



Lattice Boltzmann simulation of condensation in the presence of noncondensable gas



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ABSTRACT

In this paper we use the multiphase multispecies Lattice Boltzmann method to investigate the influence of non-condensable gas on condensation. Condensation on a horizontal cold wall as well as that on a vertical wall with droplet movement is investigated. The presence of non-condensable gas obviously reduces the condensation mass rate as well as the heat flux compared to condensation from pure vapor. The waiting time before nucleation is increased with non-condensable gas, and the wetting characteristics are also changed (the contact angles are increased), which further influences the heat transfer. Correlations of the relationship between droplet diameter and condensing time for different surface wettability, or contact angles, as well as different air mass fraction are obtained. As for condensation on a surface parallel to the gravitational force, it's demonstrated that the presence of non-condensable gas reduces the droplet departure diameter and increases the period between subsequent droplet formation and departure.

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1. Introduction

Condensation is a process commonly used in several applications such as waste heat boiler and heat exchanger due to its great performance in transferring heat through phase change. In all applications, the phase change is not that of a pure substance because of the presence of noncondensable gases such as air mixing with the condensing vapor. Under certain circumstances where the vapor is the only condensable phase, the presence of noncondensable gases plays a negative effect on heat transfer, and seriously reduce its efficiency. Overall, vapor condensation is a complex process because it involves phase change, multiphase flow and multiple components or species.

Several studies have been designed to explore boiling through numerical simulations. Direct numerical simulation based on two-film theory is one of the most widely used method to deal with condensation in the presence of noncondensable gases [1–10]. The condensing liquid and the noncondensable gas are assumed as two layers of fluid, the vapor diffuses across the noncondensable gas layer and then condenses at the interface. This method can only deal with film condensation, and cannot deal

with complex vapor-liquid flow. Another common set of approaches is based on front tracking methods for interfaces such as the volume of fluid (VOF), level-set and phase change methods [11–17]. The phase change is often parameterized with experimental correlations, while in some other cases it is solved by an energy and mass balance equation directly at the interface through source terms for the phase change [18–23]. In these methods, a bubble (or droplet) and an interface have to be set there initially because the nucleation process during condensation cannot be simulated.

In the present study, we take a different approach as we aim to solve for the nucleation and flow process together in a self-consistent way. The model we use is based on the Lattice Boltzmann method (LBM), which is a mesoscopic solver that can simulate two-phase flows with complex time evolving interfaces (deformation, coalescence, breakup, etc.). Among all the LBM multiphase methods, the pseudo-potential model (Shan-Chen model) can be easily used to calculate multiphase and multispecies problem. The pseudo-potential approach is convenient in that it is a diffuse interface approach, which implies that there is no need to track the interface between the different phases. A significant advantage of the model is that we can apply a real gas equation of state and add a phase change source term into the energy equation which simultaneously allows us to model the nucleation process. These characteristics motivated our choice for the Shan-Chen (SC) model with a double distribution

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function to deal with this multiphase (gas-liquid) multispecies (air, water vapor) phase change problem.

In the SC model, a pseudo-potential function is used to represent molecular interactions. Fluids can spontaneously separate into two phases or two species with two different densities under these interactions (spinodal decomposition). The phase interface is characterized by the variation of the fluid density for each phase [24–30]. Hazi and Markus [31] used the SC model to investigate boiling, where the source term for the phase is derived directly from the entropy balance equation based on an equation of state for real gases. Building from Hazi’s method, Cheng et al. [32,33] improved on the pseudo-potential function as well as the source term to calculate both boiling and condensation. Li et al. [34] also used the pseudo-potential model to simulate two phase flow during pool boiling, which allowed them to reproduce the boiling curve and the influence of surface wettability on boiling accurately. They, however, solved the temperature field with a traditional finite-difference scheme.

All the above literatures focus on single component model with phase change (water-vapor). Zhang et al. [35] used the multiphase multicomponent SC model to study the condensation of humid air on a rough surface, however it is assumed that condensation is isothermal and that the phase changes does not affect the temperature distribution. Chen et al. [36] recently developed a multicomponent multiphase reactive transport processes with SC model for phase change. However, in their model, the phase change between vapor and liquid is not compatible with the real gas equation of state, they rather propose a special treatment of nodes undergoing phase change, which complicates the algorithm significantly.

In summary, it remains rather challenging to simulate the multiphase multispecies phase change problem self-consistently. In the present study, we propose a model to circumvent this challenge. We use the LB method to simulate the condensation with noncondensable gas, which deals with multiphase, multispecies and phase change all together. The model allows us to study the effect of non-condensable gas (impurities) on condensation and heat transfer. Its effect on surface wettability is also investigated.

