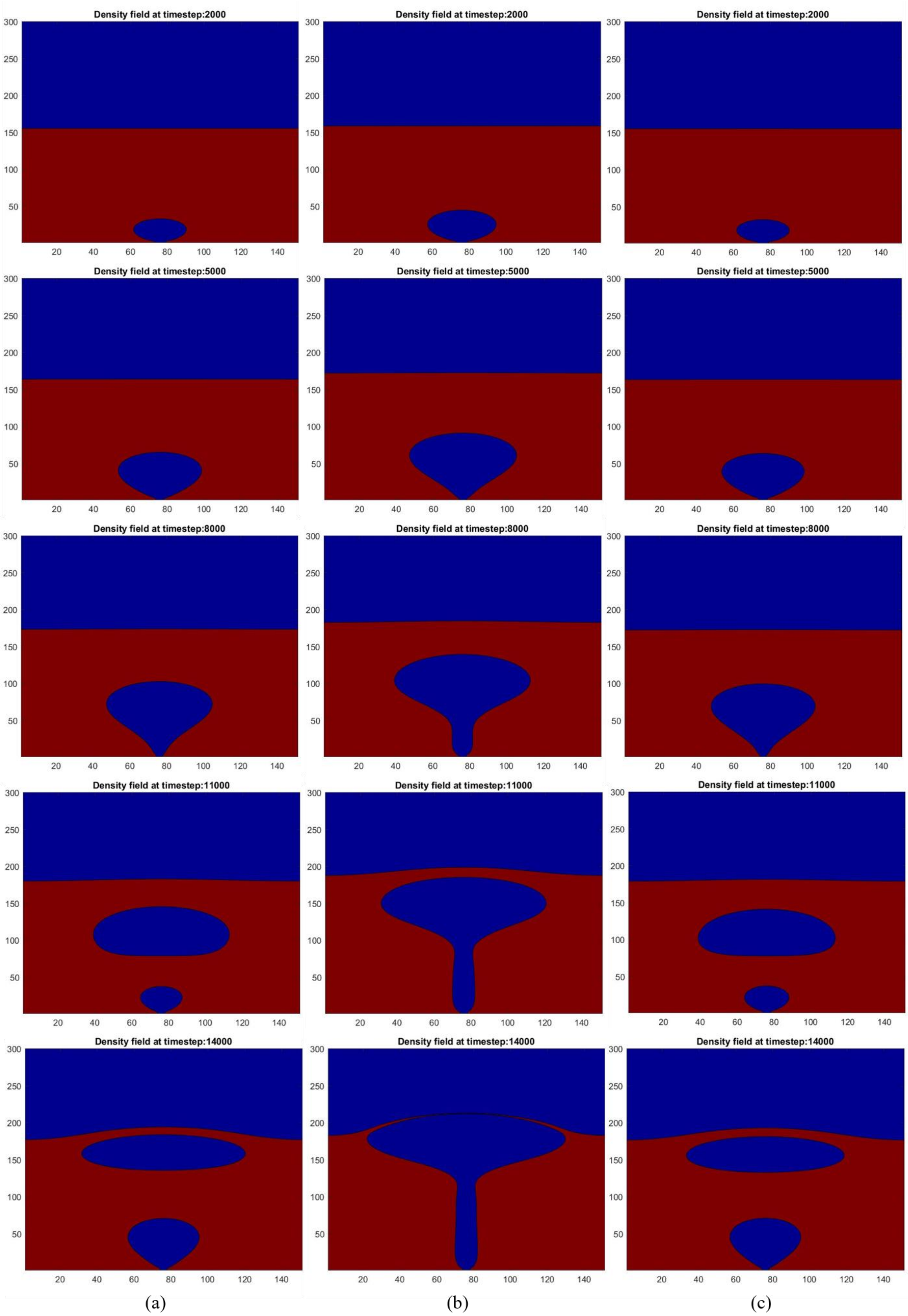

Figure 2. Nucleation of a single bubble at different timesteps: 2000, 5000, 8000, 11000 and 14000 (respectively) for different energy equations, namely (a): Presented model; (b): Gong and Cheng (2012); (c) Gong et al. (2018).

