



Liquid temperature dependence of kinetic boundary condition at vapor–liquid interface



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ARTICLE INFO

Article history:

Received 8 July 2015

Received in revised form 5 March 2016

Accepted 21 March 2016

Available online 16 April 2016

Keywords:

Kinetic boundary condition

Evaporation and condensation

Vapor–liquid interface

Kinetic theory of gases

ABSTRACT

For the accurate description of heat and mass transfer through a vapor–liquid interface, the appropriate modeling of the interface during nonequilibrium phase change (net evaporation/condensation) is a crucial issue. The aim of this study is to propose a microscopic interfacial model which should be imposed at the interface as the kinetic boundary condition for the Boltzmann equation. In this study, we constructed the kinetic boundary condition for monoatomic molecules over a wide range of liquid temperature based on mean field kinetic theory, and we validated the accuracy of the constructed kinetic boundary condition by solving the boundary value problem of the Boltzmann equation. These results showed that we can impose the kinetic boundary condition at the interface by simply specifying liquid temperature and simulate the complex vapor–liquid two-phase flow induced by net evaporation/condensation. Furthermore, we applied the constructed kinetic boundary condition to the boundary condition for the fluid-dynamic-type equations. This application enables us to deal with a large spatio-temporal scale of the interfacial dynamics in the vapor–liquid two-phase system with net evaporation/condensation.

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1. Introduction

Heat and mass transfer through a vapor–liquid interface induced by nonequilibrium phase change (net evaporation/condensation) plays an important role in dynamics of the vapor–liquid two-phase flows, such as Leidenfrost effect [1–3] and cavitation bubble collapse [4–6]. In recent years, furthermore, with the progression of micro/nanofluidic devices, the precise investigation of transport phenomena during net evaporation/condensation has been required [7].

Since net evaporation/condensation originates from the motion of molecules in the vicinity of the interface, the vapor in contact with the interface is in nonequilibrium in which the conventional continuum description is not appropriate, and the analysis of the Boltzmann equation based on kinetic theory of gases (molecular gas dynamics) is essential [8]. The Boltzmann equation governs the spatio-temporal development of the molecular velocity distribution function, $f(\mathbf{x}, \boldsymbol{\xi}, t)$, defined as $dN = (1/m)f(\mathbf{x}, \boldsymbol{\xi}, t)d\mathbf{x}d\boldsymbol{\xi}$, where $\mathbf{x} = (x, y, z)$ is position, $\boldsymbol{\xi} = (\xi_x, \xi_y, \xi_z)$ is molecular velocity, $d\mathbf{x}d\boldsymbol{\xi} = dx dy dz d\xi_x d\xi_y d\xi_z$ is an infinitesimal volume element in the six-dimensional phase space, dN is the number of molecules

in $d\mathbf{x}d\boldsymbol{\xi}$, and m is the mass of a molecule. Once the velocity distribution function f is obtained as the solution of the Boltzmann equation, the macroscopic variables, such as density, velocity, and temperature, are obtained from its moments

$$\rho = \int_{-\infty}^{\infty} f d\boldsymbol{\xi}, \quad v_i = \frac{1}{\rho} \int_{-\infty}^{\infty} \xi_i f d\boldsymbol{\xi}, \quad T = \frac{1}{3\rho R} \int_{-\infty}^{\infty} (\xi_i - v_i)^2 f d\boldsymbol{\xi}, \quad (1)$$

where ρ is density, $v_i = (v_x, v_y, v_z)$ is velocity, T is temperature, R is the gas constant and $\int_{-\infty}^{\infty} d\boldsymbol{\xi} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\xi_x d\xi_y d\xi_z$.

