

Slow flows of a vapor-gas mixture with large density and temperature variations in the near-continuum regime

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A binary mixture of a vapor and a noncondensable gas in contact with the boundary made of the condensed phase (liquid or solid) of the vapor is considered in the following situation: the amount of the noncondensable gas contained in the system is of the same order of magnitude as that of the vapor; the temperature variation along the boundary may be large; the boundary is at rest, and there is no flow at infinity when an infinite domain is considered; and the Knudsen number is small (i.e., near-continuum regime). Slow steady flows (with Mach number of the order of Knudsen number, or equivalently, with Reynolds number of the order of unity) of the mixture, mainly caused by evaporation and condensation of the vapor on the boundary, are investigated on the basis of kinetic theory. The basic system used in this work is the fluid-dynamic-type system that was derived systematically from the Boltzmann system in a previous paper [S. Takata and K. Aoki, *Transp. Theor. Stat. Phys.* **30**, 205 (2001); erratum, *ibid.* **31**, 289 (2002)] in connection with the ghost effect, and it is solved numerically by a finite-volume method. Some additional computation using the direct simulation Monte Carlo method, based on the original Boltzmann system, is also performed for comparison. The behavior of the mixture in the continuum limit in which the Knudsen number vanishes is discussed with special interest in the ghost effect. © 2007 American Institute of Physics. [DOI: [10.1063/1.2796213](https://doi.org/10.1063/1.2796213)]

I. INTRODUCTION

Study of vapor flows with evaporation and condensation on the boundary has been one of the important subjects in kinetic theory of gases in the last four decades (see, e.g., Refs. 1–6). Let us restrict ourselves to the near-continuum regime in which the Knudsen number, defined by the ratio of the mean free path of the vapor molecules to the characteristic length of the system, is small. In this case, fluid-dynamic-type systems, composed of fluid-dynamic-type equations and appropriate slip and jump boundary conditions, that describe steady flows of the vapor have been derived by systematic asymptotic analysis based on the system of the Boltzmann or its model equations.^{5–10} Some of these fluid-dynamic-type systems were extended to the vapor flows in the presence of a noncondensable gas, which neither evaporates nor condenses on the boundary, for model Boltzmann equations.^{11,12} However, some interesting phenomena for the mixture of the vapor and the noncondensable gas in the near-continuum regime (in particular in the continuum limit) were clarified rather recently.^{13–18}

In Ref. 16, the following rather general situation was considered: the amount of the noncondensable gas contained in the system is of the same order of magnitude as that of the vapor; the temperature variation along the boundary may be large; and the boundary is at rest, and there is no flow at infinity when an infinite domain is considered (see Sec. II for a more precise statement). The fluid-dynamic-type system

that describes the steady behavior of the vapor and noncondensable gas in this situation was derived from the Boltzmann system. In this reference, interest was focused on the ghost effect^{5,6,19–21} in the continuum limit where the Knudsen number goes to zero. That is, it was shown that (i) the flow of the vapor caused by evaporation and condensation vanishes in the continuum limit; however, (ii) the macroscopic flow field in the limit is affected by the invisible or infinitesimal flow. This seemingly paradoxical result is of fundamental interest and importance.

On the other hand, the fluid-dynamic-type system derived in Ref. 16 is also of practical importance because it describes slow flows (with Mach number of the order of Knudsen number, or equivalently, with Reynolds number of the order of unity) of the vapor and noncondensable gas, mainly caused by evaporation and condensation of the vapor, at small Knudsen numbers in the situation described at the beginning of the preceding paragraph. In other words, the fluid-dynamic-type system provides a tool of analysis of such flows without going back to the Boltzmann system that is much more complicated than the former system. The fluid-dynamic-type equations are not the Navier-Stokes equations but contain additional terms, the so-called Burnett terms.^{22,23} These equations as well as their boundary conditions can be derived only by kinetic considerations based on the Boltzmann system and are not obvious at all if one adheres only to macroscopic considerations.

The aim of the present paper is to show the usefulness of the fluid-dynamic-type system of Ref. 16 for practical analysis. Although the system was derived more than five years ago, its application to practical problems was not possible because it contained some coefficients in the equations as well as the boundary conditions whose numerical data were not available at that time. In the mean time, these coefficients were obtained and their databases were constructed in separate papers.^{24,25} Therefore, the fluid-dynamic-type system has been completed and is available for practical computations. The construction of a convenient numerical method for the system is also an important purpose of the present paper.

The paper is organized as follows. In Sec. II, the physical problem considered in this paper is described in a general setting. In Sec. III, the fluid-dynamic-type system of Ref. 16 is summarized with the help of Appendices A and B. In Sec. IV, a numerical solution method based on the finite-volume method²⁶ is constructed for the fluid-dynamic-type system. In Sec. V, the fluid-dynamic-type system is applied to a specific problem, and its numerical solution is presented together with some comparisons with the numerical solution of the Boltzmann system by the direct simulation Monte Carlo (DSMC) method.^{27,28} Finally in Sec. VI, brief concluding remarks are given.

II. PROBLEM AND ASSUMPTION

Let us consider a binary mixture of a vapor (A component) and a noncondensable gas (B component) in contact with the boundary with arbitrary (but smooth) shape, made of the condensed phase (liquid or solid) of the vapor. Therefore, evaporation and condensation of the vapor may take place on the boundary. We investigate the steady flow of the mixture, caused mainly by evaporation and condensation on the boundary, on the basis of kinetic theory under the following assumptions:

- (i) The amount of the noncondensable gas contained in the system is of the same order of magnitude as that of the vapor.
- (ii) The behavior of the mixture is described by the Boltzmann equation for binary gas mixtures.
- (iii) The vapor molecules leaving the surface of the condensed phase are distributed according to the half-range Maxwellian with temperature, flow velocity, and molecular number density equal to the temperature of the surface, the velocity of the surface, and the saturation number density of the vapor at the surface temperature.
- (iv) The molecules of the noncondensable gas reflected on the surface are distributed according to the half-range Maxwellian with temperature and flow velocity equal to the temperature and the velocity of the surface in such a way that the net molecular flux vanishes (diffuse reflection).
- (v) The molecules of the vapor and those of the noncondensable gas are hard spheres.
- (vi) The Knudsen number is small.
- (vii) The variation of the temperature of the boundary may be large.

- (viii) The boundary is at rest or moving (without motion in the normal direction) with a low speed, its Mach number being as small as the Knudsen number.
- (ix) In the case of an infinite domain, the vapor as well as the noncondensable gas is at rest at infinity or flowing with a low speed, its Mach number being as small as the Knudsen number.

In this situation, the behavior of the vapor and the noncondensable gas can be described by a fluid-dynamic-type system, which will be summarized in the next section.

III. FLUID-DYNAMIC-TYPE SYSTEM

In Ref. 16, a systematic asymptotic analysis for small Knudsen numbers based on the Boltzmann system was carried out in the situation described in Sec. II, and a fluid-dynamic-type system was derived. The analysis is along the lines of the asymptotic theory^{9,29,30} for a single-component gas that has been developed by Sone over the last four decades. The reader is referred to Refs. 5 and 6 for the details of the theory. In this section, we summarize the fluid-dynamic-type system derived in Ref. 16.

To begin with, we summarize the main notation appearing in what follows.

The symbol X_i denotes the rectangular coordinate system in space; n^A , p^A , v_i^A , m^A , and d^A denote the molecular number density, pressure, flow velocity, molecular mass, and molecular diameter of the vapor, respectively, and n^B , p^B , v_i^B , m^B , and d^B the corresponding quantities of the noncondensable gas; n , ρ , T , p , and v_i are the molecular number density, mass density, temperature, pressure, and barycentric flow velocity of the total mixture, respectively ($p = knT$, where k is the Boltzmann constant). The reference quantities are denoted by the subscript “0”; i.e., L_0 is the reference length of the system, m_0 the reference molecular mass, d_0 the reference molecular diameter, T_0 the reference temperature, n_0 the reference molecular number density, ρ_0 the reference mass density ($\rho_0 = m_0 n_0$), $p_0 (= kn_0 T_0)$ the reference pressure, l_0 the reference mean free path ($l_0 = 1 / \sqrt{2} \pi d_0^2 n_0$), and $\text{Kn} = l_0 / L_0$ the Knudsen number. The symbols n_i and t_i denote, respectively, the unit normal vector (pointing into the gases) and a unit tangential vector to the boundary; T_w and v_{wi} are the temperature and velocity of the boundary ($v_{wi} n_i = 0$), respectively; and n_w^A and $p_w^A (= kn_w^A T_w)$ are the saturation number density and pressure of the vapor at temperature T_w , respectively. Assumption (viii) requires that $v_{wi} / (2kT_0 / m_0)^{1/2}$ is of the order of Kn. The Greek letter α is used to express the labels “A” and “B” of the component gases (α component, n^α , T^α , etc.).

We now introduce the following dimensionless quantities:

$$\begin{aligned}
 x_i &= X_i / L_0, & \hat{m}^\alpha &= m^\alpha / m_0, \\
 \hat{d}^\alpha &= d^\alpha / d_0, & \hat{n}^\alpha &= n^\alpha / n_0, \\
 \hat{p}^\alpha &= p^\alpha / p_0, & \hat{v}_i^\alpha &= v_i^\alpha / (2kT_0 / m_0)^{1/2}, \\
 \hat{n} &= n / n_0, & \hat{\rho} &= \rho / \rho_0, & \hat{p} &= p / p_0,
 \end{aligned} \tag{1}$$

$$\hat{v}_i = v_i / (2kT_0/m_0)^{1/2}, \quad \hat{T} = T/T_0,$$

$$\hat{T}_w = T_w/T_0, \quad \hat{v}_{wi} = v_{wi} / (2kT_0/m_0)^{1/2},$$

$$\hat{n}_w^A = n_w^A/n_0, \quad \hat{p}_w^A = p_w^A/p_0,$$

where $\hat{v}_{wi}$ is a quantity of the order of Kn. Thus, $\hat{p} = \hat{n}\hat{T}$ and $\hat{p}_w^A = \hat{n}_w^A \hat{T}_w$ hold.

A. Fluid-dynamic-type equations

According to Ref. 16, the physical quantities are expanded in power series of a small parameter $\epsilon = (\sqrt{\pi}/2)\text{Kn}$. To be more specific, let h stand for any of $\hat{n}^\alpha$, $\hat{p}^\alpha$, $\hat{v}_i^\alpha$ ($\alpha=A,B$), $\hat{n}$, $\hat{p}$, $\hat{p}$, $\hat{v}_i$, and $\hat{T}$, then

$$h = h_{(0)} + h_{(1)}\epsilon + h_{(2)}\epsilon^2 + \dots, \quad (2)$$

where

$$\hat{v}_{i(0)}^\alpha = \hat{v}_{i(0)} \equiv 0. \quad (3)$$

It should be noted that the expansion for the velocities $\hat{v}_i^\alpha$ and $\hat{v}_i$ starts from the first order, which is the difference between the present expansion and the classical Hilbert expansion. The coefficients $h_{(0)}$, $h_{(1)}$, ... are governed by the fluid-dynamic-type equations.

The equations for the first two terms of the expansion for $\hat{p}$ are simply

$$\frac{\partial \hat{p}_{(0)}}{\partial x_i} = 0, \quad \frac{\partial \hat{p}_{(1)}}{\partial x_i} = 0. \quad (4)$$

The constants $\hat{p}_{(0)}$ and $\hat{p}_{(1)}$ are to be determined from conditions proper to each problem.