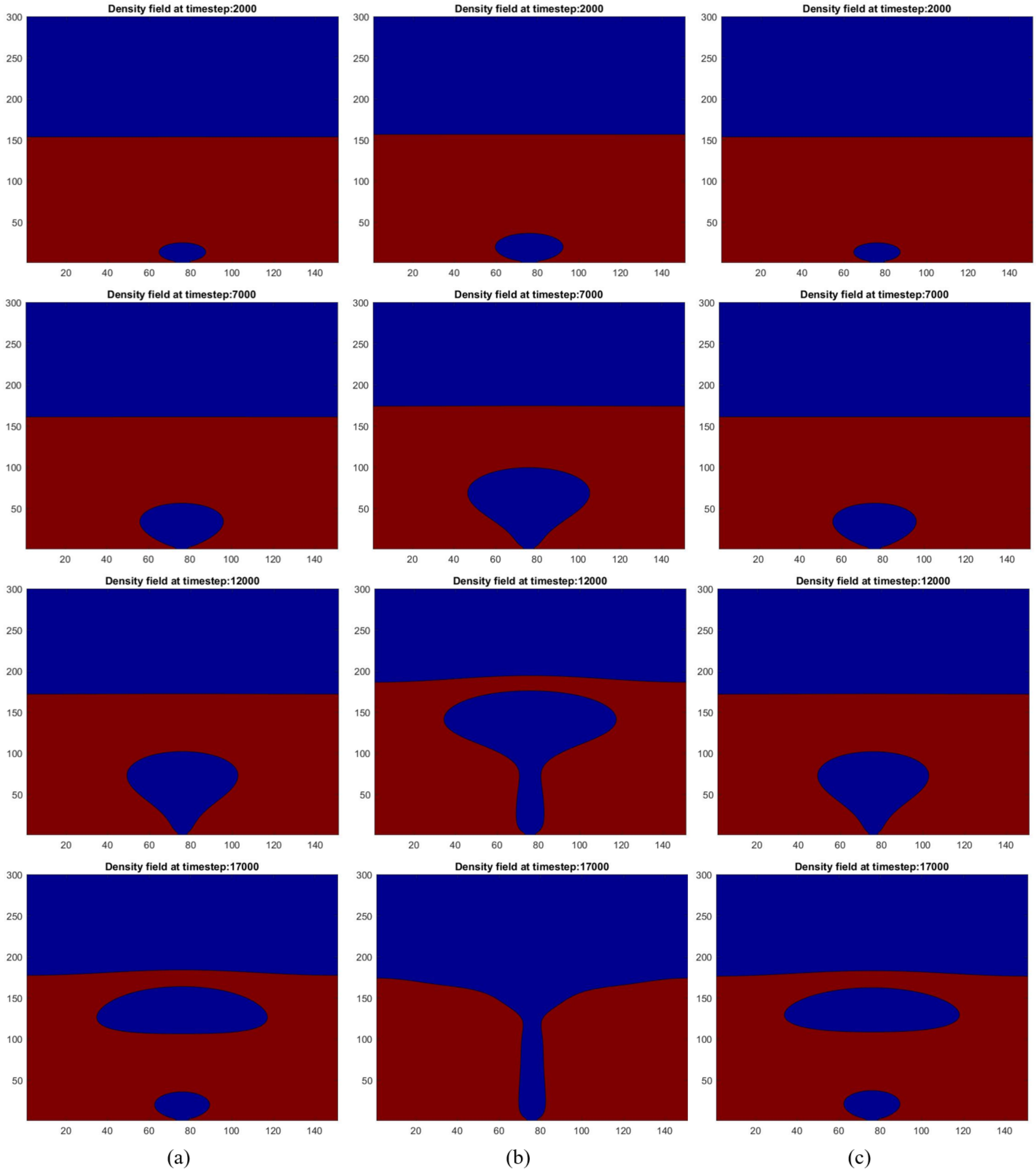

Figure 3. Nucleation of a single bubble at different timesteps: 2000, 7000, 12000 and 17000 (respectively) for different energy equations, namely (a): Presented model; (b): Gong and Cheng (2012); (c) Gong et al. (2018).

4. CONCLUSION

In this paper, a hybrid pseudopotential Lattice Boltzmann Method with the BGK collision operator was used to simulate boiling heat transfer. Different energy models were considered and their features were carefully presented and discussed. A correct energy model is obtained and commented. Results for the nucleation, growth and departure for a single bubble were presented for different energy equations. The inconsistency of some energy models used in the literature were established and confirmed with the numerical results.

5. REFERENCES

Chen, H., Chen, S., Matthaeus, W.H., 1992. "*Recovery of the Navier–Stokes equations using a lattice-gas Boltzmann method*". *Physical Review E*, Vol. 45, pp. 1 – 4.

Gong, S. and Cheng, P., 2012. "A lattice Boltzmann method for simulation of liquid–vapor phase-change heat transfer". *International Journal of Heat and Mass Transfer*, Vol. 55, pp. 4923–4927.

Gong, S. and Cheng, P., 2017. " Direct numerical simulations of pool boiling curves including heater's thermal responses and the effect of vapor phase's thermal conductivity". *International Journal of Heat and Mass Transfer*, Vol. 87, pp. 61–71.

Gong, W., Yan, Y.Y., Chen, S., Wright, E. “A modified phase change pseudopotential lattice Boltzmann model”. *International Journal of Heat and Mass Transfer*, Vol. 125, pp. 323–329.

Li, Q., Kang, Q.J., Francois, M.M., He, Y.L., Luo, K.H., 2015. "Lattice Boltzmann modeling of boiling heat transfer: The boiling curve and the effects of wettability". *International Journal of Heat and Mass Transfer*, Vol. 85, pp. 787–796

Zou, Q. and He, X., 1997. “On pressure and velocity boundary conditions for the lattice Boltzmann BGK model”. *Physics of Fluids*, Vol. 9, pp. 1591–1598.

6. RESPONSIBILITY NOTICE

The authors are the only responsible for the printed material included in this paper.