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# Mean-Field Kinetic Theory Based Study of Boundary Condition at Vapor–Liquid Interface

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*The target of this thesis is heat and mass transfer in vapor–liquid two-phase systems composed of vapor and its condensed phase. Not only can this transport phenomena be widely observed in the natural world, but these are also applied to engineering. Hence, this transport phenomenon in the vapor–liquid two-phase system has been investigated from various theoretical frameworks, such as fluid dynamics, thermodynamics, and physical chemistry. In this thesis, we especially examine heat and mass transfer associated with a mass flux in the normal direction passing through the vapor–liquid interface. The mass flux at the vapor–liquid interface arises due to the molecular motions near the vapor–liquid interface. In general, the influence of the microscopic phenomenon is confined to a sufficiently small region, and it does not affect the macroscopic phenomenon. On the other hand, it is known that the mass flux in the normal direction passing through the vapor–interface affects the vapor flow beyond the region in the vicinity of the interface. Naturally, such a mass flux should be predicted based on the microscopic theory. However, simplified models that ignore the microscopic phenomenon near the vapor–liquid interface are widely used as the boundary condition in the macroscopic theory, namely, fluid dynamics. The objective of this thesis is to propose a proper boundary condition at the vapor–liquid interface from the microscopic theories, namely, the mean-field kinetic theory and molecular gas dynamics. To achieve this objective, we investigate the boundary condition in molecular gas dynamics by utilizing the molecular simulation based on the mean-field kinetic theory. This investigation is the main content of this thesis. With the use of this boundary condition obtained by the molecular simulation, we can derive the boundary condition in fluid dynamics by the molecular gas dynamics analysis.*

## 1 Introduction

### 1.1 Importance of mass flux at vapor–liquid interface

In this section, we detail our target, which is heat and mass transfer in vapor–liquid two-phase systems composed of single-component vapor and its condensed phase. Fundamentally, liquid and vapor are composed of molecules and are essentially discrete.

However, when the molecular collisions sufficiently take place in the domain under consideration, liquid and vapor can be assumed as the continuum mediums in which liquid and vapor are in local or global equilibrium. This assumption is the basis of continuum mechanics, namely, fluid dynamics. On the other hand, the presence of the interface between liquid and vapor often interrupts the application of continuum mechanics because the macroscopic variables change drastically. Thus, we have to impose the rule regarding the mass, momentum, and energy passing through the vapor–liquid interface.

A fundamental rule is the conservation law of fluxes. The conservation laws of the mass flux $\mathcal{M}$, the momentum flux $\mathcal{P}_i$, and the energy flux $\mathcal{E}$ are described as follows:

$$\mathcal{M} \equiv \rho_{\mathrm{L}}(v_{\mathrm{L}j} - v_{\mathrm{w}j})n_j = \rho_{\mathrm{V}}(v_{\mathrm{V}j} - v_{\mathrm{w}j})n_j, \tag{1}$$

$$\mathcal{P}_i \equiv [\rho_{\mathrm{L}} v_{\mathrm{L}i}(v_{\mathrm{L}j} - v_{\mathrm{w}j}) + p_{\mathrm{L}ij}]n_j = [\rho_{\mathrm{V}} v_{\mathrm{V}i}(v_{\mathrm{V}j} - v_{\mathrm{w}j}) + p_{\mathrm{V}ij}]n_j, \tag{2}$$

$$\begin{aligned}\mathcal{E} &\equiv [\rho_{\mathrm{L}}(e_{\mathrm{L}} + \frac{1}{2}v_{\mathrm{L}i}^2)(v_{\mathrm{L}j} - v_{\mathrm{w}j}) + p_{\mathrm{L}ij}v_{\mathrm{L}i} + q_{\mathrm{L}j}]n_j \\ &= [\rho_{\mathrm{V}}(e_{\mathrm{V}} + \frac{1}{2}v_{\mathrm{V}i}^2)(v_{\mathrm{V}j} - v_{\mathrm{w}j}) + p_{\mathrm{V}ij}v_{\mathrm{V}i} + q_{\mathrm{V}j}]n_j,\end{aligned} \tag{3}$$

where the subscripts L and V represent the variables in liquid and vapor, respectively, $n_i$ is the unit vector in the direction normal to the vapor–liquid interface pointing toward vapor, $\rho$ is the density, $v_i$ is the flow velocity vector, $v_{\mathrm{w}i}$ is the velocity vector of the motion of the interface (advection and deformation), $p_{ij}$ is the stress tensor, $e$ is the internal energy, and $q_i$ is the heat flux vector.

When $\mathcal{M} = 0$, given the condition as to whether $v_{\mathrm{L}i}$ and $v_{\mathrm{V}i}$ follow $v_{\mathrm{w}i}$ (the slip or non-slip boundary condition), we can readily obtain the expressions of the stress tensor and the heat flux vector in the direction normal to the vapor–liquid interface. In contrast, when $\mathcal{M} \neq 0$, we have to specify a certain $\mathcal{M}$ to obtain these expressions because the terms related to $\mathcal{M}$ are included in $\mathcal{P}_i$ and $\mathcal{E}$. Therefore, a proper specification of the mass flux at the vapor–liquid interface is necessary to predict heat and mass transfer in the vapor–liquid two-phase system.

In this thesis, we mainly discuss the case of $\mathcal{M} \neq 0$, especially the nonequilibrium case which cannot be handled as thermodynamic equilibrium. In such nonequilibrium cases, the state that the mass flux leaving from liquid to vapor ($(v_i - v_{\mathrm{w}i})n_i > 0$) is referred to as *net evaporation*, and the mass flux in the direction opposite to net evaporation ($(v_i - v_{\mathrm{w}i})n_i < 0$) is referred to as *net condensation*. It is known that the influence of net evaporation/condensation is dominant in some vapor–liquid two-phase flow problems, namely, dynamics of bubbles and droplets [1–6].