The first nontrivial set of the fluid-dynamic-type equations are as follows:

$$\frac{\partial}{\partial x_j} (\hat{n}_{(0)}^A \hat{v}_{j(1)}^A) = 0, \quad (5a)$$

$$\frac{\partial}{\partial x_j} (\hat{n}_{(0)}^B \hat{v}_{j(1)}^B) = 0, \quad (5b)$$

$$\begin{aligned} 2\hat{p}_{(0)}\hat{v}_{j(1)}\frac{\partial \hat{v}_{i(1)}}{\partial x_j} = & -\frac{\partial \hat{p}_{(2)}}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\hat{\mu} \hat{T}_{(0)}^{1/2} \frac{\partial \hat{v}_{i(1)}}{\partial x_j} \right) - \frac{\partial}{\partial x_j} \left(\frac{\hat{Y}_1}{\hat{p}_{(0)}} \frac{\partial \hat{T}_{(0)}}{\partial x_i} \frac{\partial \hat{T}_{(0)}}{\partial x_j} \right) - \frac{\partial}{\partial x_j} \left[\frac{1}{\hat{n}_{(0)}} \frac{\partial}{\partial x_j} \left(\hat{Y}_2 \frac{\partial \hat{T}_{(0)}}{\partial x_i} \right) \right] \\ & - \frac{\partial}{\partial x_j} \left(\frac{\hat{Y}_4}{\hat{n}_{(0)}} \frac{\partial X^A}{\partial x_j} \frac{\partial \hat{T}_{(0)}}{\partial x_i} \right) - \frac{\partial}{\partial x_j} \left[\frac{\hat{T}_{(0)}}{\hat{n}_{(0)}} \frac{\partial}{\partial x_j} \left(\hat{Y}_5 \frac{\partial X^A}{\partial x_i} \right) \right], \end{aligned} \quad (5c)$$

$$\begin{aligned} \frac{\partial}{\partial x_j} \left(\hat{\lambda} \hat{T}_{(0)}^{1/2} \frac{\partial \hat{T}_{(0)}}{\partial x_j} \right) - \frac{\partial}{\partial x_j} [k_T \hat{p}_{(0)} (\hat{v}_{j(1)}^A - \hat{v}_{j(1)}^B)] \\ - \frac{5}{2} (\hat{n}_{(0)}^A \hat{v}_{j(1)}^A + \hat{n}_{(0)}^B \hat{v}_{j(1)}^B) \frac{\partial \hat{T}_{(0)}}{\partial x_j} = 0, \end{aligned} \quad (5d)$$

$$\hat{v}_{i(1)}^A - \hat{v}_{i(1)}^B = -\frac{\hat{T}_{(0)}^{1/2}}{\hat{n}_{(0)}} \frac{\hat{D}_{AB}}{X^A X^B} \left(\frac{\partial X^A}{\partial x_i} + k_T \frac{\partial \ln \hat{T}_{(0)}}{\partial x_i} \right), \quad (5e)$$

where

$$\hat{n}_{(0)} = \hat{n}_{(0)}^A + \hat{n}_{(0)}^B, \quad (6a)$$

$$\hat{p}_{(0)} = \hat{m}^A \hat{n}_{(0)}^A + \hat{m}^B \hat{n}_{(0)}^B, \quad (6b)$$

$$\hat{v}_{i(1)} = (\hat{m}^A \hat{n}_{(0)}^A \hat{v}_{i(1)}^A + \hat{m}^B \hat{n}_{(0)}^B \hat{v}_{i(1)}^B) / \hat{p}_{(0)}, \quad (6c)$$

$$\hat{p}_{(0)} = \hat{n}_{(0)} \hat{T}_{(0)}, \quad (6d)$$

$$X^\alpha = \hat{n}_{(0)}^\alpha / \hat{n}_{(0)}, \quad (6e)$$

$$\overline{A_{ij}} = A_{ij} + A_{ji} - (2/3) A_{kk} \delta_{ij}. \quad (6f)$$

Here, X^α is the local concentration of the α component in the zeroth-order ($X^A + X^B = 1$). The coefficients $\hat{\mu}$, $\hat{\lambda}$, $\hat{D}_{AB}$, k_T , $\hat{Y}_1$, $\hat{Y}_2$, $\hat{Y}_3$, $\hat{Y}_4$, and $\hat{Y}_5$ (transport coefficients, for short), which depend on $\hat{m}^\alpha$ and $\hat{d}^\alpha$, are functions of the local concentration X^A . The $\hat{\mu}$, $\hat{\lambda}$, and $\hat{D}_{AB}$ correspond to the viscosity μ , thermal conductivity λ , and mutual-diffusion coefficient D_{AB} , respectively; more specifically, they are related as $\mu = (\sqrt{\pi}/2)(2kT_0/m_0)^{-1/2} p_0 l_0 \hat{T}_{(0)}^{1/2} \hat{\mu}$, $\lambda = (\sqrt{\pi}k/m_0)(2kT_0/m_0)^{-1/2} p_0 l_0 \hat{T}_{(0)}^{1/2} \hat{\lambda}$, and $D_{AB} = (\sqrt{\pi}/2) \times (2kT_0/m_0)^{1/2} l_0 (\hat{T}_{(0)}^{1/2} / \hat{n}_{(0)}) \hat{D}_{AB}$. The k_T is the thermal-diffusion ratio, i.e., the ratio of the thermal-diffusion coefficient to the mutual-diffusion coefficient. The definitions of these transport coefficients are given in Appendix A.

Equations (5a)–(5e), with the help of Eqs. (6a)–(6e), form a closed set of equations for $\hat{n}_{(0)}^A$, $\hat{n}_{(0)}^B$, $\hat{n}_{(0)}$, X^A , X^B , $\hat{p}_{(0)}$, $\hat{T}_{(0)}$, $\hat{v}_{i(1)}^A$, $\hat{v}_{i(1)}^B$, $\hat{v}_{i(1)}$, and $\hat{p}_{(2)}$, which can finally be reduced to a set of partial differential equations for $\hat{n}_{(0)}^A$ (or X^A), $\hat{T}_{(0)}$, $\hat{v}_{i(1)}$, and $\hat{p}_{(2)}$. The partial pressure $\hat{p}_{(0)}^\alpha$ of each component is then given by

$$\hat{p}_{(0)}^\alpha = \hat{n}_{(0)}^\alpha \hat{T}_{(0)}. \quad (7)$$

It should be remarked here that the functional forms of the transport coefficients $\hat{\mu}$, $\hat{\lambda}$, $\hat{D}_{AB}$, k_T , $\hat{Y}_1$, $\hat{Y}_2$, $\hat{Y}_3$, $\hat{Y}_4$, and $\hat{Y}_5$, as functions of the local concentration X^A of the vapor, cannot be obtained explicitly. However, for application of Eqs. (5a)–(5e) to practical problems, the functional forms are indispensable. Therefore, in Ref. 24, the functional forms were obtained numerically, and their database was constructed. By making use of the database, Eqs. (5a)–(5e) become applicable to concrete problems at least at the numerical level.

It should be mentioned that equations similar to Eqs. (5a)–(5e) had been derived from the so-called Burnett equations for a mixture of noncondensable gases in a more intuitive way in Ref. 23, where convection is shown to be induced by the imbalance of the concentration stress.

B. Boundary conditions

The boundary conditions on the surface of the condensed phase for the fluid-dynamic-type equations (5a)–(5e) are obtained by analyzing the Knudsen layer, the thin layer of thickness of the order of the mean free path adjacent to the surface. The boundary conditions taken from Ref. 16 are summarized as follows:

$$\hat{n}_{(0)}^A = \hat{n}_w^A (= \hat{p}_w^A / \hat{T}_w), \quad (8a)$$

$$\hat{T}_{(0)} = \hat{T}_w, \quad (8b)$$

$$\hat{v}_{i(1)}^B n_i = 0, \quad (8c)$$

$$(\hat{v}_{i(1)} - \hat{U}_i) t_i = -\hat{T}_{(0)}^{1/2} \left(b_7 \frac{1}{\hat{p}_{(0)}} \frac{\partial \hat{T}_{(0)}}{\partial x_i} t_i + b_9 \frac{1}{\hat{n}_{(0)}} \frac{\partial X^A}{\partial x_i} t_i \right). \quad (8d)$$

Here, the velocity of the boundary $\hat{v}_{wi}$ has been written as

$$\hat{v}_{wi} = \hat{U}_i \epsilon, \quad (9)$$

with $\hat{U}_i$ being of $O(1)$, and b_7 and b_9 , which depend on $\hat{m}^\alpha$ and $\hat{\lambda}^\alpha$, are functions of the local concentration X^A of the vapor. The term containing b_7 in Eq. (8d) indicates the velocity slip due to the temperature variation along the boundary (the thermal slip or thermal creep), whereas the term containing b_9 the velocity slip due to the variation of the local concentration of the vapor along the boundary (the diffusion slip). The b_7 (thermal-slip coefficient) and b_9 (diffusion-slip coefficient) were obtained by the analysis of the two fundamental half-space problems of the linearized Boltzmann equation.²⁵ Note that (b_7, b_9) (here and in Ref. 16) $= (-b_I, -b_{II})$ (Ref. 25). In this reference, a database from which accurate values of b_7 and b_9 can be obtained instantaneously for a given X^A is constructed. The details are summarized in Appendix B.

The thermal slip is a classical phenomenon in kinetic theory^{31,32} and has been investigated by many authors. Here, we only refer to a few papers that seem to be of some

importance out of many existing works: Refs. 21 and 32–37 for a single-component gas and Refs. 25 and 38–42 for a gaseous mixture. The diffusion slip, which is peculiar to a gaseous mixture, is also a classical problem, about which we refer to Refs. 25, 38, 40, and 42–46.

C. Remarks on continuum limit

In this subsection, we give a short remark on the continuum limit where Kn or ϵ vanishes. In this limit, the macroscopic variables $\hat{n}^A$, $\hat{n}^B$, $\hat{n}$, $\hat{T}$, $\hat{v}_i^A$, $\hat{v}_i^B$, $\hat{v}_i$, $\hat{p}$, etc., reduce to their respective leading-order terms in the expansion (2); for instance, $(\hat{n}^A, \hat{n}^B, \hat{T}, \hat{p}) \rightarrow (\hat{n}_{(0)}^A, \hat{n}_{(0)}^B, \hat{T}_{(0)}, \hat{p}_{(0)})$ and $(\hat{v}_i^A, \hat{v}_i^B, \hat{v}_i) \rightarrow (0, 0, 0)$ [cf. Eq. (3)]. That is, in this limit, the flow velocity vanishes, and thus evaporation and condensation of the vapor stop. Therefore, one might expect that the temperature field in this limit is given by the steady heat-conduction equation (for a binary mixture) with the no-jump boundary condition, which is considered to describe the temperature field in a stationary gas in the continuum limit. However, this is not the case. The leading-order terms $\hat{n}_{(0)}^A$, $\hat{n}_{(0)}^B$, and $\hat{T}_{(0)}$ are determined together with the first-order velocity fields $\hat{v}_{i(1)}^A$ and $\hat{v}_{i(1)}^B$ (and $\hat{v}_{i(1)}$) by the fluid-dynamic-type system described in Secs. III A and III B, which is different from the heat-conduction equation. An example demonstrating this discrepancy will be shown in Fig. 9(d) in Sec. V B. This means that, in spite of the fact that there is no flow, the temperature and density fields in the continuum limit are affected by the infinitesimal flow [note that $\hat{v}_i^\alpha = \hat{v}_{i(1)}^\alpha \epsilon + \dots \rightarrow 0$, but $\hat{v}_{i(1)}^\alpha$ is of $O(1)$]. This is an example of the *ghost effect*.¹⁹ Since this effect has been discussed in many places, we avoid repeating the discussion, referring to the literature, such as Refs. 20, 21, 5, 47, 48, and 6, and the references in Refs. 5 and 6 (for a gas mixture, see Refs. 15, 16, 49, and 50). We just mention that the ghost effect associated with the present fluid-dynamic-type system is discussed in detail in Ref. 16.

IV. NUMERICAL METHOD

A. Preliminaries

We first rewrite the fluid-dynamic-type equations in a different form that is more convenient for our numerical method.

The continuity equation for each component can be combined to obtain a continuity equation for the barycentric velocity merely by using the definition of $\hat{\rho}_{(0)}$,

$$\frac{\partial}{\partial x_i} (\hat{\rho}_{(0)} \hat{v}_{i(1)}) = 0. \quad (10)$$

Using the definition of the barycentric velocity and Eq. (5e), we can write each velocity component as

$$\hat{v}_{i(1)}^A = \hat{v}_{i(1)} - \frac{\hat{m}^B \hat{D}_{AB} \hat{T}_{(0)}^{1/2}}{\hat{\rho}_{(0)} X^A} \left(\frac{\partial X^A}{\partial x_i} + \frac{k_T}{\hat{T}_{(0)}} \frac{\partial \hat{T}_{(0)}}{\partial x_i} \right), \quad (11a)$$

$$\hat{v}_{i(1)}^B = \hat{v}_{i(1)} + \frac{\hat{m}^A \hat{D}_{AB} \hat{T}_{(0)}^{1/2}}{\hat{\rho}_{(0)} (1 - X^A)} \left(\frac{\partial X^A}{\partial x_i} + \frac{k_T}{\hat{T}_{(0)}} \frac{\partial \hat{T}_{(0)}}{\partial x_i} \right). \quad (11b)$$

With expression (11a), the vapor continuity equation (5a) can be rewritten as

$$\begin{aligned} & \frac{\partial}{\partial x_i} \left(\frac{\hat{\rho}_{(0)}}{\hat{T}_{(0)}} \hat{v}_{i(1)} X^A \right) \\ &= \frac{\partial}{\partial x_i} \left[\frac{\hat{D}_{AB} \hat{T}_{(0)}^{1/2}}{(\hat{m}^A/\hat{m}^B - 1)X^A + 1} \left(\frac{\partial X^A}{\partial x_i} + \frac{k_T}{\hat{T}_{(0)}} \frac{\partial \hat{T}_{(0)}}{\partial x_i} \right) \right]. \end{aligned} \quad (12)$$

Similarly, the energy equation (5d) can be rewritten as

$$\begin{aligned} & \frac{\partial}{\partial x_i} \left(\frac{5 \hat{\rho}_{(0)}}{2 \hat{T}_{(0)}} \hat{v}_{i(1)} \hat{T}_{(0)} \right) \\ &= \frac{\partial}{\partial x_i} \left[\hat{\lambda} \hat{T}_{(0)}^{1/2} \frac{\partial \hat{T}_{(0)}}{\partial x_i} \right] \\ & - \frac{\partial}{\partial x_i} \left[\gamma \hat{T}_{(0)}^{3/2} \left(\frac{\partial X^A}{\partial x_i} + \frac{k_T}{\hat{T}_{(0)}} \frac{\partial \hat{T}_{(0)}}{\partial x_i} \right) \right], \end{aligned} \quad (13)$$

where an additional coefficient γ has been defined, related to the other coefficients as

$$\gamma \equiv \hat{D}_{AB} \left[\frac{5}{2} \frac{\hat{m}^A/\hat{m}^B - 1}{(\hat{m}^A/\hat{m}^B - 1)X^A + 1} - \frac{k_T}{X^A(1 - X^A)} \right]. \quad (14)$$

Like the other coefficients, it depends only on the molecular properties $\hat{m}^\alpha$ and $\hat{d}^\alpha$ and the local concentration X^A . Note that the definition of k_T is such that γ retains a finite value even when the gas concentration of either component approaches zero.