In this analysis, we have to specify a molecular velocity distribution function composed of molecules outgoing from the liquid into the vapor phase, f_{out} , which should be imposed at the interface as the kinetic boundary condition (KBC) for the Boltzmann equation. Since it has been found that the KBC significantly affects the macroscopic variables obtained from Eq. (1)[8,9] during net evaporation and condensation, the proper specification of the KBC at the interface is critical. One of the most conventional forms of the KBC is shown as follows:

$$f_{\text{out}} = [\alpha_e \rho^*(T_L) + (1 - \alpha_c) \sigma] \hat{f}, \quad \xi_z > 0, \quad (2)$$

where ρ^* is the saturated vapor density, α_e and α_c are evaporation and condensation coefficients, respectively, ξ_z is the molecular velocity in the direction normal to the interface, $\xi_z > 0$ denotes the direction of molecular velocity outgoing from the liquid into the vapor phase, and \hat{f} is a normalized molecular velocity

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distribution function; the normalized Maxwellian distribution at liquid temperature, T_L ,

$$\hat{f} = \frac{1}{(\sqrt{2\pi RT_L})^3} \exp\left(-\frac{\xi_i^2}{2RT_L}\right) \quad (3)$$

is assumed conventionally. σ is related to a molecular velocity distribution function composed of molecules colliding onto the liquid from the vapor phase ($\xi_z < 0$), f_{coll} . Its definition is

$$\sigma \sqrt{\frac{RT_L}{2\pi}} = - \int_{\xi_z < 0} \xi_z f_{\text{coll}} d\xi = J_{\text{coll}}, \quad (4)$$

where J_{coll} is the molecular mass flux colliding onto the liquid from the vapor phase and $\int_{\xi_z < 0} d\xi = \int_{-\infty}^0 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\xi_x d\xi_y d\xi_z$. f_{coll} at each time is obtained by solving the initial boundary value problem of the Boltzmann equation [8]; σ has a unit of density and is equal to ρ^* in the vapor–liquid equilibrium.

One of the most important issues in the construction of the KBC during net evaporation/condensation lies in the determination of the evaporation coefficient α_e and the condensation coefficient α_c . As for the definitions of α_e and α_c , some different models were proposed [10–14]. We adopt the following definitions of α_e and α_c as a widely-used model [12,15–20].

$$\alpha_e = \frac{J_{\text{evap}}}{J_{\text{out}}}, \quad \alpha_c = \frac{J_{\text{cond}}}{J_{\text{coll}}}, \quad (5)$$

where J_{evap} is evaporation molecular mass flux, J_{cond} is condensation molecular mass flux, and J_{out} is molecular mass flux outgoing from the liquid into the vapor phase; star (*) superscripts denote quantities at the vapor–liquid equilibrium and $J_{\text{out}}^* = J_{\text{coll}}^* = \rho^* \sqrt{(RT_L/2\pi)}$. The relations of each molecular mass flux are as follows:

$$J_{\text{out}} = J_{\text{evap}} + J_{\text{ref}}, \quad J_{\text{coll}} = J_{\text{cond}} + J_{\text{ref}}, \quad (6)$$

where J_{ref} is molecular mass flux reflecting to the vapor phase (reflection molecular mass flux). The next task is to distinguish between J_{evap} and J_{ref} to estimate these molecular mass fluxes and then to determine α_e and α_c .

In the vapor–liquid equilibrium, α_e is equal to α_c from the definition of Eq. (5), and that is confirmed based on molecular dynamics [12,17,18]. On the other hand, during net evaporation/condensation, several studies to determine α_e and α_c based on molecular dynamics have been proposed to date [15,16,19,20]. For instance, Ishiyama et al. [19,20] proposed a concept of *spontaneous evaporation* to avoid the ambiguities of assigning J_{evap} and J_{ref} . They showed that α_e and α_c for monoatomic (argon) molecules take almost the same value during net evaporation/condensation. Meland et al. [15] distinguished these molecular mass fluxes by using *interphase boundary* and pointed out that α_e and α_c for monoatomic (argon) molecules vary with the increase in the Mach number of vapor far from the interface. Kryukov et al. [16] also found the increase in α_c by accounting for monoatomic (argon and helium) molecules.

Neither α_e nor α_c has been indisputably determined after all, even though each of different coefficients had been derived from the same definition (Eq. (5)) with the use of simple monoatomic molecules. In other words, the distinction between J_{evap} and J_{ref} has still remained ambiguity. Furthermore, these studies [15,16,19,20] investigated only a few cases of liquid temperature. It would be advantageous that the molecular dynamics simulations can deal with practical monoatomic and polyatomic molecules; however, it is extremely hard to conduct a systematic investigation of the KBC in consideration of the liquid temperature dependence because of its high computational cost.