A typical example is the vapor bubble collapse problem. Fujikawa and Akamatsu [1] derived the equation of motion for single spherical bubble accompanied with net evaporation/condensation for the first time. The result of the numerical simulation of this equation of motion implied that a purely vaporous bubble produce a strong pressure wave in liquid at the instant the rebound process begins. This equation of motion is commonly used in the numerical simulation of a bubble accompanied with net evaporation/condensation. Akhatov *et al.* [2] proposed the numerical simulation of the single spherical bubble collapse and rebound processes accompanied with net evapo-

ration/condensation by the Euler equation and showed that the temporal evolution of a bubble radius agrees with that obtained by the experiment for a laser induced bubble. Jinbo *et al.* [3] investigated the influence of net evaporation/condensation on the single nonspherical bubble collapse processes by the Euler equation and indicated that the temperature and pressure fields in a bubble vary locally according to net evaporation/condensation. These results implied that net evaporation/condensation affects the temperature and pressure fields in the inside and the outside of a bubble. Furthermore, on the basis of these results, we can naturally predict that net evaporation/condensation affects the shock wave propagation and the liquid jet formulation attributed to the bubble collapse process.

In these studies, well-known boundary conditions at the vapor–liquid interface, namely, the Hertz-Knudsen-Langmuir model and the Hertz-Knudsen-Schrage model, are utilized to estimate the mass flux induced by net evaporation/condensation. Some studies, however, threw doubt on the accuracy of these models [7]. We detail these models in the next section.

Moreover, from an application point of view, several studies [8, 9] proposed the basis of therapeutic applications by using the shock wave and the liquid jet attributed to the bubble collapse process. For example, Ohl *et al.* [9] tried to apply the liquid jet to deliver noninvasively large-sized molecules into cells, and Kobayashi *et al.* [8] estimated the interaction between the shock wave and the bubble for the extracorporeal shock-wave lithotripsy. However, in these therapeutic applications, we have to take into account the influence of net evaporation/condensation in addition to the effect of the complex bubble interaction and the noncondensable gas. At least, if we can treat the influence of net evaporation/condensation with the accurate model, it will be helpful for developing the basis of these therapeutic applications.

## 1.2 Boundary condition at vapor–liquid interface

As was mentioned above, a proper specification of the mass flux at the vapor–liquid interface is necessary to predict heat and mass transfer in the vapor–liquid two-phase system. The well-known boundary conditions to estimate the mass flux induced by net evaporation/condensation are the Hertz-Knudsen-Langmuir (HKL) model and the Hertz-Knudsen-Schrage (HKS) model [10]. The previous studies introduced in the above section [1–3] utilized the HKL and HLS models. Even in studies other than those introduced, these models are very commonly used. The recent researches regarding these models are reviewed by Persad *et al.* [11]. However, the accuracy of these models are questionable [7].

Here, we state the critical issue of the HKL and HKS models and the objective of this thesis. The mass flux at the vapor–liquid interface obtained by the HKL and HLS

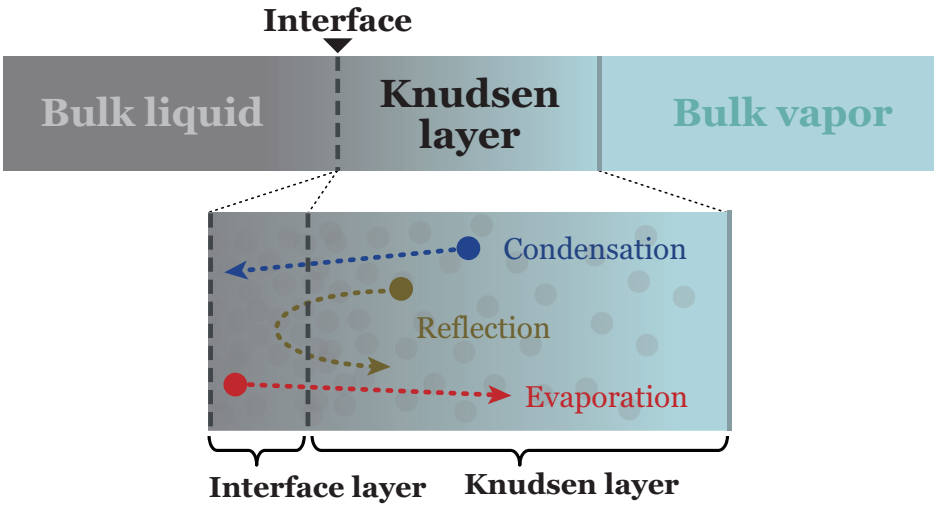


Figure 1: Physical picture of the vapor–liquid two-phase system.

models are as follows:

$$\mathcal{M}_{\mathrm{HKL}} = \frac{\alpha}{\sqrt{2\pi R}} \left( \frac{p^*}{\sqrt{T_{\mathrm{L}}}} - \frac{p}{\sqrt{T}} \right), \tag{4}$$

$$\mathcal{M}_{\mathrm{HKS}} = \frac{2\alpha}{(2-\alpha)\sqrt{2\pi R}} \left( \frac{p^*}{\sqrt{T_{\mathrm{L}}}} - \frac{p}{\sqrt{T}} \right), \tag{5}$$

where $\alpha$ is an unknown dimensionless parameter, $R$ is the gas constant, $T_{\mathrm{L}}$ is the liquid temperature, $p^*$ is the saturated vapor pressure at the liquid temperature, $p$ and $T$ are the pressure and the temperature, respectively. The critical issue of Eqs. (4) and (5) lies in the determination of $p$ and $T$.

To detail the critical issue of the HKL and HKS models, we explain the physical picture of the vapor–liquid two-phase system as shown in Fig. 1. As illustrated in Fig. 1, there is a transition layer between bulk liquid and bulk vapor. This transition layer in which the characteristic length scale is the mean free path is called the *Knudsen layer* [12]. The lower part of Fig. 1 is the enlarged view of the vapor–liquid interface and the Knudsen layer. In the macroscopic point of view, the vapor–liquid interface is the discontinuity surface, while in the microscopic point of view, the macroscopic variables transit smoothly between bulk liquid and bulk vapor. As illustrated in Fig. 1, the region in contact with the vapor–liquid interface in which the characteristic length scale is the molecular diameter is referred to as the *interface layer* in this thesis. The interface layer is equivalent to the vapor–liquid interface with zero thickness in the macroscopic point of view. With this microscopic point of view, we can capture the essence that net evaporation/condensation occurs as a consequence of the unbalance (nonequilibrium) of the number of molecules in the interface layer. Such nonequilibrium of molecules accommodates to local equilibrium through the molecular interactions in the Knudsen layer. We postulate, throughout this thesis, the physical picture of the vapor–liquid

two-phase system shown in Fig. 1.