The equation of motion (5c) can be rewritten as (see Sec. 5.3 in Ref. 21)

$$\begin{aligned} \frac{\partial}{\partial x_j} (\hat{\rho}_{(0)} \hat{v}_{j(1)} \hat{v}_{i(1)}) &= -\frac{1}{2} \frac{\partial \hat{p}_{(2)}^\dagger}{\partial x_i} + \frac{1}{2} \frac{\partial}{\partial x_j} \left[\hat{\mu} \hat{T}_{(0)}^{1/2} \frac{\partial \hat{v}_{i(1)}}{\partial x_j} \right] + \frac{1}{2} \frac{\partial}{\partial x_j} \left[\hat{\mu} \hat{T}_{(0)}^{1/2} \frac{\partial \hat{v}_{j(1)}}{\partial x_i} \right] - \frac{1}{3} \frac{\partial}{\partial x_i} \left[\hat{\mu} \hat{T}_{(0)}^{1/2} \frac{\partial \hat{v}_{j(1)}}{\partial x_j} \right] \\ &+ \frac{1}{2} \frac{\partial}{\partial x_j} \left[2 \frac{\hat{Y}_1 - \hat{Y}_2}{\hat{\rho}_{(0)}} \frac{\partial \hat{T}_{(0)}}{\partial x_i} \frac{\partial \hat{T}_{(0)}}{\partial x_j} + 2 \hat{Y}_3 \frac{\hat{T}_{(0)}^2}{\hat{\rho}_{(0)}} \frac{\partial X^A}{\partial x_i} \frac{\partial X^A}{\partial x_j} + \frac{\hat{T}_{(0)}}{\hat{\rho}_{(0)}} \left(\hat{Y}_4 + \frac{d\hat{Y}_2}{dX^A} - 4\hat{Y}_5 \right) \frac{\partial X^A}{\partial x_j} \frac{\partial \hat{T}_{(0)}}{\partial x_i} \right. \\ &\left. + \frac{\hat{T}_{(0)}}{\hat{\rho}_{(0)}} \left(\hat{Y}_4 - \frac{d\hat{Y}_2}{dX^A} \right) \frac{\partial X^A}{\partial x_i} \frac{\partial \hat{T}_{(0)}}{\partial x_j} \right], \end{aligned} \quad (15)$$

by using the chain rule to expand the derivatives, and defining a modified pressure $\hat{p}_{(2)}^\dagger$:

$$\begin{aligned} \hat{p}_{(2)}^\dagger &\equiv \hat{p}_{(2)} + \frac{2}{3} \frac{\hat{Y}_1}{\hat{\rho}_{(0)}} \left(\frac{\partial \hat{T}_{(0)}}{\partial x_j} \right)^2 - \frac{4}{3} \frac{\hat{T}_{(0)}}{\hat{\rho}_{(0)}} \frac{\partial}{\partial x_j} \left(\hat{Y}_2 \frac{\partial \hat{T}_{(0)}}{\partial x_j} \right) \\ &- \frac{2\hat{Y}_2}{\hat{\rho}_{(0)}} \left(\frac{\partial \hat{T}_{(0)}}{\partial x_j} \right)^2 + \frac{2}{3} \hat{Y}_3 \frac{\hat{T}_{(0)}^2}{\hat{\rho}_{(0)}} \left(\frac{\partial X^A}{\partial x_j} \right)^2 \\ &+ \frac{2}{3} \hat{Y}_4 \frac{\hat{T}_{(0)}}{\hat{\rho}_{(0)}} \frac{\partial \hat{T}_{(0)}}{\partial x_j} \frac{\partial X^A}{\partial x_j} - \frac{4}{3} \frac{\hat{T}_{(0)}^2}{\hat{\rho}_{(0)}} \frac{\partial}{\partial x_j} \left(\hat{Y}_5 \frac{\partial X^A}{\partial x_j} \right) \\ &- \frac{4\hat{T}_{(0)}\hat{Y}_5}{\hat{\rho}_{(0)}} \frac{\partial \hat{T}_{(0)}}{\partial x_j} \frac{\partial X^A}{\partial x_j}. \end{aligned} \quad (16)$$

That is, the terms of gradient form arising from the non-Navier-Stokes terms are put inside $\hat{p}_{(2)}^\dagger$. By introducing the modified pressure, the apparent third-order derivatives of $\hat{T}_{(0)}$ and X^A in Eq. (5c) are eliminated, and the number of deriva-

tive terms to be approximated numerically is reduced.

In summary, we are going to solve, instead of Eqs. (5a)–(5e), the equation system (10), (12), (13), and (15), the unknowns of which are $\hat{v}_{i(1)}$, $\hat{T}_{(0)}$, X^A , and $\hat{p}_{(2)}^\dagger$. The variable $\hat{\rho}_{(0)}$ is not counted among the unknowns since it depends on X^A and $\hat{T}_{(0)}$ as

$$\hat{\rho}_{(0)} = \frac{\hat{\rho}_{(0)}}{\hat{T}_{(0)}} [(\hat{m}^A - \hat{m}^B)X^A + \hat{m}^B]. \quad (17)$$

Nevertheless, it is retained in the equations to keep the resemblance to the equations of conventional gas dynamics.

B. Finite-volume method

Let us note that Eqs. (12), (13), and (15) can be expressed in the following concise form:

$$\frac{\partial}{\partial x_j}(M_j \phi) = \frac{\partial}{\partial x_j} \left(\Gamma \frac{\partial \phi}{\partial x_j} \right) + b, \quad (18)$$

where ϕ stands for X^A , $\hat{T}_{(0)}$, or the individual components of $\hat{v}_{i(1)}$, and M_i , Γ , and b , in general, depend on X^A , $\hat{T}_{(0)}$, and $\hat{v}_{i(1)}$ [and $\hat{p}_{(2)}^\dagger$ in Eq. (15)]. To be more specific,

$$\phi = X^A, \quad M_j = (\hat{p}_{(0)}/\hat{T}_{(0)})\hat{v}_{j(1)}, \quad (19)$$

$$\Gamma = \hat{D}_{AB} \hat{T}_{(0)}^{1/2} [(\hat{m}^A/\hat{m}^B - 1)X^A + 1]^{-1},$$

for Eq. (12),

$$\phi = \hat{T}_{(0)}, \quad M_j = (5/2)(\hat{p}_{(0)}/\hat{T}_{(0)})\hat{v}_{j(1)}, \quad (20)$$

$$\Gamma = \hat{\lambda} \hat{T}_{(0)}^{1/2},$$

for Eq. (13), and

$$\phi = \hat{v}_{i(1)}, \quad M_j = \hat{p}_{(0)}\hat{v}_{j(1)}, \quad (21)$$

$$\Gamma = (1/2)\hat{\mu}\hat{T}_{(0)}^{1/2},$$

for Eq. (15); b 's are the rest of the terms in the respective equations.

We try to solve Eq. (18) using the iteration scheme

$$\frac{\partial}{\partial x_j}(M_j^{m-1} \phi^m) = \frac{\partial}{\partial x_j} \left(\Gamma^{m-1} \frac{\partial \phi^m}{\partial x_j} \right) + b^{m-1}, \quad (22)$$

under the boundary conditions (8) with appropriate discretization. Here, ϕ^m denotes ϕ at the m th iteration, and M_j^{m-1} , Γ^{m-1} , and b^{m-1} mean M_j , Γ , and b evaluated by using X^A , $\hat{T}_{(0)}$, $\hat{v}_{i(1)}$, and $\hat{p}_{(2)}^\dagger$ at the $(m-1)$ th iteration. More specifically, we construct a sequence $\{\phi^1, \phi^2, \dots\}$, which is expected to converge, on the basis of Eq. (22) with an appropriate initial function ϕ^0 and regard the limit (i.e., ϕ^m with a sufficiently large m) as an approximate solution of Eq. (18). Note that Eq. (22) is linear in each step in the iteration process. Also note that to ensure the stability and fast convergence, the change in each variable in one iteration should be limited. In the actual computation, we use the under-relaxation technique to limit the change. That is, if ϕ^m is obtained from Eq. (22), $\phi^m + \beta_\phi(\phi^{m-1} - \phi^m)$, rather than ϕ^m itself is used for the next step of iteration [i.e., Eq. (22) with $m=m+1$]. The optimum under-relaxation factors β_ϕ are problem dependent. Not using under-relaxation may slow or prevent convergence.

The computational domain is divided into a number of small control volumes. Let us consider a single control volume Ω with boundary $\partial\Omega$. If we integrate Eq. (22) over this control volume, we obtain, after application of Gauss' theorem,

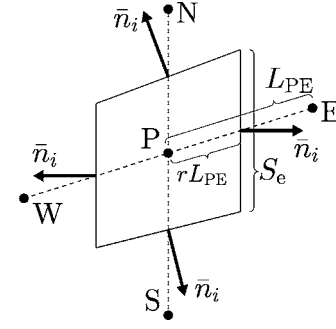


FIG. 1. A control volume.

$$\int_{\partial\Omega} \bar{n}_j M_j^{m-1} \phi^m dS = \int_{\partial\Omega} \bar{n}_j \Gamma^{m-1} \frac{\partial \phi^m}{\partial x_j} dS + \int_{\Omega} b^{m-1} dV, \quad (23)$$

where $\bar{n}_i$ is the outward unit normal vector to the surface $\partial\Omega$, dS is the surface element on $\partial\Omega$ in the dimensionless x_i space, and dV is the volume element in the same space. For simplicity, we explain the discretization of Eq. (23) in the case of two-dimensional problems (i.e., the problems where the physical quantities are independent of x_3 and $\hat{v}_{3(1)}=0$). The generalization to three-dimensional problems is straightforward.

We consider a two-dimensional control volume Ω (with boundary $\partial\Omega$), which is assumed to be a quadrilateral, as depicted in Fig. 1. The center (barycenter) of this control volume is denoted by “P,” and the centers of the neighboring control volumes are denoted by “E,” “W,” “N,” and “S.” The physical quantities are stored at the grid points located at the centers of the control volumes.

To save space, the method of discretization for the surface integrals in Eq. (23) will be described only for the cell face $\partial\Omega_e$ between points P and E, but it is done analogously for other cell faces. We denote by L_{PE} the distance between grid points P and E and by S_e the area (the length times the unit width in the x_3 direction) of the surface $\partial\Omega_e$.