In contrast to these studies, the authors [21] have proposed a novel method of determining the KBC for the monoatomic

(hard-sphere) molecules based on mean field kinetic theory [22,23]. This method can construct the KBC without distinguishing each molecular mass flux. The constructed KBC can describe accurate macroscopic variables, such as vapor density, velocity, and temperature, in the case of liquid temperature near the triple point. Furthermore, incorporating mean field kinetic theory, we can succeed to reduce the computational cost compared with the molecular dynamics simulations. However, any dependence of the KBC constructed by this method with liquid temperature has yet to be explored.

In this study, we conduct a systematic investigation of the KBC during net evaporation/condensation by considering the liquid temperature dependence. First, we construct the KBC during net evaporation/condensation by using this method over a wide range of liquid temperatures (Section 3.2). Then, we validate the accuracy of the constructed KBC by solving the boundary value problem of the Boltzmann equation (Section 3.3). Finally, we comment on the application of the constructed KBC to the boundary condition for the fluid-dynamic-type equations (Section 3.4).

2. Method

2.1. Numerical simulation of the Enskog–Vlasov equation

In this study, we utilize a DSMC-based numerical scheme employing the Enskog–Vlasov equation to construct the KBC. This numerical scheme provides the reasonable description of the vapor–liquid two-phase flow.

The Enskog–Vlasov equation [22,23] is a kinetic equation based on mean field kinetic theory, which describes the hard-sphere fluid interaction by Sutherland potential, $\phi(r)$, defined as

$$\phi(r) = \begin{cases} +\infty & (r < a) \\ -\phi_a \left(\frac{r}{a}\right)^{-\gamma} & (r \geq a), \end{cases} \quad (7)$$

where r is intermolecular distance, a is a molecular diameter, ϕ_a and γ are constants; γ is set as six to follow the attractive tail of the 12–6 Lennard–Jones intermolecular potential. In terms of a one-particle velocity distribution function, the Enskog–Vlasov equation is expressed as

$$\frac{\partial f}{\partial t} + \xi_i \frac{\partial f}{\partial x_i} + \frac{F_i(x_i, t)}{m} \frac{\partial f}{\partial \xi_i} = C_E, \quad (8)$$

$$C_E = a^2 \int \left\{ Y \left[n \left(x_i + \frac{a}{2} K_i, t \right) \right] f(x_i + aK_i, \xi'_{1i}, t) f(x_i, \xi'_i, t) \right. \\ \left. - Y \left[n \left(x_i - \frac{a}{2} K_i, t \right) \right] \times f(x_i - aK_i, \xi_{1i}, t) f(x_i, \xi_i, t) \right\} \\ \times H(\xi_{ri} K_i) (\xi_{ri} K_i) d\xi_1 d^2 \mathbf{K},$$

where t is time, x_i is position (x , y , and z), Y is a pair correlation function, n is number density, K_i is the unit vector defined as $K_i = (x_{1i} - x_i) / (\|x_{1i} - x_i\|)$, H is the Heaviside function, ξ_i and ξ_{1i} denote the molecular velocity of two colliding molecules; prime (') superscripts denote quantities of post-collisional molecules, ξ_{ri} denotes the relative velocity $\xi_{ri} = \xi_i - \xi_{1i}$, and F_i is a self-consistent force field determined from Eq. (7) [24]

$$F_i(x_i, t) = \int_{\|x_{1i} - x_i\| > a} \frac{d\phi}{dr} \frac{x_{1i} - x_i}{\|x_{1i} - x_i\|} n(x_{1i}, t) dx_{1i}, \quad (9)$$

where x_i and x_{1i} denote the molecular position of two colliding molecules.

As for the equation of state for hard-sphere molecules, we utilized Carnahan and Stirling approximation [25]. According to this equation of state, the critical temperature of hard-sphere molecules is given as follows [24]:

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