Let us now go back to the HKL and HKS models (Eqs. (4) and (5)). The critical issue of the HKL and HKS models is that these models ignore the molecular interactions in the Knudsen layer. In other words, $p$ and $T$ in these models can be specified independently of the molecular interactions in the Knudsen layer. Since the outside of the Knudsen layer reaches local equilibrium as a consequence of the molecular interactions in the Knudsen layer, there is no basis that a proper mass flux can be predicted from the HKL and HKS models by specifying $p$ and $T$ that ignore such molecular interactions. It would be advantageous that the HKL and HKS models can omit the complex analysis in the Knudsen layer, but the molecular interactions there play a major role in the mass flux induced by net evaporation/condensation. The aim of this thesis is to propose a physically proper boundary condition at the vapor–liquid interface that takes into account such microscopic phenomenon.

We then describe the strategy of this thesis. In this thesis, we postulate a phenomenological model of the molecular motions to discuss the microscopic phenomenon near the vapor–liquid interface. The key processes according to this model are *evaporation*, *reflection*, and *condensation*. As illustrated in Fig. 1, the process from the interface layer into the Knudsen layer is called evaporation, that from the Knudsen layer into the interface layer is called condensation, and that accompanied by the change in the direction in the interface layer is referred to as reflection. When the number of the evaporation molecules is greater than that of the condensation molecules, net evaporation occurs at the vapor–liquid interface, while when the number of condensation molecules is greater than that of the evaporation molecules, net condensation occurs at the vapor–liquid interface.

To examine these molecular processes, we have to carry out the molecular simulation for the vapor–liquid two-phase system including the interface layer and the Knudsen layer. We refer to the simulation that tracks the temporal evolution of the positions and the velocities of molecules under a certain intermolecular potential as the molecular simulation. With the development of high-performance computing from the 1990s, the molecular simulations for the vapor–liquid two-phase system have been performed to examine the molecular processes, such as evaporation, reflection, and condensation [13–20]. However, the results of the molecular simulation cannot be directly applied as the boundary condition in the macroscopic theory, namely, fluid dynamics.

The most accurate way to derive the boundary condition in fluid dynamics by replacing the microscopic information obtained from the molecular simulation with relevant macroscopic variables is the molecular gas dynamics analysis [12]. In a sense, molecular gas dynamics bridges between the microscopic theory and the macroscopic theory. In the molecular gas dynamics analysis, the microscopic phenomenon in the interface layer is taken into the boundary condition (the kinetic boundary condition). However, the conventional kinetic boundary condition that has been used in the molecular gas dynamics analysis is mere mathematical model. The main content of this thesis is to investigate the kinetic boundary condition at the vapor–liquid interface by utilizing the molecular simulation in the vapor–liquid two-phase system including the interface layer

and the Knudsen layer.

## 2 Molecular gas dynamics analysis

Here, we briefly explain the theoretical framework of molecular gas dynamics, the conventional kinetic boundary condition, and the derivation method of the boundary condition in fluid dynamics. The contents of this section are based on the literature [7, 12].

### 2.1 Velocity distribution function

In the following, we consider gas or vapor consisting of single-component monatomic molecules with the influence range of the intermolecular force $a$. The motion of these molecules is governed by Newton's equation of motion. A sufficient number of molecules are present in the system under consideration; there is also many molecules in the volume elements taken in the system in which the number density is $n$. In the limit when $n \to \infty$ and $a \to 0$, we assume that $na^3 \to 0$ holds. This condition means that the total volume where the intermolecular forces are effective is negligibly small compared with the volume of gas or vapor, that is, the ideal gas condition. Also, the limiting that $n \to \infty$ and $a \to 0$ with fixed $na^2$ is called the Grad-Boltzmann limit. The inverse of $na^2$ is the order of the mean free path, which is the distance of molecules traveling before the subsequent collision.

Under the limiting that $m \to 0$ and $n \to \infty$ with keeping $mn$ is fixed at a finite value, we can define the velocity distribution function $f$, which is a function representing the statistical properties of molecules in the volume element, as follows:

$$m\mathrm{d}N = f(\boldsymbol{x}, \boldsymbol{\xi}, t)\mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{\xi}, \tag{6}$$

where $\mathrm{d}\boldsymbol{x}$ is the volume element in the physical space ($\mathrm{d}\boldsymbol{x} = \mathrm{d}x\mathrm{d}y\mathrm{d}z$), $\mathrm{d}\boldsymbol{\xi}$ is the volume element in the molecular velocity space ($\mathrm{d}\boldsymbol{\xi} = \mathrm{d}\xi_x\mathrm{d}\xi_y\mathrm{d}\xi_z$), and $m$ is the mass of a molecule. In Eq. (6), $\mathrm{d}N$ is the number of molecules in $\mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{\xi}$ at time $t$, the position $x_i = (x, y, z)$, and molecular velocity $\xi_i = (\xi_x, \xi_y, \xi_z)$ in the 6-dimensional phase space. This $f$ defined in Eq. (6) is the only unknown variable in molecular gas dynamics. Note that we use vector notation and tensor notation without notice, such as $x_i = \boldsymbol{x}$ and $\xi_i = \boldsymbol{\xi}$, if necessary.

### 2.2 Boltzmann equation

As mentioned above, we deal with numerous molecules whose motion is governed by Newton's equation of motion. Here, we regard the gas or vapor as an ensemble of particles and examine the motion of this ensemble, which is governed by the Liouville equation. Although the Liouville equation is exact, it is often too detailed to describe the motion of gas or vapor, and it is too complex to be solved. A more convenient starting point to describe the $N$-particle system is the Bogolyubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy equation. The BBGKY hierarchy equation connects the evolution

of an $N$-particle distribution function to an $N+1$ particle distribution function; this equation is not closed generally because both distribution functions are unknown.