We first consider the first term on the right-hand side of Eq. (23). In the case of a Cartesian grid, the term $\bar{n}_j(\partial\phi^m/\partial x_j)$ can be approximated by a finite difference using the values of ϕ^m at the nodes E and P. On a non-Cartesian grid, however, since the normal vector at the cell surface does not in general coincide with the line connecting E and P, we need to incorporate the values of ϕ^m at other nodes to approximate the derivative $\bar{n}_j(\partial\phi^m/\partial x_j)$. On the other hand, we wish to avoid using more node values than necessary for this approximation. This can be achieved by the deferred correction approach suggested by Muzaferija.⁵³ That is, if ξ_i is the unit vector pointing from node P to node E, then the term under consideration on $\partial\Omega_e$ is approximated as

$$\int_{\partial\Omega_e} \bar{n}_j \Gamma^{m-1} \frac{\partial \phi^m}{\partial x_j} dS = S_e \Gamma_e^{m-1} \frac{\phi_E^m - \phi_P^m}{L_{PE}} + S_e \Gamma_e^{m-1} (\bar{n}_j - \xi_j) \times \left(\frac{\partial \phi^{m-1}}{\partial x_j} \right)_e, \quad (24)$$

where ϕ_P^m and ϕ_E^m are the values of ϕ^m at node points P and

E, and the subscript “e” means that the stored value has been interpolated to the cell surface at its intersection with the line PE. The point here is that the correction term required when $\bar{n}_i \neq \xi_i$ is evaluated using the value of $(\partial \phi^{m-1} / \partial x_j)_e$ at the $(m-1)$ th iteration. The term $(\partial \phi^{m-1} / \partial x_j)_e$ on the surface $\partial \Omega_e$ is obtained by interpolation using the corresponding gradient terms at cell centers. The latter terms are computed by taking the average over the control volume, with the integral rewritten using Gauss’ theorem so that it can be expressed through grid point values interpolated to cell surfaces. For example, in the x_1 direction, we obtain

$$\left(\frac{\partial \phi^{m-1}}{\partial x_1} \right)_P = \frac{1}{\Delta \Omega} \int_{\Omega} \frac{\partial}{\partial x_j} \phi^{m-1} \delta_{1j} d\Omega = \frac{1}{\Delta \Omega} \int_{\partial \Omega} \phi^{m-1} \bar{n}_1 dS. \quad (25)$$

Here, $\Delta \Omega$ is the cell volume (the area times the unit width in the x_3 direction in the present two-dimensional case).

Although technically the approximation equation (24) is of only first-order accuracy on a nonuniform grid (and non-uniformness is required because high accuracy demands smaller cells in some parts of the computational domain, e.g., in the vicinity of walls), the approximation is asymptotically of second order, as demonstrated in Ref. 26.

The left-hand side of Eq. (23) on $\partial \Omega_e$ is discretized through linear interpolation

$$\int_{\partial \Omega_e} \bar{n}_j M_j^{m-1} \phi^m dS = S_e M_e^{m-1} [r \phi_E^m + (1-r) \phi_P^m], \quad (26)$$

where r is a parameter associated with the nonuniformity of the grid ($0 < r < 1$; $r=0.5$ for a uniform grid; see Fig. 1), and M_e^{m-1} indicates $\bar{n}_j M_j^{m-1}$ at the point where the line between nodes P and E crosses the cell surface.

On the other hand, the source term (the second term on the right-hand side) in Eq. (23) is approximated by taking the values at the grid point multiplied by the cell volume, i.e.,

$$\int_{\Omega} b^{m-1} dV = \Delta \Omega b_P^{m-1}. \quad (27)$$

After the discretization described above, Eq. (23) can be written in the form

$$a_P^{m-1} \phi_P^m = (a_E^{m-1} \phi_E^m + a_W^{m-1} \phi_W^m + a_N^{m-1} \phi_N^m + a_S^{m-1} \phi_S^m) + B^{m-1}, \quad (28)$$

where each of the coefficients a_P^{m-1} , a_E^{m-1} , a_W^{m-1} , a_N^{m-1} , and a_S^{m-1} , and the source term B^{m-1} are evaluated by the use of the values of the physical quantities at the previous step $[(m-1)$ th step] at the nodes {P, E, W, N, S}. Equation (28) is also valid at boundary control volumes if the coefficients $a_E^{m-1}, \dots, a_S^{m-1}$ that correspond to boundary nodes are set to be zero, and the boundary conditions are implemented by incorporating them in B^{m-1} (the treatment of the boundary condition will be discussed in Sec. IV C). Thus the linear system of equations obtained by writing Eq. (28) for each control volume is closed and can be solved by standard numerical methods. In this way, a discretized solution ϕ^m for the m th step is obtained.

So far we have described how to construct the m th approximation of X^A , $\hat{T}_{(0)}$, and $\hat{v}_{i(1)}$ from their $(m-1)$ th approximation using Eqs. (12), (13), and (15). Now we must also deal with the modified pressure $\hat{p}_{(2)}^\dagger$. However, there is no equation dominated by $\hat{p}_{(2)}^\dagger$; in fact, the only occurrence of $\hat{p}_{(2)}^\dagger$ is in the form of a gradient in the momentum equation (15). This is a feature that the fluid-dynamic-type equations in this paper share with the incompressible Navier-Stokes equation, so it is suitable to attempt similar solution techniques. A well-known method is the SIMPLE algorithm.^{26,51,52} In its original formulation,⁵¹ it was described for a staggered grid; i.e., flow velocities were stored at cell surfaces rather than cell centers. For complicated geometries, however, it is more suitable to use a co-located grid, i.e., a grid system where all variables are stored at cell centers. A description of how to construct a solution method for a co-located grid in the case of the incompressible Navier-Stokes equation is found in Ref. 26.

The main idea is to use the continuity equation (10) to derive an equation from which an updated value of $\hat{p}_{(2)}^\dagger$ can be obtained. We assume that from the previous step in the iterative process we already have a velocity field $\hat{v}_{i(1)}^{m-1}$ satisfying continuity, and a corresponding modified pressure field $\hat{p}_{(2)}^{\dagger m-1}$. Using these values to calculate the relevant coefficients and solving the linear algebraic system [Eq. (28) with P running all nodes], we obtain a velocity field $\hat{v}_{i(1)}^*$ that cannot be expected to satisfy continuity. Therefore, we introduce corrections $\hat{p}_{(2)}^{\dagger'}$ and $\hat{v}_{i(1)}'$, and set

$$\hat{p}_{(2)}^{\dagger m} = \hat{p}_{(2)}^{\dagger m-1} + \hat{p}_{(2)}^{\dagger'}, \quad (29a)$$

$$\hat{v}_{i(1)}^m = \hat{v}_{i(1)}^* + \hat{v}_{i(1)}'. \quad (29b)$$

We then assume that Eq. (10) is satisfied with $\hat{p}_{(0)} = \hat{p}_{(0)}^{m-1}$ $[(m-1)$ th approximation of $\hat{p}_{(0)}]$ and $\hat{v}_{i(1)} = \hat{v}_{i(1)}^m$ and integrate it over a control volume to obtain

$$\int_{\partial \Omega} \bar{n}_j \hat{p}_{(0)}^{m-1} \hat{v}_{j(1)}^m dS = 0. \quad (30)$$

If we assume that there is a relation between the velocity correction and the pressure correction, for example, of the form

$$\hat{v}_{i(1)}' = c \frac{\partial \hat{p}_{(2)}^{\dagger'}}{\partial x_i}, \quad (31)$$

we then have, from Eqs. (29b) and (30),

$$\int_{\partial \Omega} \bar{n}_j \hat{p}_{(0)}^{m-1} \hat{v}_{j(1)}^* dS + c \int_{\partial \Omega} \bar{n}_j \hat{p}_{(0)}^{m-1} \frac{\partial \hat{p}_{(2)}^{\dagger'}}{\partial x_j} dS = 0. \quad (32)$$

This relation, which is similar to Eq. (23), leads to a linear algebraic system for the values of $\hat{p}_{(2)}^{\dagger'}$ at the grid points. However, the matrix for the resulting algebraic system is symmetric, and in addition it should be solved with high accuracy in each iteration to ensure convergence, so that in actual implementation it might be more appropriate to use a different solver for the linear algebraic system.

There is some freedom to choose a suitable relation (31) because for the converged solution the corrections should all go to zero. However, since we also want the velocity field to satisfy the conservation of momentum, a reasonable choice could be a relation based on the momentum equation. If we insert Eqs. (29a) and (29b) into the discretized momentum equation, Eq. (28) with $\phi = \hat{v}_{i(1)}$, and neglect the influence of the velocity corrections at the neighboring nodes, we then have the relation

$$\hat{v}'_{i(1)} = - \frac{\Delta\Omega}{2a_p^{m-1}(\hat{v}_{k(1)})} \frac{\partial \hat{p}'_{(2)}}{\partial x_i}, \quad (33)$$

where $a_p^{m-1}(\hat{v}_k)$ indicates a_p^{m-1} [see Eq. (28)] when $\phi = \hat{v}_k$. Note that a_p^{m-1} should be equal for $\hat{v}_{1(1)}$ and $\hat{v}_{2(1)}$ for computational efficiency. In particular, this should be kept in mind in implementation of the boundary conditions. Equation (33) is known as the SIMPLE approximation. In the present study, we use Eq. (33) as the relation (31).

Ideally, the same discretization of the pressure gradient term should be used in both the momentum equation (15) and the pressure correction equation (32). Unfortunately, doing this on a co-located grid gives rise to oscillations in the pressure field. To avoid these oscillations, we adopt the pressure-velocity coupling of Rhie and Chow.⁵⁴ The details are omitted here (see Ref. 26).

C. Boundary conditions

The solution process described in Sec. IV B is performed under the boundary conditions (8). The boundary conditions for X^A , $\hat{T}_{(0)}$, and the tangential component of $\hat{v}_{i(1)}$ can be implemented straightforwardly from Eq. (8) after substituting $\hat{n}_{(0)} = \hat{p}_{(0)}/\hat{T}_{(0)}$ and $X^A = \hat{n}_{(0)}^A/\hat{n}_{(0)}$. For example, Eqs. (8a) and (8b) give the condition for X^A , i.e.,

$$X^A = \hat{p}_{(0)}^A/\hat{p}_{(0)}. \quad (34)$$

On the other hand, the boundary condition for the normal component of the barycentric velocity can be obtained from Eq. (8c) in combination with Eqs. (5e) and (6c):

$$n_i \hat{v}_{i(1)} = - \frac{\hat{m}^A \hat{D}_{AB} \hat{T}_{(0)}^{1/2}}{\hat{p}_{(0)}(1 - X^A)} n_i \left(\frac{\partial X^A}{\partial x_i} + \frac{k_T}{\hat{T}_{(0)}} \frac{\partial \hat{T}_{(0)}}{\partial x_i} \right). \quad (35)$$

When the mixture is confined in a closed domain V, it may be more natural to specify the average amount of the noncondensable gas inside the domain, rather than to specify the constant $\hat{p}_{(0)}$ directly. As the former quantity, we choose a dimensionless parameter n_{av}^B/n_0 , where n_{av}^B is the (dimensional) average number density of the noncondensable gas in the domain, which is expressed as

$$\frac{n_{av}^B}{n_0} = \frac{1}{V} \int_V \hat{n}_{(0)}^B dV, \quad (36)$$

with the condition $\int_V \hat{n}_{(m)}^B dV = 0$ ($m \geq 1$), where V is the volume of V in the x_i space. Then, $\hat{p}_{(0)}$ is expressed in the following form:

$$\hat{p}_{(0)} = \left(\int \frac{1}{\hat{T}_{(0)}} (1 - X^A) dV \right)^{-1} V \frac{n_{av}^B}{n_0}. \quad (37)$$

Therefore, $\hat{p}_{(0)}$ is computed as a part of the iterative process.

It should be noted that a factor $(1 - X^A)$ is contained in the denominator in Eq. (35). The expression is theoretically sound even in the case where the local concentration of noncondensable gas approaches zero, because the concentration gradient and the coefficient k_T both also go to zero in the limit. However, when the expression is discretized in the course of numerical analysis, the induced error could be large and cause divergence. This is more likely to occur for small values of n_{av}^B . In fact, if $\hat{p}_{(0)}$ is computed from Eq. (37) during the iteration process, it is quite possible that at some point $\hat{p}_{(0)} < \hat{p}_w^A$ which unphysically implies that $X^A > 1$. Although this will cause trouble for the boundary condition (35), the rest of the equations are not greatly affected, and will still converge towards a solution. If in the final solution $X^A \leq 1$ everywhere, we can overlook the fact that somewhere during the solution process there was an unphysical solution. It is therefore enough to find an alternate boundary condition for the normal flow velocity in the case where X^A is close to unity, for example by setting the boundary normal velocity so that the continuity equation is satisfied in the control volume next to the wall.

Furthermore, our treatment of pressure requires continuity to be satisfied globally in each iteration, and thus the normal velocity boundary condition must be consistent with continuity. The evaporation and condensation should balance each other exactly. In the general case it cannot be known beforehand exactly where on the boundary evaporation takes place and where condensation takes place. The part of the wall that has condensation can be identified by checking where the normal velocity is directed towards the wall. Integrating the normal velocity across this area, the total amount of condensation C_{tot} is obtained. In a similar way, the total amount of evaporation E_{tot} can be obtained. The normal velocity boundary value in the evaporating region is then multiplied by C_{tot}/E_{tot} everywhere to make the evaporation and condensation balance.