2. Model description

2.1. Multiphase multicomponent pseudo-potential LBM model

In the case of two components where only one component goes through phase change, a two-component multiphase LBM is required. The multicomponent multiphase SC model treats each component with a corresponding distribution function. Based on the assumption of a single relaxation time commonly referred to as the Bhatnagar–Gross–Krook (BGK) model, the evolution equation for each component is given by:

$$f_i^\sigma(\vec{x} + \vec{e}_i^\sigma \delta t, t + \delta t) - f_i^\sigma(\vec{x}, t) = -\frac{1}{\tau_\sigma} (f_i^\sigma(\vec{x}, t) - f_i^{\text{eq},\sigma}(\vec{x}, t)) \quad (1)$$

where f_i^σ is the density distribution function of the component σ at position \vec{x} and time t , τ is the relaxation time. \vec{e}_i is the discrete velocity along the i th lattice direction, and f_i^{eq} is the equilibrium distribution. For the D2Q9 scheme,

$$\vec{e}_i = \begin{cases} 0, & i = 0 \\ (\cos[(i-1)\pi/2], \sin[(i-1)\pi/2]), & i = 1, 2, 3, 4 \\ \sqrt{2}(\cos[(i-5)\pi/2 + \pi/4], \sin[(i-5)\pi/2 + \pi/4]), & i = 5, 6, 7, 8 \end{cases} \quad (2)$$

and

$$f_i^{\text{eq}}(\vec{x}, t) = \omega_i \rho \left[1 + \frac{\vec{e}_i \cdot \vec{u}}{c_s^2} + \frac{(\vec{e}_i \cdot \vec{u})^2}{2c_s^4} - \frac{\vec{u}^2}{2c_s^2} \right] \quad (3)$$

where ω_i are the weight factors and are given by $\omega_0 = 4/9$, $\omega_{1-4} = 1/9$ and $\omega_{5-8} = 1/36$. The lattice sound speed c_s is defined as $c_s^2 = c^2/3$, and $c = \delta x/\delta t$ with δx and δt the lattice spacing and time spacing respectively (set to 1). The fluid density ρ and fluid velocity \vec{u} are obtained from the statistical moments of the distributions

$$\rho^\sigma = \sum_i f_i^\sigma \quad (4)$$

$$\rho^\sigma \vec{u}^\sigma = \sum_i \vec{e}_i f_i^\sigma \quad (5)$$

Finally, the kinematic viscosity is given by $\nu^\sigma = c_s^2(\tau^\sigma - 0.5)\delta t$.

For a multicomponent system, there exists both intra- and inter-molecular interaction forces. The interaction potential ψ^σ is introduced in the SC model to include the interaction forces between particles. The intra-molecular interaction is generally defined as

$$\vec{F}_f^{\sigma\sigma}(\vec{x}) = -G^{\sigma\sigma} \psi^\sigma(\vec{x}) \sum_i \omega(\vec{e}_i^\sigma) \psi^\sigma(\vec{x} + \vec{e}_i) \vec{e}_i \quad (6)$$

where $\psi^\sigma(\vec{x})$ is the pseudo-potential function, G is a coefficient that sets the strength of the interaction and $\omega(\vec{e}_i^\sigma)$ are weighting factors. The latter are set to $\omega(\vec{e}_i^\sigma) = 1/3$ for the four nearest neighbors and $1/12$ for the neighbors along the diagonal [37].

The interaction force between two components is shown as:

$$\vec{F}_f^{\sigma\bar{\sigma}}(\vec{x}) = -G^{\sigma\bar{\sigma}} \varphi^\sigma(\vec{x}) \sum_i \omega(\vec{e}_i^\sigma) \varphi^{\bar{\sigma}}(\vec{x} + \vec{e}_i) \vec{e}_i \quad (7)$$

where φ^σ and $\varphi^{\bar{\sigma}}$ are different from ψ^σ and $\psi^{\bar{\sigma}}$ [36]. For two components system φ^1 and φ^2 are designed to enforce the proper distribution of the two components at equilibrium. It was shown that $\varphi^1(\rho_2) = 1 - \exp(-\rho_2/\rho_{20})$ and $\varphi^2(\rho_1) = a_0 - \exp(-\rho_1/\rho_{10})$, providing a suitable set of functions [36]. The value of $G^{\sigma\bar{\sigma}}$, a_0 , ρ_{10} and ρ_{20} are critical for the multicomponent multiphase system and also control the magnitude of the mutual diffusivity in the gas phase. After many test simulations, we set $G^{12} = G^{21} = 0.00001$, $a_0 = 0.9$, $\rho_{10} = 6$ and $\rho_{20} = 6$ which provide a set of parameters that recovers Laplace law accurately [36–39].

The interaction force between solid and fluid, which controls wetting, is given by:

$$\vec{F}_s^{\sigma}(\vec{x}) = -g_s^\sigma \psi^\sigma(\vec{x}) \sum_i \omega(\vec{e}_i^\sigma) \psi(\rho_w) s(\vec{x} + \vec{e}_i) \vec{e}_i \quad (8)$$

where g_s^σ is a coefficient that sets the strength of the fluid–solid interaction for component σ , $s(\vec{x} + \vec{e}_i)$ is the indicator function flagging the solid when its value is 1 and fluid when equals to 0.

In this paper, component 1 and 2 refer to the condensable and noncondensable gas, respectively. The noncondensable gas component is considered an ideal fluid, which requires G^{22} to be zero. The condensable component is treated as non-ideal fluid following the P-R EOS [34,40]:

$$p_{\text{EOS}} = \frac{\rho R t}{1 - b\rho} - \frac{a\alpha(T)\rho^2}{1 + 2b\rho - b^2\rho^2} \quad (9)$$

where

$$\alpha(T) = \left[1 + (0.37464 + 1.54226\omega - 0.26992\omega^2) \times (1 - \sqrt{T/T_c}) \right]^2, \\ a = 3.0/49.0, b = 2.0/21.0 \text{ and } R = 1.0. \text{ The effective mass of condensable component is then } \psi^1(\vec{x}) = \sqrt{2(p_{\text{EOS}} - \rho c_s^2)/g_c^2} \text{ [40].}$$

The velocity shift force scheme [24] is used here by replacing velocity in Eq. (5) with:

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