In fact, to obtain the macroscopic variables and the fluxes that we are interested in, we only require the lowest order distribution function defined in Eq. (6). However, the two-particle distribution function is required to solve the BBGKY hierarchy equation for the one-particle distribution function, and this equation is not closed after all. We introduce the following correlation function to close the BBGKY hierarchy equation.

$$f_2(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{\xi}_1, \boldsymbol{\xi}_2, t) = Y f_1(\boldsymbol{x}_1, \boldsymbol{\xi}_1, t) f_1(\boldsymbol{x}_2, \boldsymbol{\xi}_2, t), \tag{7}$$

where $f_1$ indicates the one-particle distribution function, which is equivalent to $f$ defined in Eq. (6), $f_2$ indicates the two-particle distribution function, $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ indicate the positions of two molecules, $\boldsymbol{\xi}_1$ and $\boldsymbol{\xi}_2$ indicate the velocities of two molecules, and $Y$ is a pair correlation. In the Grad-Boltzmann limit, $Y$ can be set to unity, which is called the molecular chaos assumption, and thereby $f_2$ is transferred to the product of $f_1$. Also, the intermolecular collisions are events that occur at one point in time and space. Since the collision frequency of the triple or more multiple collisions is sufficiently small in the Grad-Boltzmann limit, we can only consider the binary event.

By the above procedure, the Boltzmann equation which is an equation governing the evolution of the one-particle distribution function in the system without the external force is derived as follows [21]:

$$\frac{\partial f}{\partial t} + \xi_i \frac{\partial f}{\partial x_i} = C_{\mathrm{B}}, \tag{8}$$

where the left-hand side of Eq. (8) represents the effect of the evolution of $f$ along the path of free molecular motion, and the right-hand side of Eq. (8) represents the effect of the intermolecular collision and is called *collision integral* or *Boltzmann collision term*,

$$C_{\mathrm{B}} = \frac{1}{m} \int_{\text{all } K_i,\ \text{all } \xi_{1i}} [f(\boldsymbol{x}, \boldsymbol{\xi}_1', t) f(\boldsymbol{x}, \boldsymbol{\xi}', t) - f(\boldsymbol{x}, \boldsymbol{\xi}_1, t) f(\boldsymbol{x}, \boldsymbol{\xi}, t)] B \mathrm{d}\Omega(\boldsymbol{K}) \mathrm{d}\boldsymbol{\xi}_1, \tag{9}$$

where $\xi_i$ indicates the velocity of a molecule under consideration, $\xi_{1i}$ indicates the velocity of a molecule colliding with the molecule having the velocity $\xi_i$, $K_i$ is a unit vector along the direction of the molecular velocity before and after the collision, $\mathrm{d}\Omega(\boldsymbol{K})$ is a solid angle element in the $K_i$ direction, and $B$ is a nonnegative function determined by the intermolecular force model and $B = a^2 |K_j(\xi_{1j} - \xi_j)|/2$ for hard-sphere molecules having a diameter $a$. In Eq. (9), $\xi_i'$ and $\xi_{1i}'$ indicate the molecular velocities after the collision and are determined by considering the elastic collision,

$$\xi_i' = \xi_i + K_i K_j (\xi_{1j} - \xi_j), \qquad \xi_{1i}' = \xi_{1i} + K_i K_j (\xi_{1j} - \xi_j). \tag{10}$$

The details of the derivation of Eqs. (8) and (9) are given in the literature [12, 21].

## 2.3 Kinetic boundary condition

The Boltzmann equation regulates the evolution of the velocity distribution function along the path in $(\boldsymbol{x}, t)$ space of the molecules having the velocity $\xi_i$. If $f$ in the domain under consideration at the initial time is given and how the molecules are scattered at the boundary at the arbitrary time is determined, we can determine the behavior of $f$ by the Boltzmann equation. In other words, the boundary condition for the Boltzmann equation is an outgoing velocity distribution function to gas or vapor, $f_{\mathrm{out}}$, as a consequence of molecules colliding and scattering at the boundary. The boundary condition for the Boltzmann equation is called the kinetic boundary condition (KBC). Similar to other boundary conditions, we cannot derive the KBC from the framework of molecular gas dynamics. Although we have to investigate the molecular interaction with the boundary in order to impose the KBC, in the molecular gas dynamics analysis, mathematical models have often been utilized as the KBC [12, 22–24].

We hereafter consider the KBC in the system composed of monatomic vapor and its condensed phase (liquid) with the planar vapor–liquid interface. The conventional KBC, which is widely used in the molecular gas dynamics analysis [12, 22–24], is shown as follows:

$$f_{\mathrm{out}} = [\alpha\rho^* + (1-\alpha)\sigma]\hat{f}^*, \qquad (\xi_i - v_{\mathrm{w}i})n_i > 0, \tag{11}$$

where $n_i$ is the unit vector in the direction normal to the vapor–liquid interface pointing vapor, $\rho^*$ is the saturated vapor density at the liquid temperature $T_{\mathrm{L}}$, $\hat{f}^*$ is the normalized velocity distribution function of the KBC and is assumed the normalized Maxwellian distribution at $T_{\mathrm{L}}$,

$$\hat{f}^* = \frac{1}{\sqrt{2\pi R T_{\mathrm{L}}}^3} \exp\left(-\frac{(\xi_i - v_{\mathrm{w}i})^2}{2RT_{\mathrm{L}}}\right), \tag{12}$$

$\sigma$ is a parameter having the dimension of the density, and its definition is related to the velocity distribution function of molecules colliding with the vapor–liquid interface from vapor, $f_{\mathrm{coll}}$,

$$\sigma\sqrt{\frac{RT_{\mathrm{L}}}{2\pi}} = -\int_{(\xi_i - v_{\mathrm{w}i})n_i<0} (\xi_j - v_{\mathrm{w}j})n_j f_{\mathrm{coll}} \mathrm{d}\boldsymbol{\xi}, \tag{13}$$

where $\int_{(\xi_i - v_{\mathrm{w}i})n_i<0} \mathrm{d}\boldsymbol{\xi}$ indicates that the domain of the integration is $-\infty$ to zero for the molecular velocity in the direction normal to the vapor–liquid interface and $-\infty$ to $\infty$ for that in the tangential direction. Equation (11) is a mere mathematical model; $\alpha$ is a parameter and is often set to unity for simplicity, and the functional form of $\hat{f}^*$ is an assumption.