V. NUMERICAL EXAMPLES

In this section, we apply the fluid-dynamic-type system summarized in Sec. III to a specific problem.

A. Problem

Let us consider a slightly rarefied gas mixture of a vapor and a noncondensable gas, contained between two walls of sinusoidal shape, located at

$$X_2 = \pm (L_0/2) [1 - \hat{D} \sin(2\pi X_1/L_0)], \quad (38)$$

where $0 \leq \hat{D} < 1$ (Fig. 2). Both walls, consisting of the condensed phase of the vapor, have a common temperature T_w . We assume that the wall temperature T_w and the corresponding saturation number density n_w^A have the following sinusoidal distribution:

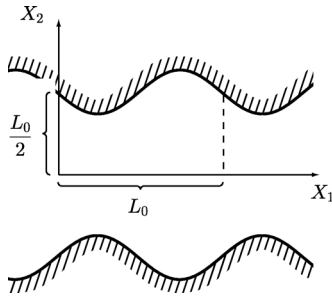


FIG. 2. Geometry.

$$T_w = T_0[1 - \hat{T}_c \cos(2\pi x_1/L_0)], \quad (39a)$$

$$n_w^A = n_0[1 - \hat{n}_c^A \cos(2\pi x_1/L_0)], \quad (39b)$$

where $0 \leq \hat{T}_c < 1$ and $0 \leq \hat{n}_c^A < 1$. In terms of the dimensionless variables, Eqs. (38), (39a), and (39b) become

$$x_2 = \pm (1/2)[1 - \hat{D} \sin(2\pi x_1)], \quad (40a)$$

$$\hat{T}_w = 1 - \hat{T}_c \cos(2\pi x_1), \quad (40b)$$

$$\hat{n}_w^A = 1 - \hat{n}_c^A \cos(2\pi x_1). \quad (40c)$$

We assume that the solution is symmetric with respect to $x_2=0$ and is periodic with period 1 in x_1 and consider the domain $0 \leq x_1 \leq 1$ and $0 \leq x_2 \leq (1/2)[1 - \hat{D} \sin(2\pi x_1)]$, imposing the symmetry condition at $x_2=0$, and the periodic condition at $x_1=0$ and 1. Thus, n_{av}^B is the average molecular number density in this domain. We analyze the behavior of the gas mixture numerically, using the fluid-dynamic-type system in Sec. III, under the assumption that the amount of noncondensable gas is comparable to that of the vapor, i.e., n_{av}^B/n_0 is of the order of unity. If we take m^A and d^A as the reference molecular mass m_0 and diameter d_0 , then the problem is characterized by the following dimensionless parameters: m^B/m^A , d^B/d^A , $\hat{D}$, $\hat{T}_c$, $\hat{n}_c^A$, and n_{av}^B/n_0 .

In the following, we mainly show the result in the case of plane ($\hat{D}=0$) and isothermal ($\hat{T}_c=0$) walls. The assumption of isothermal walls seems unphysical because the saturation pressure p_w^A (or the saturation number density n_w^A) depends on the temperature T_w . However, we consider an idealized case to simplify the physical situation. This idealization is acceptable because of the fact that in general a small variation of T_w results in a large variation of p_w^A . Incidentally, the configuration of the problem is not a model of a specific real problem but is designed to demonstrate the capability of the present numerical method for fully two-dimensional flows. Once its efficiency is confirmed, we can apply the method to practical problems, such as evaporation of droplets into a background gas.⁵⁵

B. Numerical results

In Figs. 3–7, we show some results for different mass ratios in the case of $d^B/d^A=1$, $\hat{D}=0$ (plane walls), $\hat{T}_c=0$ (isothermal walls), $\hat{n}_c^A=0.5$, and $n_{av}^B/n_0=0.8$. Figure 3 shows

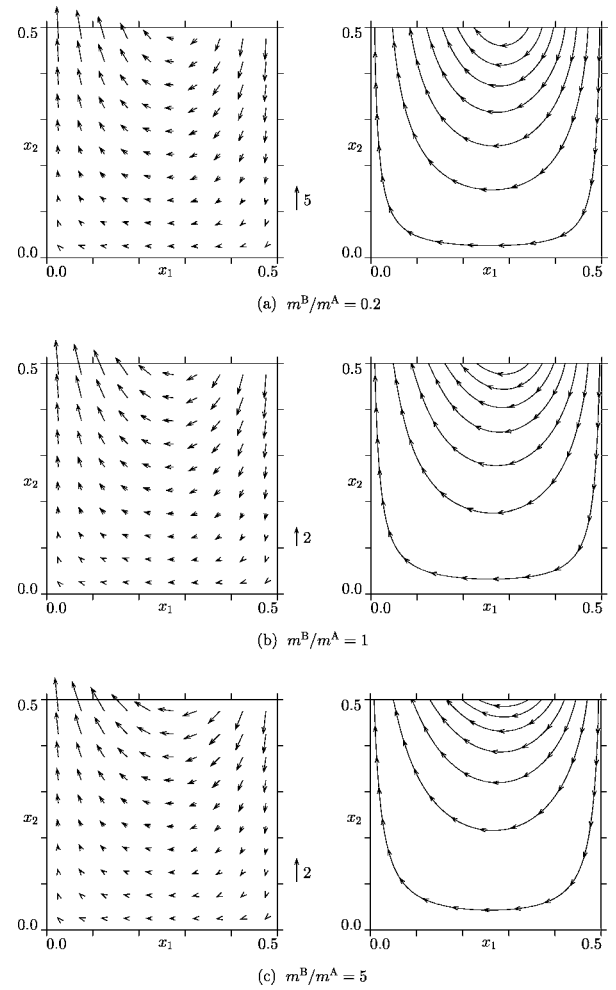


FIG. 3. The first-order coefficient $\hat{v}_{i(1)}^A$ of the flow velocity of the vapor for different m^B/m^A in the domain $0 \leq x_1 \leq 1/2$ and $0 \leq x_2 \leq 1/2$ [$d^B/d^A=1$, $\hat{D}=0$ (plane walls), $\hat{T}_c=0$ (isothermal walls), $\hat{n}_c^A=0.5$, and $n_{av}^B/n_0=0.8$]. (a) $m^B/m^A=0.2$, (b) $m^B/m^A=1$, and (c) $m^B/m^A=5$. In the left-hand figures, the arrow indicates the flow velocity vector $\hat{v}_{i(1)}^A$ in the x_1 - x_2 plane at its starting point, and its scale is shown in each figure. The right-hand figures show the streamlines of the corresponding flow velocities.

the first-order coefficient of the vapor flow velocity $\hat{v}_{i(1)}^A$, Fig. 4 that of the noncondensable gas flow velocity $\hat{v}_{i(1)}^B$, and Fig. 5 that of the barycentric flow velocity $\hat{v}_{i(1)}$; in each figure, panel (a) shows the result for $m^B/m^A=0.2$, panel (b) for $m^B/m^A=1$, and panel (c) for $m^B/m^A=5$. Since the flow field is symmetric with respect to $x_1=1/2$ in the case of plane walls, only the part $0 \leq x_1 \leq 1/2$ and $0 \leq x_2 \leq 1/2$ is shown in the figures. In the left-hand figures, the arrow indicates the flow velocity vector $\hat{v}_{i(1)}^A$, $\hat{v}_{i(1)}^B$, or $\hat{v}_{i(1)}$ in the x_1 - x_2 plane at its starting point, and its scale is shown in each figure. The right-hand figures show the streamlines of the corresponding flow velocities. Figure 6, on the other hand, shows the isolines of the concentration of the vapor X^A based on the leading-order number density for $m^B/m^A=0.2$, 1, and 5 in the same domain. Figure 7 shows the distribution of the leading-order temperature $\hat{T}_{(0)}$ along the lines $x_1=0$ and 0.5 for various values of m^B/m^A in the case where the other parameters are the same as in Figs. 3–6.

The vapor evaporating from the part of the wall with

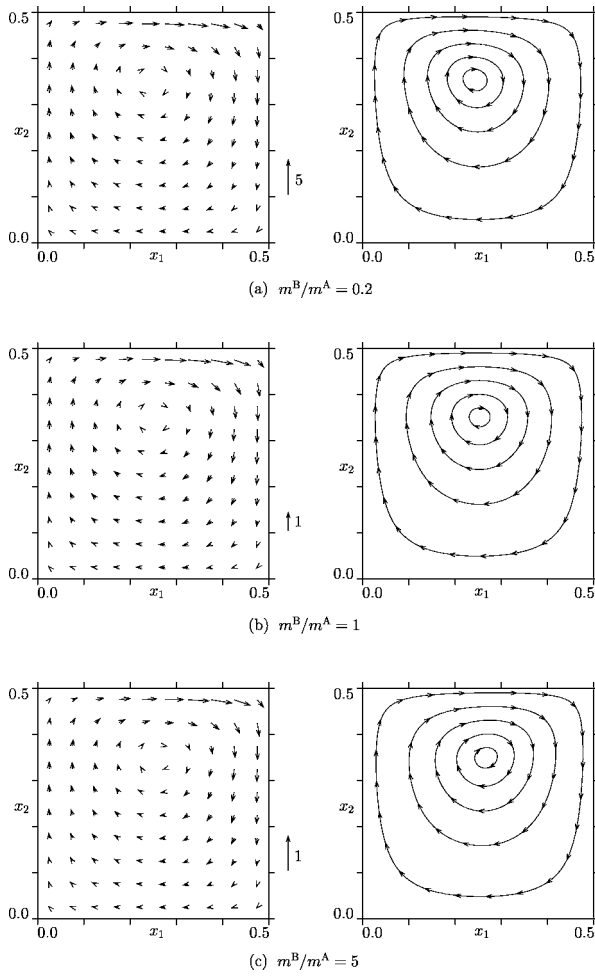


FIG. 4. The first-order coefficient $\hat{v}_{i(1)}^B$ of the flow velocity of the noncondensable gas for different m^B/m^A in the domain $0 \leq x_1 \leq 1/2$ and $0 \leq x_2 \leq 1/2$ [$d^B/d^A=1$, $\hat{D}=0$ (plane walls), $\hat{T}_c=0$ (isothermal walls), $\hat{n}_c^A=0.5$, and $n_{av}^B/n_0=0.8$]. (a) $m^B/m^A=0.2$, (b) $m^B/m^A=1$, and (c) $m^B/m^A=5$. In the left-hand figures, the arrow indicates the flow velocity vector $\hat{v}_{i(1)}^B$ in the x_1 - x_2 plane at its starting point, and its scale is shown in each figure. The right-hand figures show the streamlines of the corresponding flow velocities.

high saturation number density, flows back to the wall forming half-loop streamlines, and condenses on the part with low saturation number density ($n_w^A < n_0$) (Fig. 3). This flow of the vapor induces a circulating flow of the noncondensable gas (Fig. 4). As the molecular mass of the noncondensable gas increases ($m^B/m^A=0.2 \rightarrow 1 \rightarrow 5$), the speed of the vapor flow as well as that of the resulting noncondensable gas flow decreases because the impeding effect on evaporation and condensation caused by the presence of the noncondensable gas increases. The barycentric velocity is subject to the velocity slip on the wall described by Eq. (8d). In the case of isothermal walls, the velocity slip is due to the diffusion slip (the slip proportional to b_9). When $m^B/m^A=1$ (and $d^B/d^A=1$), the coefficient b_9 becomes zero, so that the tangential component of the barycentric flow velocity vanishes on the wall [Fig. 5(b)]. The diffusion slip is leftward in Fig. 5(a) and rightward in Fig. 5(c). As the result, a circulation appears in the latter figure. According to Fig. 6, the distribution of the concentration of the vapor is almost independent of m^B/m^A near the walls. Although the temperature