## 2.4 Knudsen layer analysis

Sone *et al.* [12,22] have systematically investigated the method for deriving the boundary condition in fluid dynamics, which is consistent with the fluid dynamic equations. As

stated in the former section, the HKL and HKS models (Eqs. (4) and (5)) have the problem in determining $p$ and $T$ included in these models. In the method proposed by Sone *et al.* [12, 22], $p$ and $T$, which take into account the molecular interactions in the Knudsen layer, can be obtained by solving the Boltzmann equation with the KBC. We here introduce the result by utilizing the conventional KBC (Eq. (11)).

The procedure to derive the boundary condition for the fluid dynamic equations by solving the Boltzmann equation in the Knudsen layer is called the Knudsen layer analysis [12, 22]. It becomes possible to replace the microscopic information in the Knudsen layer with the relevant macroscopic variables by this analysis. The Knudsen layer analysis is a boundary value problem to obtain the solution of the Boltzmann equation and its existence condition under the KBCs at the vapor–liquid interface and at the end of the Knudsen layer (infinitely far from the vapor–liquid interface). The existence condition of the solution of this boundary value problem means the states of the pressure $p$, the temperature $T$, and the velocity $v_i$ at the end of the Knudsen layer,

$$\frac{p - p^*}{p^*} = \left( C_4^* - 2\sqrt{\pi} \frac{1-\alpha}{\alpha} \right) \frac{(v_i - v_{\mathrm{w}i}) n_i}{\sqrt{2RT_{\mathrm{L}}}}, \tag{14}$$

$$\frac{T - T_{\mathrm{L}}}{T_{\mathrm{L}}} = d_4^* \frac{(v_i - v_{\mathrm{w}i}) n_i}{\sqrt{2RT_{\mathrm{L}}}}, \tag{15}$$

that is, the slip boundary condition [12, 22]. In Eqs. (14) and (15), $C_4^*$ and $d_4^*$ are the slip coefficients, which include the microscopic information in the Knudsen layer and these are obtained by determining the molecular model. The slip coefficients of various molecular models are summarized in the literature [12].

From Eq. (14) and the equation of state for the ideal gas, the mass flux at the end of the Knudsen layer can be found as follows:

$$\mathcal{M}_{\mathrm{MGD}} = \frac{1}{2\sqrt{\pi}\frac{1-\alpha}{\alpha} - C_4^*} \sqrt{\frac{2}{R}} \left( \frac{p^*}{\sqrt{T_{\mathrm{L}}}} - \frac{p}{\sqrt{T_{\mathrm{L}}}} \right), \tag{16}$$

where the term $O[((v_i - v_{\mathrm{w}i}) n_i / \sqrt{2RT_{\mathrm{L}}})^2]$ is neglected because the slip boundary condition is derived under the condition $|(v_i - v_{\mathrm{w}i}) n_i / \sqrt{2RT_{\mathrm{L}}}| \ll 1$. With the use of Eqs. (16) and (15) or Eqs. (14) and (15) as the boundary conditions, the fluid dynamic equations can be closed. Equations (14), (15), and (16) are, strictly speaking, the boundary conditions at the end of the Knudsen layer, but we call those the *boundary conditions at the vapor–liquid interface* because we do not have to solve the Knudsen layer in the fluid dynamics analysis.

## 3 Contents of this thesis

The objective of this thesis is to propose a physically proper boundary condition at the vapor–liquid interface with net evaporation/condensation. After summarizing the topics so far, we then clarify the remaining issue and state the scope of this thesis.

### 3.1 Clarification of remaining issue

To summarize the preceding sections, what we have to do to propose the boundary condition at the vapor–liquid interface are (i) to conduct the molecular simulation to construct the KBC and (ii) to conduct the Knudsen layer analysis to derive the boundary condition for the fluid dynamic equations. As for (ii), it has been systematically investigated by Sone *et al.* [12, 22]; hence, as long as these results are available, the only thing we should study in this thesis is (i).

According to the physical picture shown in Fig. 1, the KBC is the outgoing velocity distribution function from the interface layer at the vapor–liquid interface. Numerous studies [25–38] examined this velocity distribution function by the molecular simulation in the vapor–liquid two-phase system including the interface layer and the Knudsen layer.

In some previous studies, $\alpha$ is divided into two different coefficients, namely, the evaporation coefficient $\alpha_{\mathrm{e}}$ and the condensation coefficient $\alpha_{\mathrm{c}}$, as a kind of physical properties. These coefficients are defined in relation to the molecular processes illustrated in Fig. 1. Some different definitions have been proposed for $\alpha_{\mathrm{e}}$ and $\alpha_{\mathrm{c}}$. For instance, Tsuruta *et al.* [30] defined $\alpha_{\mathrm{e}}$ and $\alpha_{\mathrm{c}}$ by the number of molecules at the vapor–liquid interface and expressed these coefficients as the functions of the liquid temperature and the translational energy in the direction normal to the vapor–liquid interface. Ishiyama *et al.* [32,33] defined $\alpha_{\mathrm{e}}$ and $\alpha_{\mathrm{c}}$ by the molecular mass fluxes at the vapor–liquid interface and indicated that these coefficients depend only on the liquid temperature. Naturally, such a different tendency arises from the different definitions of $\alpha_{\mathrm{e}}$ and $\alpha_{\mathrm{c}}$. However, it should be emphasized that even if these coefficients are calculated according to the same definitions as Ishiyama *et al.* [32, 33], these coefficients vary with the degree of net evaporation/condensation [26, 36]. These results indicate that neither $\alpha_{\mathrm{e}}$ nor $\alpha_{\mathrm{c}}$ has been indisputably determined after all.

In addition, some previous studies [33, 37, 39, 40] pointed out that the normalized velocity distribution function of the KBC deviates from the normalized Maxwellian distribution (Eq. (12)) when the vapor–liquid interface is in strong net evaporation or condensation. Thus, the construction of the KBC at the vapor–liquid interface is an issue open to question.

To clarify this remaining issue, we consider the following generalized KBC [41].

$$f_{\mathrm{out}} = \mathcal{A}\hat{f}^*, \qquad (\xi_i - v_{\mathrm{w}i})n_i > 0, \tag{17}$$

where we assume that $\hat{f}^*$ is to be the normalized Maxwellian distribution (Eq. (12)). The conditions of $\mathcal{A}$ is shown as follows: (1) $\mathcal{A}$ is the nonnegative function, (2) $\mathcal{A}$ is allowable to be the function of the liquid temperature $T_{\mathrm{L}}$ and/or $\sigma$ (Eq. (13)), and (3) $\mathcal{A}$ is independent of the molecular velocity. Note that some KBCs proposed by the previous molecular simulations do not satisfy these conditions. We extract the part related to the liquid temperature $\mathcal{A}_0(T_{\mathrm{L}})$ from $\mathcal{A}$ and rewrite Eq. (17) as

$$\mathcal{A} = \mathcal{A}_0(T_{\mathrm{L}}) + [\mathcal{A} - \mathcal{A}_0(T_{\mathrm{L}})]. \tag{18}$$

When $\mathcal{A} = \alpha_\mathrm{e}\rho^* + (1-\alpha_\mathrm{c})\sigma$, $\alpha_\mathrm{e}$ and $\alpha_\mathrm{c}$ are defined by

$$\alpha_\mathrm{e} = \frac{\mathcal{A}_0(T_\mathrm{L})}{\rho^*}, \qquad \alpha_\mathrm{c} = 1 - \frac{\mathcal{A} - \mathcal{A}_0(T_\mathrm{L})}{\sigma}. \tag{19}$$

In Eq. (19), the selection of $\mathcal{A}_0(T_\mathrm{L})$ is arbitrary. In other words, under the assumption that $\hat{f}^*$ is to be the normalized Maxwellian distribution (Eq. (12)), there is an infinite number of $\alpha_\mathrm{e}$ and $\alpha_\mathrm{c}$ pairs corresponding to arbitrary $\mathcal{A}_0(T_\mathrm{L})$. To determine $\alpha_\mathrm{e}$ and $\alpha_\mathrm{c}$ uniquely, we have to clarify the physical requirement that $\mathcal{A}_0(T_\mathrm{L})$ should satisfy. Also, if $\alpha_\mathrm{e}$ and $\alpha_\mathrm{c}$ is related to the molecular processes illustrated in Fig. 1, the physical requirement that $\mathcal{A}_0(T_\mathrm{L})$ should satisfy is synonymous with the definitions of these molecular processes. That is why $\alpha_\mathrm{e}$ and $\alpha_\mathrm{c}$ have not been determined so far.

## 3.2 Scope of this thesis

To break through the issue stated in above, we consider $\alpha_\mathrm{e}$ and $\alpha_\mathrm{c}$ from a more fundamental rule, that is, the conservation law of the mass flux extended to the microscopic point of view. This fundamental rule holds regardless of any condition. The conservation law of the mass flux extended to the microscopic point of view represents the relation between the mass flux in the macroscopic and microscopic points of view as shown in the following.

$$\begin{aligned}
\mathcal{M} &= \rho(v_j - v_{\mathrm{w}j})n_j \\
&= \int_{\text{all } \xi_i} (\xi_j - v_{\mathrm{w}j})n_j f(\boldsymbol{x}, \boldsymbol{\xi}, t)\mathrm{d}\boldsymbol{\xi} \\
&= \int_{(\xi_i - v_{\mathrm{w}i})n_i > 0} (\xi_j - v_{\mathrm{w}j})n_j f_\mathrm{out}\mathrm{d}\boldsymbol{\xi} + \int_{(\xi_i - v_{\mathrm{w}i})n_i < 0} (\xi_j - v_{\mathrm{w}j})n_j f_\mathrm{coll}\mathrm{d}\boldsymbol{\xi},
\end{aligned} \tag{20}$$

where $\int_{(\xi_i - v_{\mathrm{w}i})n_i > 0} \mathrm{d}\boldsymbol{\xi}$ indicates that the domain of the integration is zero to $\infty$ for the molecular velocity in the direction normal to the vapor–liquid interface and $-\infty$ to $\infty$ for that in the tangential direction. Equation (20) clearly shows that the mass flux induced by net evaporation/condensation is caused by the difference in the mass flux related to the velocity distribution functions $f_\mathrm{out}$ and $f_\mathrm{coll}$. When $f_\mathrm{out}$ is the generalized KBC (Eq. (17)), we get the following expression.

$$\rho(v_i - v_{\mathrm{w}i})n_i = (\mathcal{A} - \sigma)\sqrt{\frac{RT_\mathrm{L}}{2\pi}}, \tag{21}$$

For example, when $\mathcal{A} = \alpha_\mathrm{e}\rho^* + (1-\alpha_\mathrm{c})\sigma$, Eq. (21) becomes

$$\rho(v_i - v_{\mathrm{w}i})n_i = (\alpha_\mathrm{e}\rho^* - \alpha_\mathrm{c}\sigma)\sqrt{\frac{RT_\mathrm{L}}{2\pi}}. \tag{22}$$

We hereafter call Eq. (21) the *mass flux relation* for simplicity. In this thesis, we investigate Eq. (21) by the molecular simulation. From this result, we can determine $\alpha_\mathrm{e}$

and $\alpha_c$ without explicitly defining the molecular processes illustrated in Fig. 1. Also, after determining $\alpha_e$ and $\alpha_c$ in this way, we can consider their physical meanings by investigating the relation between these coefficients and the molecular processes.