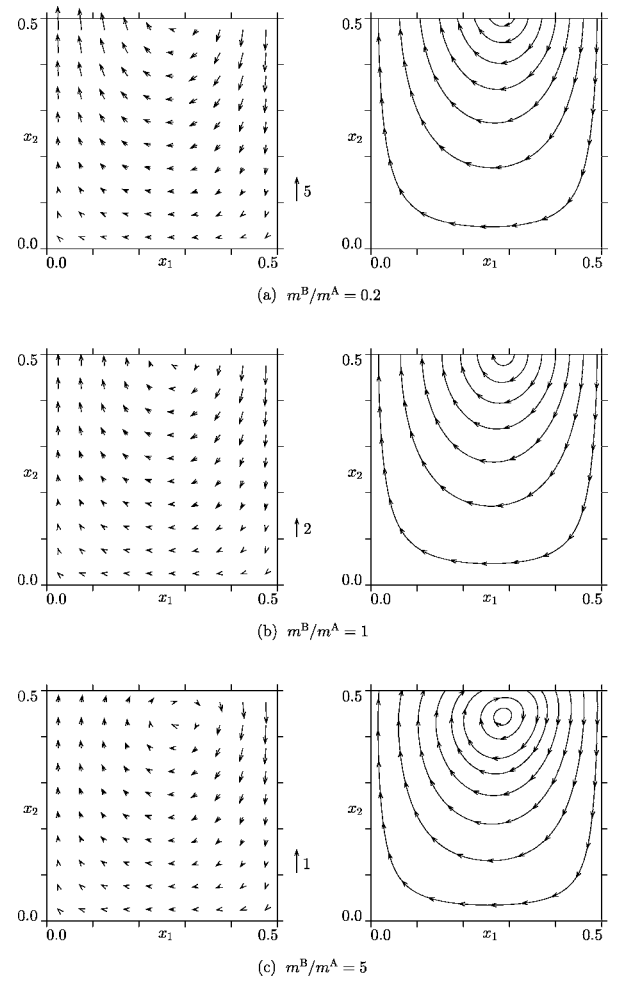


FIG. 5. The first-order coefficient $\hat{v}_{i(1)}$ of the barycentric flow velocity for different m^B/m^A in the domain $0 \leq x_1 \leq 1/2$ and $0 \leq x_2 \leq 1/2$ [$d^B/d^A=1$, $\hat{D}=0$ (plane walls), $\hat{T}_c=0$ (isothermal walls), $\hat{n}_c^A=0.5$, and $n_{av}^B/n_0=0.8$]. (a) $m^B/m^A=0.2$, (b) $m^B/m^A=1$, and (c) $m^B/m^A=5$. In the left-hand figures, the arrow indicates the flow velocity vector $\hat{v}_{i(1)}$ in the x_1 - x_2 plane at its starting point, and its scale is shown in each figure. The right-hand figures show the streamlines of the corresponding flow velocities.

of the walls is uniform, there appears a slight nonuniformity in the temperature $\hat{T}_{(0)}$, as shown in Fig. 7. That is, there is a slight heating for $m^B/m^A > 1$ and cooling for $m^B/m^A < 1$, the temperature being uniform for $m^B/m^A=1$ (although the temperature distribution is shown only at $x_1=0$ and 0.5 in Fig. 7, the above statement is true for any other x_1).

If one tries to solve the present problem within the framework of continuum fluid dynamics, natural fluid-dynamic equations would be the compressible Navier-Stokes equations with slow motion, which is equivalent to Eqs. (5a)–(5e) with $\hat{Y}_1=\hat{Y}_2=\hat{Y}_3=\hat{Y}_4=\hat{Y}_5=0$. On the other hand, the boundary condition corresponding to Eq. (8a) is usually assumed from considerations on the physical nature of the surface of the condensed phase and the structure of the Navier-Stokes equations. Other boundary conditions based on macroscopic considerations would be the conditions equivalent to Eqs. (8b) and (8c), and the no-slip condition for the tangential flow velocity, i.e., Eq. (8d) with $b_7=b_9=0$. Therefore, we call the system consisting of Eqs. (5a)–(5e)

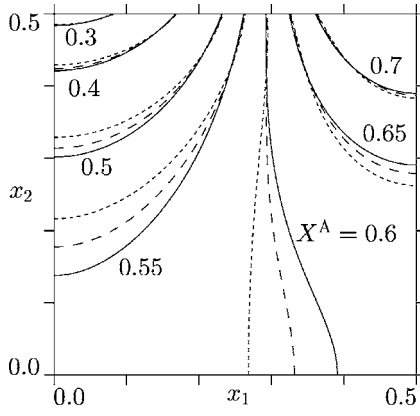


FIG. 6. The isolines of the concentration of the vapor X^A based on the leading-order molecular number density for different m^B/m^A in the domain $0 \leq x_1 \leq 1/2$ and $0 \leq x_2 \leq 1/2$ [$d^B/d^A=1$, $\hat{D}=0$ (plane walls), $\hat{T}_c=0$ (isothermal walls), $\hat{n}_c^A=0.5$, and $n_{av}^B/n_0=0.8$]. The short dashed line indicates the result for $m^B/m^A=0.2$, the long dashed line that for $m^B/m^A=1$, and the solid line that for $m^B/m^A=5$.

with $\hat{Y}_1=\hat{Y}_2=\hat{Y}_3=\hat{Y}_4=\hat{Y}_5=0$ and boundary conditions (8a)–(8d) with $b_7=b_9=0$ the Navier-Stokes system.^{52,56–59} An example of the difference between the full fluid-dynamic-type system and the Navier-Stokes system is demonstrated in Fig. 8. More specifically, the streamlines of $\hat{v}_{i(1)}$ [Fig. 8(a)] and the isolines of X^A [Fig. 8(b)] obtained by the respective systems are compared for $m^B/m^A=5$, $d^B/d^A=1$, $\hat{D}=0$ (plane walls), $\hat{T}_c=0$ (isothermal walls), $\hat{n}_c^A=0.5$, and $n_{av}^B/n_0=0.8$. A decisive difference is that there is a circulation in the barycentric velocity field in the case of the full fluid-dynamic-type system [Fig. 8(a)]. The difference in the concentration is less significant [Fig. 8(b)].

Figure 9 shows the result when a sinusoidal temperature distribution is imposed along the wall, i.e., when $\hat{T}_c=0.3$, in the case of $m^B/m^A=5$, $d^B/d^A=1$, $\hat{D}=0$ (plane walls), $\hat{n}_c^A=0.5$, and $n_{av}^B/n_0=0.8$. Figure 9(a) shows the flow velocity vector of the barycentric velocity $\hat{v}_{i(1)}$, Fig. 9(b) the corresponding streamlines, Fig. 9(c) the isolines of the concentration of the vapor X^A , and Fig. 9(d) those of the temperature $\hat{T}_{(0)}$. The dashed line in Fig. 9(d) will be commented in the following paragraph. The corresponding isothermal case is shown in Figs. 5(c) and 6; more precisely, Fig. 5(c) corresponds to Figs. 9(a) and 9(b), and Fig. 6 (for $m^B/m^A=5$) to

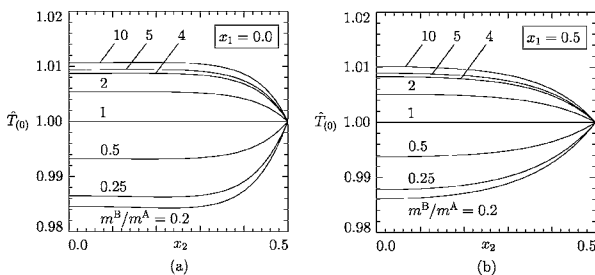


FIG. 7. The distribution of the leading-order temperature $\hat{T}_{(0)}$ along the lines $x_1=0$ and 0.5 for various values of m^B/m^A [$d^B/d^A=1$, $\hat{D}=0$ (plane walls), $\hat{T}_c=0$ (isothermal walls), $\hat{n}_c^A=0.5$, and $n_{av}^B/n_0=0.8$]. (a) $x_1=0$, (b) $x_1=0.5$.

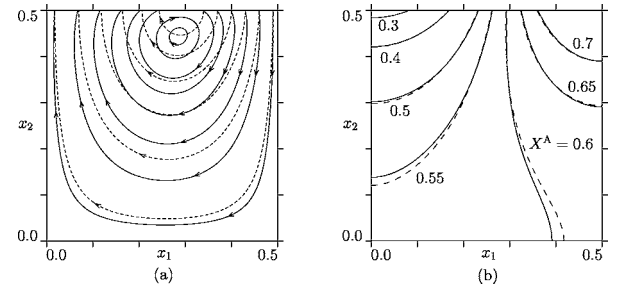


FIG. 8. The difference between the full fluid-dynamic-type system and the Navier-Stokes system [$m^B/m^A=5$, $d^B/d^A=1$, $\hat{D}=0$ (plane walls), $\hat{T}_c=0$ (isothermal walls), $\hat{n}_c^A=0.5$, and $n_{av}^B/n_0=0.8$]. (a) Streamlines of $\hat{v}_{i(1)}$, and (b) isolines of X^A . Here, the solid line indicates the result by the full fluid-dynamic-type system, and the dashed line that by the Navier-Stokes system.

Fig. 9(c). The flow pattern changes because the thermal slip [cf. Eq. (8d)] caused by the rightward temperature gradient enhances the velocity slip in the same direction.

Let us consider the continuum limit in the case of Fig. 9. As commented in Sec. III C, in this limit, the flow vanishes and the temperature field reduces to $\hat{T}_{(0)}$, which is shown by the solid line in Fig. 9(d). On the other hand, the dashed line in the same figure indicates the corresponding isolines of the temperature field given by the steady heat-conduction equation, that is, the solution of Eqs. (5d) and (5e) with $\hat{v}_{j(1)}^A=\hat{v}_{j(1)}^B=0$ and the boundary condition (8b) for the same values of the parameters. In this case, in place of the condition (8a), we need to specify a parameter associated with the amount of the component A. Here, the total amount of the component A is set to be equal to that of the vapor in the

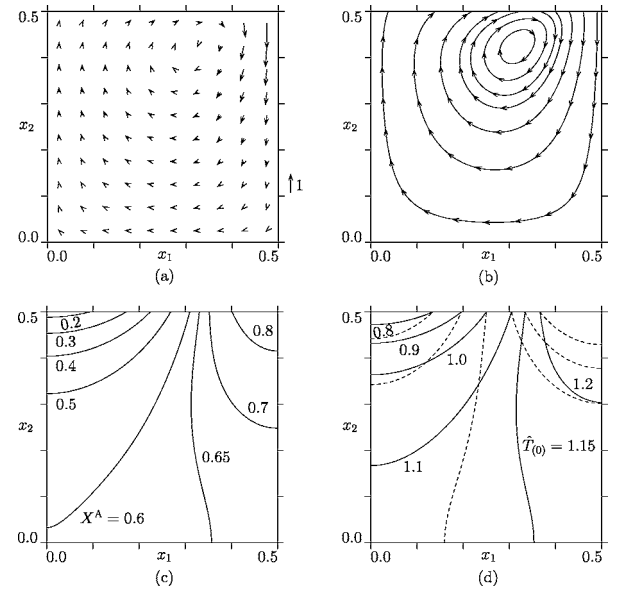


FIG. 9. Flow field with a temperature variation along the walls [$m^B/m^A=5$, $d^B/d^A=1$, $\hat{D}=0$ (plane walls), $\hat{T}_c=0.3$, $\hat{n}_c^A=0.5$, and $n_{av}^B/n_0=0.8$]. (a) Flow velocity field of $\hat{v}_{i(1)}$, (b) streamlines of $\hat{v}_{i(1)}$, (c) isolines of X^A , and (d) isolines of $\hat{T}_{(0)}$ (solid line). In (a), the arrow indicates the flow velocity vector $\hat{v}_{i(1)}$ in the x_1 - x_2 plane at its starting point, and its scale is shown in the figure. In (d), the dashed line indicates the corresponding isolines of the temperature field by the steady heat-conduction equation (see the fifth paragraph in Sec. V B).

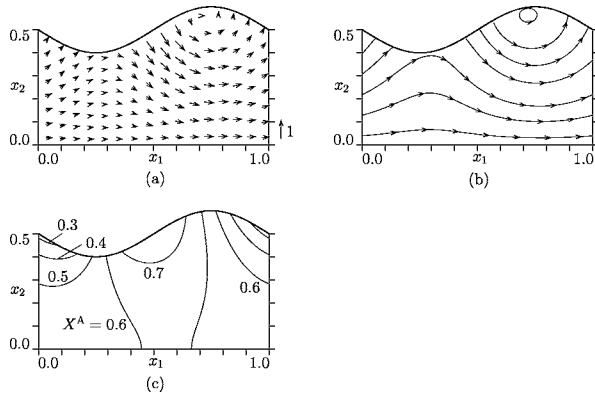


FIG. 10. Flow field for the isothermal walls of sinusoidal shape ($m^B/m^A=5$, $d^B/d^A=1$, $\hat{D}=0.1$, $\hat{T}_c=0$, $\hat{n}_c^A=0.5$, and $n_{av}^B/n_0=0.8$). (a) Flow velocity field of $\hat{v}_{i(1)}$, (b) streamlines of $\hat{v}_{i(1)}$, and (c) isolines of X^A . In (a), the arrow indicates the vector $\hat{v}_{i(1)}$, and its scale is shown in the figure.

numerical result in the case of the mixture of the vapor and noncondensable gas. Since the dashed lines coincide with the corresponding solid lines on the wall, their labels are omitted. As is seen from the figure, the correct temperature field differs significantly from that given by the heat-conduction equation. This discrepancy is caused by the ghost effect.

In Figs. 10 and 11, the result for walls of sinusoidal shape ($\hat{D}=0.1$) is shown for $\hat{T}_c=0$ (Fig. 10) and 0.3 (Fig. 11) in the case of $m^B/m^A=5$, $d^B/d^A=1$, $\hat{n}_c^A=0.5$, and $n_{av}^B/n_0=0.8$. Since the flow field is not symmetric with respect to $x_1=0.5$, it is shown in the full period $0 \leq x_1 \leq 1$. In each figure, panel (a) shows the barycentric flow velocity vector $\hat{v}_{i(1)}$, panel (b) the corresponding streamlines, and panel (c) the isolines of the concentration of the vapor X^A . Figure 11(d) shows the isolines of the temperature $\hat{T}_{(0)}$. Since the temperature variation is very small in the case of Fig. 10, the isothermal lines are not shown there.

The fluid-dynamic-type system has been solved on a 240×120 nonuniform grid with finer control volumes near the wall (although for some cases the solution has been compared with the solution of double grid-size to ensure the accuracy). Furthermore it has been confirmed that the present

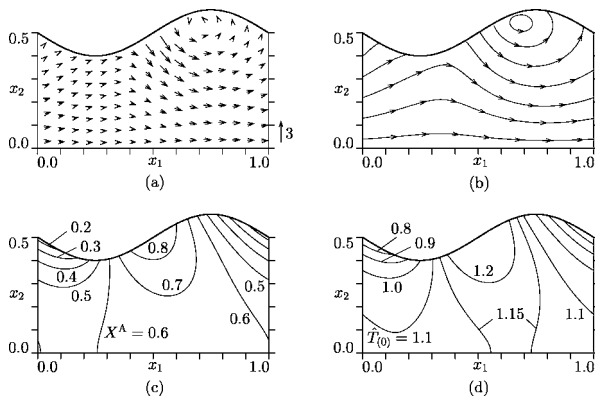


FIG. 11. Flow field for the nonisothermal walls of sinusoidal shape ($m^B/m^A=5$, $d^B/d^A=1$, $\hat{D}=0.1$, $\hat{T}_c=0.3$, $\hat{n}_c^A=0.5$, and $n_{av}^B/n_0=0.8$). (a) Flow velocity field of $\hat{v}_{i(1)}$, (b) streamlines of $\hat{v}_{i(1)}$, (c) isolines of X^A , and (d) isolines of $\hat{T}_{(0)}$. See the caption of Fig. 10.

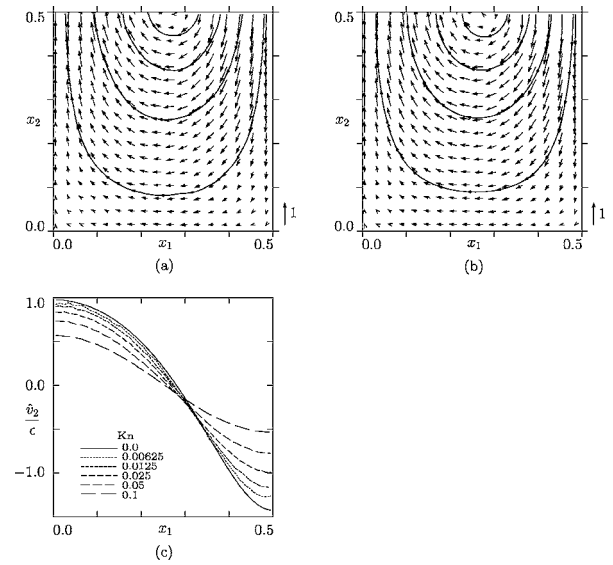


FIG. 12. Comparison between the DSMC result and the continuum limit: barycentric flow velocity ($\hat{D}=\hat{T}_c=0$, $m^B/m^A=d^B/d^A=1$, $\hat{n}_c^A=0.5$, and $n_{av}^B/n_0=1$). (a) $\hat{v}_i/\epsilon=(2/\sqrt{\pi})(\hat{v}_i/\text{Kn})$ at $\text{Kn}=0.00625$. (b) $\hat{v}_{i(1)}=\lim_{\epsilon \rightarrow 0}(\hat{v}_i/\epsilon)$ obtained by the fluid-dynamic-type system. (c) Distribution of $\hat{v}_2/\epsilon=(2/\sqrt{\pi})(\hat{v}_2/\text{Kn})$ on the wall ($x_2=0.5$) at various Kn and the continuum limit $\hat{v}_{2(1)}=\lim_{\epsilon \rightarrow 0}(\hat{v}_2/\epsilon)$. In (a) and (b), the arrow indicates the vector $\hat{v}_i/\epsilon$ [(a)] or $\hat{v}_{i(1)}=\lim_{\epsilon \rightarrow 0}(\hat{v}_i/\epsilon)$ [(b)] at its starting point, and its scale is shown in the figures. The corresponding streamlines are also shown in the figures.

code yields the same results as Ref. 14 for a one-dimensional problem (two-surface problem of evaporation and condensation in the presence of the noncondensable gas). All computations were carried out on a Dell™ Workstation running an Intel® Pentium® 4 (2.2 GHz) CPU, or a computer of equivalent capacity.

C. Comparison with DSMC result

We also investigate the same problem, in the case of plane ($\hat{D}=0$) and isothermal ($\hat{T}_c=0$) walls, numerically on the basis of kinetic theory, using the DSMC method.^{27,28} In this subsection, we show some results, which will be compared with the results based on the fluid-dynamic-type system. Since the flow field is symmetric with respect to $x_2=0$, $x_1=0$, and $x_1=0.5$, the computation is performed in the domain $0 \leq x_1 \leq 0.5$ and $0 \leq x_2 \leq 0.5$ with the specular reflection condition on $x_2=0$, $x_1=0$, and $x_1=0.5$. The DSMC method is explained in many places, so that we only show the results, omitting the description of the method.

Figures 12 and 13 contain the results for $m^B/m^A=1$, $d^B/d^A=1$, $\hat{n}_c^A=0.5$, and $n_{av}^B/n_0=1$. Figure 12(a) shows the flow velocity vector magnified by the Knudsen number, i.e., $\hat{v}_i/\epsilon=(2/\sqrt{\pi})(\hat{v}_i/\text{Kn})$, at $\text{Kn}=0.00625$ and the corresponding streamlines, and Fig. 12(b) the corresponding figure in the continuum limit, $\lim_{\epsilon \rightarrow 0}\hat{v}_i/\epsilon=\hat{v}_{i(1)}$, obtained from the fluid-dynamic type system. Figure 12(c) shows the distribution of the normal component of the velocity, magnified by ϵ , i.e., $\hat{v}_2/\epsilon$, along the wall at $x_2=0.5$ for $\text{Kn}=0.1$, 0.05, 0.025, 0.0125, and 0.00625. In the figure, the result for the continuum limit, $\lim_{\epsilon \rightarrow 0}\hat{v}_2/\epsilon=\hat{v}_{2(1)}$, is also shown. Figure 13(a)

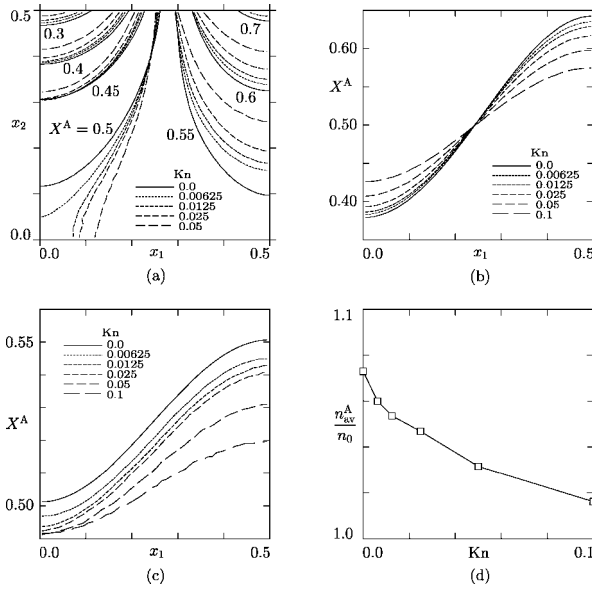


FIG. 13. Comparison between the DSMC result and the continuum limit: concentration and average molecular number density of the vapor ($\hat{D} = \hat{T}_c = 0$, $m^B/m^A = d^B/d^A = 1$, $\hat{n}_c^A = 0.5$, and $n_{av}^B/n_0 = 0.8$). (a) Isolines of the concentration of the vapor $\chi^A = \hat{n}^A / \hat{n}$ at various Kn including the continuum limit $\text{Kn} \rightarrow 0$. (b) Distribution of χ^A along $x_2 = 0.405$. (c) Distribution of χ^A along $x_2 = 0.105$. (d) Average molecular number density n_{av}^A vs Kn.

shows the isolines of the concentration of the vapor, i.e., $\chi^A = \hat{n}^A / (\hat{n}^A + \hat{n}^B)$, for $\text{Kn} = 0.05, 0.025, 0.0125$, and 0.00625 , together with the corresponding result in the continuum limit, i.e., $\lim_{\text{Kn} \rightarrow 0} \chi^A = X^A$. Figures 13(b) and 13(c) are, respectively, the distribution of the concentration of the vapor χ^A along $x_2 = 0.405$ and that along $x_2 = 0.105$ for $\text{Kn} = 0.1, 0.05, 0.025, 0.0125$, and 0.00625 . Figure 13(d) shows the average molecular number density of the vapor n_{av}^A over the computational domain versus Kn. As is seen from Figs. 12 and 13, the DSMC result tends to approach the continuum limit obtained by the fluid-dynamic-type system as the Knudsen number becomes small. However, a closer look at Figs. 13(a) and 13(c) reveals that the speed of approach to the continuum limit is not monotonic near the center line ($x_2 = 0$). The curve in Fig. 13(d) also exhibits a slightly unnatural behavior for small Kn. Such behavior may be true physically. At the same time, we cannot exclude the possibility that it is attributed to insufficient accuracy of the DSMC computation. This point will be discussed below.

Figures 14–16 show the results for $m^B/m^A = 5$, $d^B/d^A = 1$, $\hat{n}_c^A = 0.5$, and $n_{av}^B/n_0 = 0.8$. Figure 14(a) shows the flow velocity vector magnified by the Knudsen number, i.e., $\hat{v}_i/\epsilon = (2/\sqrt{\pi})(\hat{v}_i/\text{Kn})$, at $\text{Kn} = 0.0125$ and the corresponding streamlines, and Fig. 14(b) is the corresponding figure in the continuum limit, $\lim_{\text{Kn} \rightarrow 0} \hat{v}_i/\epsilon = \hat{v}_{i(1)}$, obtained by the fluid-dynamic type system. Figure 14(c) shows the distribution of the normal component of the velocity magnified by ϵ , i.e., $\hat{v}_2/\epsilon$, along the wall ($x_2 = 0.5$) for $\text{Kn} = 0.1, 0.05, 0.025$, and 0.0125 , and Fig. 14(d) is the corresponding figure for the tangential component, i.e., $\hat{v}_1/\epsilon$. In the figures, the results for the continuum limits, i.e., $\lim_{\text{Kn} \rightarrow 0} \hat{v}_2/\epsilon = \hat{v}_{2(1)}$ and $\lim_{\text{Kn} \rightarrow 0} \hat{v}_1/\epsilon = \hat{v}_{1(1)}$, are also shown. Figure 15(a) shows the isolines of the concentration of the vapor, i.e.,

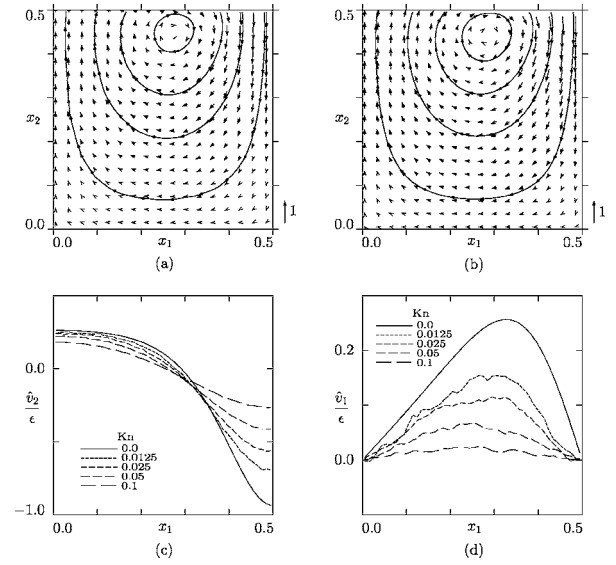


FIG. 14. Comparison between the DSMC result and the continuum limit: barycentric flow velocity ($\hat{D} = \hat{T}_c = 0$, $m^B/m^A = 5$, $d^B/d^A = 1$, $\hat{n}_c^A = 0.5$, and $n_{av}^B/n_0 = 0.8$). (a) $\hat{v}_i/\epsilon = (2/\sqrt{\pi})(\hat{v}_i/\text{Kn})$ at $\text{Kn} = 0.0125$. (b) $\hat{v}_{i(1)} = \lim_{\text{Kn} \rightarrow 0} (\hat{v}_i/\epsilon)$ obtained by the fluid-dynamic-type system. (c) Distribution of $\hat{v}_2/\epsilon = (2/\sqrt{\pi})(\hat{v}_2/\text{Kn})$ on the wall ($x_2 = 0.5$) at various Kn and the continuum limit $\hat{v}_{2(1)} = \lim_{\text{Kn} \rightarrow 0} (\hat{v}_2/\epsilon)$. (d) Distribution of $\hat{v}_1/\epsilon = (2/\sqrt{\pi})(\hat{v}_1/\text{Kn})$ on the wall ($x_2 = 0.5$) at various Kn and the continuum limit $\hat{v}_{1(1)} = \lim_{\text{Kn} \rightarrow 0} (\hat{v}_1/\epsilon)$. See the caption of Fig. 12. In (a) and (b), the arrow indicates the vector $\hat{v}_i/\epsilon$ [(a)] or $\hat{v}_{i(1)} = \lim_{\text{Kn} \rightarrow 0} (\hat{v}_i/\epsilon)$ [(b)] at its starting point, and the corresponding streamlines are also shown.