Let us now detail how to investigate and what to clarify together with the scope of this thesis. In Chapter 2, we first explain the vapor–liquid two-phase system to be considered. The system considered in this thesis is a steady one-dimensional net evaporation/condensation problem in vapor between two liquid slabs with the different temperature. This problem is often called the two-surface problem. After explaining the one-dimensional problem of net evaporation/condensation, we introduce the features of the two-surface problem from the results of the previous studies. Next, we explain the molecular simulation method. The investigation of Eq. (21) requires to exhaustively and precisely obtain $\rho(v_i - v_{wi})n_i$ under the various cases of net evaporation/condensation. However, the molecular dynamics simulation, which has been utilized as a molecular simulation, requires a high computational cost. Actually, in the previous studies [26, 28, 30, 31, 33–37], only in the several limited cases of net evaporation/condensation have been examined. In contrast, we focus on the novel molecular simulation method based on the mean-field kinetic theory proposed by Frezzotti *et al.* [42]. We can perform the molecular simulation for the one-dimensional net evaporation/condensation problem with less computational cost than the molecular dynamics simulation by utilizing this novel method.

In Chapter 3, we examine the mass flux relation (Eq. (21)) to find a pair of $\alpha_e$ and $\alpha_c$ defined by Eq. (19) by the molecular simulation based on the mean-field kinetic theory. We perform the molecular simulation for the two-surface problem in 160 cases of the temperature differences between two liquids. First, we confirm whether the normalized velocity distribution function of the KBC obeys Eq. (12) because the results of the previous studies [33, 37, 38, 40] indicated that the normalized velocity distribution function of the KBC deviates from Eq. (12) under strong net evaporation/condensation. Next, we formulate the mass flux relation at each liquid temperature by using $\rho(v_i - v_{wi})n_i$ obtained by the molecular simulation and corresponding $\sigma$ (Eq. (13)), and then we discuss $\alpha_e$ and $\alpha_c$ defined by Eq. (19) by comparing the formulated mass flux relation with Eq. (21). In this way, we can find a pair of $\alpha_e$ and $\alpha_c$ without explicitly defining the molecular processes illustrated in Fig. 1.

In Chapter 4, we consider the physical meaning of $\alpha_e$ and $\alpha_c$ obtained in Chapter 3. To determine $\alpha_e$ and $\alpha_c$ uniquely, we have to clarify the definitions of the molecular processes illustrated in Fig. 1. Although this definition has not been clarified, if we assume a certain condition, these molecular processes can be distinguished. We here consider a hypothesis of the spontaneous evaporation [32, 43]. According to this hypothesis, $\alpha_e$ and $\alpha_c$ are defined by the mass fluxes related to the molecular processes. $\alpha_e$ and $\alpha_c$ according to this hypothesis can be obtained from the virtual vacuum simulation [25, 32] and the net evaporation and condensation simulation [33]. However, the virtual vacuum simulation is inappropriate when the liquid temperature becomes relatively high; hence, we apply a new method, which is called the *two-boundary method*, proposed by Kobayashi *et al.* [29] to estimate $\alpha_e$ and $\alpha_c$ according to the hypothesis of the spon-

taneous evaporation. First, we confirm whether the normalized velocity distribution function of the evaporation molecules is to be the normalized Maxwellian distribution (Eq. (12)), which is the premise of the hypothesis of the spontaneous evaporation. Next, we discuss the correspondence of the hypothesis of the spontaneous evaporation with $\alpha_{\mathrm{e}}$ and $\alpha_{\mathrm{c}}$ obtained in Chapter 3 by examining the mass fluxes of evaporation and condensation molecules in both the vapor–liquid equilibrium and net evaporation/condensation cases. In this way, we can find the relation among $\alpha_{\mathrm{e}}$, $\alpha_{\mathrm{c}}$ obtained in Chapter 3, and the molecular processes illustrated in Fig. 1.

In Chapter 6, we verify the accuracy of $\alpha_{\mathrm{e}}$ and $\alpha_{\mathrm{c}}$ obtained in Chapter 3 and Chapter 4. We perform the molecular simulation for the different two vapor–liquid two-phase systems, which are distinct from that considered in the preceding chapters. First, in these two systems, we confirm whether the normalized velocity distribution function of the KBC obeys the normalized Maxwellian distribution (Eq. (12)). Next, we compare the macroscopic variables in vapor, namely, the velocity and the temperature, in these two systems obtained from the numerical simulation of the Boltzmann equation with the KBC, which is specified by $\alpha_{\mathrm{e}}$ and $\alpha_{\mathrm{c}}$ obtained in the preceding chapters, and those obtained from the molecular simulation based on the mean-field kinetic theory. Since it has been pointed out that the KBC significantly affects the macroscopic variables in the numerical simulation of the Boltzmann equation [44–46], the proper specification of the KBC is critical. In other words, the KBC at the vapor–liquid interface with net evaporation/condensation is validated if and only if the macroscopic variables in vapor obtained from these two simulations accurately agree with each other. This simple validation method has often been performed in the molecular dynamics simulation [44,45]. Finally, we compare the liquid temperature dependence of $\alpha_{\mathrm{e}}$ and $\alpha_{\mathrm{c}}$ in these two systems with those obtained in Chapter 3. In this way, we can verify whether $\alpha_{\mathrm{e}}$ and $\alpha_{\mathrm{c}}$ obtained in Chapter 3 and Chapter 4 depend on the simulation systems.

## 4 Concluding remarks

The target of this thesis is heat and mass transfer in a two-phase system composed of single-component monatomic vapor and its condensed phase (liquid). We especially examined heat and mass transfer associated with a mass flux in the direction normal to the vapor–liquid interface (net evaporation/condensation). The objective of this thesis is to propose a physically proper boundary condition at the vapor–liquid interface. What we have to do to propose the boundary condition are (i) to conduct the molecular simulation to construct the boundary condition for the Boltzmann equation (KBC) and (ii) to conduct the Knudsen layer analysis to derive the boundary condition for the fluid dynamic equations. As for (ii), it has been systematically investigated by Sone *et al.* [12, 22]; hence, as long as these results are available, the only thing we should study in this thesis is (i).

To construct the KBC, we have to specify the unknown parameters included in the KBC, namely, the evaporation coefficient $\alpha_{\mathrm{e}}$ and condensation coefficient $\alpha_{\mathrm{c}}$. In this thesis, to specify these coefficients, we investigated a fundamental rule at the vapor–

liquid interface by the molecular simulation based on the mean-field kinetic theory (the EV-DSMC simulation). This fundamental rule holds regardless of any condition, that is, the conservation law of the mass flux extended to the microscopic point of view (the mass flux relation). A feature of this thesis is to utilize the molecular simulation based on the mean-field kinetic theory (the EV-DSMC simulation). The EV-DSMC simulation for the spatially one-dimensional flow runs about 50–60 times faster than an equivalent molecular dynamics simulation, which is well-used simulation method for the vapor–liquid two-phase system, with the same number of molecules. In the following, we summarize the results of the main chapters and propose the boundary condition at the vapor–liquid interface based on these results.

## 4.1 Chapter 3

On the basis of the results in Chapter 3, we formulated the following mass flux relation at the vapor–liquid interface.

$$\frac{\rho v_z}{J^*_{\mathrm{out}}} = \beta \left( 1 - \frac{\sigma}{\rho^*} \right), \tag{23}$$

where $\beta$ is a decreasing function of the liquid temperature. Also, we proposed the following KBC at the vapor–liquid interface by using the relation $\alpha_{\mathrm{e}} = \alpha_{\mathrm{c}} = \beta(T_{\mathrm{L}})$.

$$f_{\mathrm{out}} = [\beta(T_{\mathrm{L}})\rho^* + (1 - \beta(T_{\mathrm{L}}))\sigma]\hat{f}^*. \tag{24}$$

This KBC is essentially equivalent to what we set $\mathcal{A} = \alpha_{\mathrm{e}}\rho^* + (1-\alpha_{\mathrm{c}})\sigma$ in the generalized KBC (Eq. (17)) because of the relation $\alpha_{\mathrm{e}} = \alpha_{\mathrm{c}} = \beta(T_{\mathrm{L}})$. An important result is that we can find the relation $\alpha_{\mathrm{e}} = \alpha_{\mathrm{c}} = \beta(T_{\mathrm{L}})$ by formulating the mass flux relation at the vapor–liquid interface with high accuracy. However, the results in this chapter have only found a pair of $\alpha_{\mathrm{e}}$ and $\alpha_{\mathrm{c}}$ defined by Eq. (19) at each liquid temperature, and the relation between these coefficients and the molecular processes illustrated in Fig. 1 is not clear.

## 4.2 Chapter 4

On the basis of the results of Chapter 4, the following definition of $\mathcal{A}_0(T_{\mathrm{L}})$ in Eq. (19) can be obtained.

$$\mathcal{A}_0(T_{\mathrm{L}}) = \mathcal{B}(T_{\mathrm{L}}) \equiv \frac{J^*_{\mathrm{evap}}}{\sqrt{RT_{\mathrm{L}}/(2\pi)}}. \tag{25}$$

Although this result includes some assumptions, we succeeded to clarify the relation between $\beta(T_{\mathrm{L}})$ and the molecular processes illustrated in Fig. 1 by specifying $\mathcal{A}_0(T_{\mathrm{L}})$.

## 4.3 Chapter 5

On the basis of the results in Chapter 5, we suggested that the KBC (Eq. (24)), which is specified by $\alpha_{\mathrm{e}} = \alpha_{\mathrm{c}} = \beta(T_{\mathrm{L}})$, can be applied to not only a specific system but also

other systems, namely, the quasi-steady pseudo half-space and unsteady two-surface problems. Needless to say, these results do not indicate that the KBC (Eq. (24)) can be applied to all net evaporation/condensation problems. For example, we set the length of the vapor phase to approximately the mean free path in all simulation systems. If we set this length as a variable, further investigation should be required. Furthermore, in the molecular gas dynamics analysis, the solution of the Boltzmann equation have been examined on exhaustively various net evaporation/condensation problems. It is almost impossible to verify the KBC in all the net evaporation/condensation problems by using the molecular simulation. Therefore, we examined only some of the typical problems and conditions in this thesis. However, we emphasize that if we consider the formulated mass flux relation (Eq. (23)) is a fundamental physical law, the KBC proposed in this thesis can be established regardless the systems.

### 4.4 Boundary condition at vapor–liquid interface

We succeeded to propose the KBC at the vapor–liquid interface based on the results in Chapter 3–5. The pressure $p$ and the temperature $T$ at the end of the Knudsen layer can eventually be obtained by the Knudsen layer analysis with the KBC proposed in this thesis,

$$\frac{p - p^*}{p^*} = \left( C_4^* - 2\sqrt{\pi} \frac{1 - \beta(T_\mathrm{L})}{\beta(T_\mathrm{L})} \right) \frac{(v_i - v_{\mathrm{w}i}) n_i}{\sqrt{2RT_\mathrm{L}}},$$
$$\frac{T - T_\mathrm{L}}{T_\mathrm{L}} = d_4^* \frac{(v_i - v_{\mathrm{w}i}) n_i}{\sqrt{2RT_\mathrm{L}}}.$$

Furthermore, the mass flux at the end of the Knudsen layer can also be obtained as

$$\mathcal{M}_\mathrm{MGD} = \frac{1}{2\sqrt{\pi} \frac{1-\beta(T_\mathrm{L})}{\beta(T_\mathrm{L})} - C_4^*} \sqrt{\frac{2}{R}} \left( \frac{p^*}{\sqrt{T_\mathrm{L}}} - \frac{p}{\sqrt{T_\mathrm{L}}} \right).$$

Although these expressions seem to be the same as Eqs. (14), (15), and (16), it is advantageous in that these expressions is derived by using the KBC that is constructed based on the precise investigation by the molecular simulation. With the use of this mass flux, or the pressure, and the temperature as the boundary conditions, the fluid dynamic equations can be closed and then the solution that takes into account the molecular interactions in the interface layer and the Knudsen layer can be obtained.

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