$\chi^A = \hat{n}^A / (\hat{n}^A + \hat{n}^B)$, for $\text{Kn} = 0.05, 0.025$, and 0.0125 , together with the corresponding results in the continuum limit, i.e., $\lim_{\text{Kn} \rightarrow 0} \chi^A = X^A$. Figures 15(b) and 15(c) are, respectively, the distribution of the concentration of the vapor χ^A along $x_2 = 0.405$ and that along $x_2 = 0.105$ for $\text{Kn} = 0.1, 0.05, 0.025$, and 0.0125 . Figure 15(d) shows the average molecular number density of the vapor n_{av}^A over the computational domain versus Kn. Figure 16 shows the distribution of the temperature $\hat{T}$ along $x_2 = 0.005$ at various Knudsen numbers. The tendency of approach of the DSMC result to the continuum limit based on the fluid-dynamic-type system is more or less similar to the previous case (Figs. 12 and 13). One thing to be stressed here is the fact that, as is clearly seen from Figs. 8(a) and 14, the DSMC velocity field does not approach the velocity field based on the Navier-Stokes system [the dashed line in Fig. 8(a)].

The aim of the present DSMC computation is to show that its results approach the continuum limit obtained by the correct fluid-dynamic-type system as the Knudsen number becomes small. As is well known, the DSMC method has difficulties for computation in the near continuum regime. However, in the present problem, additional and more serious difficulties associated with the ghost effect manifest themselves. As discussed in Sec. III C, when the Knudsen number is small, the density and temperature fields are affected by the flow velocity that is of the order of the Knudsen number and thus vanishes in the continuum limit. Therefore, in order to obtain reliable density and temperature fields by the DSMC method, we have to obtain the velocity field accurately in such a way that $\hat{v}_i^A/\text{Kn}$, $\hat{v}_i^B/\text{Kn}$, and $\hat{v}_i/\text{Kn}$ are

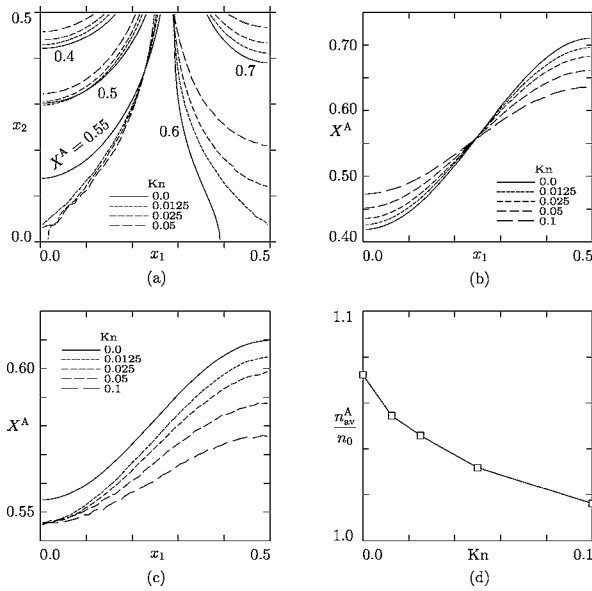


FIG. 15. Comparison between the DSMC result and the continuum limit: concentration (or molecular number density) of the vapor ($\hat{D} = \hat{T}_c = 0$, $m^B/m^A = 5$, $d^B/d^A = 1$, $\hat{n}_c^A = 0.5$, and $n_{av}^B/n_0 = 0.8$). (a) Isolines of the concentration of the vapor $\chi^A = \hat{n}^A / \hat{n}$ at various Kn including the continuum limit $\text{Kn} \rightarrow 0$. (b) Distribution of χ^A along $x_2 = 0.405$. (c) Distribution of χ^A along $x_2 = 0.105$. (d) Average molecular number density n_{av}^A vs Kn.

accurate enough. This requirement becomes increasingly difficult to fulfill as the Knudsen number approaches zero. In the present computation, the computational domain $0 \leq x_1 \leq 0.5$ and $0 \leq x_2 \leq 0.5$ is divided into 100×100 cells, and the average number of particles per cell in the final steady state is about 100 for the vapor and about 100 (or 80) for the noncondensable gas in the case of Figs. 12 and 13 (or Figs. 14–16). In the most difficult case of $\text{Kn} = 0.00625$ in Figs. 12 and 13, 16 independent computations were carried out. The averages of necessary moments of the velocity distribution function are taken over 150×10^4 time steps, after a steady state seems to be established, for each of 16 independent computations. The averages of the 16 time averages are then regarded as the steady states of the moments. Each independent computation took 600 h (including the time required to reach a steady state) on a Pentium® 4 3.6 GHz CPU. Other DSMC computations were carried out on a Dell™ Workstation running an Intel® Pentium® 4 2.2 GHz CPU.

As pointed out earlier, we cannot exclude the possibility that the approach to the continuum limit demonstrated in Figs. 13(a), 13(c), and 13(d) and in Figs. 15(a), 15(c), and 15(d), which seems to be slightly unnatural, is not true, and is attributed to inaccuracy of the DSMC computation. However, noting the small scales of the ordinates in Figs. 13(c) and 15(c), one can claim that the present computation shows the approach to the continuum limit with a sufficient accuracy. In order to resolve the ambiguity, we need finer cells and more particles. However, such computation is quite hard with normally accessible computational environments. Keeping this in mind, we should stress that the fluid-dynamic-type system summarized in Sec. III is a very powerful and practical tool to deal with the problems described in Sec. II.

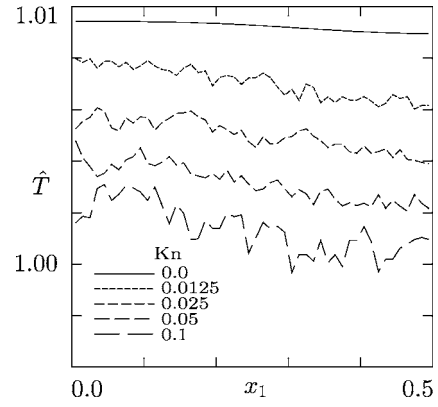


FIG. 16. Comparison between the DSMC result and the continuum limit: temperature ($\hat{D} = \hat{T}_c = 0$, $m^B/m^A = 5$, $d^B/d^A = 1$, $\hat{n}_c^A = 0.5$, and $n_{av}^B/n_0 = 0.8$). The temperature $\hat{T}$ along $x_2 = 0.005$ is shown for various Kn including the continuum limit $\text{Kn} \rightarrow 0$.

VI. CONCLUDING REMARKS

In the present paper, we considered slow steady flows of a mixture of a vapor and a noncondensable gas, caused mainly by evaporation and condensation of the vapor, at small Knudsen numbers in the situation described in Sec. II. A fluid-dynamic-type system that describes such flows was derived in Ref. 16 by a systematic asymptotic analysis for small Knudsen numbers on the basis of the Boltzmann system. However, the fluid-dynamic-type system could not be applied immediately to practical problems because it contained some coefficients whose numerical data were not available in the equations as well as the boundary conditions. Some years later, these coefficients were obtained numerically in separate papers,^{24,25} so that the fluid-dynamic-type system is now ready for application. One of the important purposes of the present paper was to summarize the fluid-dynamic-type system in a concise and usable form putting together the pieces of information obtained so far. This was done in Sec. III with the help of Appendices A and B. In Sec. IV, we constructed a numerical solution method for the fluid-dynamic-type system that is flexible for different geometries, with the help of the finite-volume method for the incompressible Navier-Stokes equations. The new method was applied to solving specific physical problems in Sec. V, and the numerical results were discussed. Some results were also compared with the numerical results obtained from the original Boltzmann system by the DSMC method. As discussed in Sec. V C, because of the special structure of the physical situation under consideration, it becomes extremely hard to obtain a reliable result by the DSMC method as the Knudsen number decreases. Therefore, the fluid-dynamic-type system treated in the present paper is a powerful tool to analyze the flows of a mixture of a vapor and a noncondensable gas in the situation described in Sec. II.

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APPENDIX A: TRANSPORT COEFFICIENTS AND THEIR DATABASE

In this appendix, we give the definitions of the transport coefficients occurring in Eqs. (5c)–(5e). In addition to α , other Greek letters (β , γ , and κ) will be used to indicate the labels “A” and “B.”

Let us denote by $A^\alpha(\zeta)$, $B^\alpha(\zeta)$, and $D^{(\beta)\alpha}(\zeta)$ the solutions of the following equations, where the independent variable ζ indicates the magnitude of a vector $(\zeta_1, \zeta_2, \zeta_3)$, i.e., $\zeta = (\zeta_i^2)^{1/2}$. That is, $A^\alpha(\zeta)$ is the solution of

$$\sum_{\beta=A,B} \hat{K}^{\beta\alpha} X^\beta \tilde{L}^{\beta\alpha}(\zeta_i A^\beta, \zeta_i A^\alpha) = -\zeta_i (\hat{m}^\alpha \zeta^2 - 5/2), \quad (A1)$$

with the subsidiary condition

$$\sum_{\beta=A,B} \hat{m}^\beta X^\beta I_4^\beta(A^\beta) = 0, \quad (A2)$$

$B^\alpha(\zeta)$ is the solution of

$$\sum_{\beta=A,B} \hat{K}^{\beta\alpha} X^\beta \tilde{L}^{\beta\alpha}(c_{ij} B^\beta, c_{ij} B^\alpha) = -2\hat{m}^\alpha c_{ij}, \quad (A3)$$

where

$$c_{ij} = \zeta_i \zeta_j - (1/3) \zeta^2 \delta_{ij}, \quad (A4)$$

and $D^{(\beta)\alpha}(\zeta)$ is the solution of

$$\begin{aligned} \sum_{\beta=A,B} \hat{K}^{\beta\alpha} X^\beta \tilde{L}^{\beta\alpha}(\zeta_i D^{(\gamma)\beta}, \zeta_i D^{(\gamma)\alpha}) \\ = -\zeta_i (\delta_{\alpha\gamma} - \hat{m}^\alpha \hat{n}_{(0)}^\alpha / \hat{\rho}_{(0)}), \end{aligned} \quad (A5)$$

with the subsidiary condition

$$\sum_{\beta=A,B} \hat{m}^\beta X^\beta I_4^\beta(D^{(\alpha)\beta}) = 0. \quad (A6)$$

Here,

$$\tilde{L}^{\beta\alpha}(f, g) = [\hat{J}^{\beta\alpha}(f E^\beta, E^\alpha) + \hat{J}^{\beta\alpha}(E^\beta, g E^\alpha)](E^\alpha)^{-1}, \quad (A7a)$$

$$\begin{aligned} \hat{J}^{\beta\alpha}(f, g) = \frac{1}{4\sqrt{2}\pi} \int [f(\zeta_{*i}^{\beta\alpha}) g(\zeta_i^{\beta\alpha}) - f(\zeta_{*i}) g(\zeta_i)] \\ \times |e_j V_j| d\Omega(e_i) d^3 \zeta_*, \end{aligned} \quad (A7b)$$

$$I_n^\alpha(F) = (8\pi/15) \int_0^\infty \zeta^n F(\zeta) E^\alpha(\zeta) d\zeta, \quad (A7c)$$

$$E^\alpha(\zeta) = (\hat{m}^\alpha / \pi)^{3/2} \exp(-\hat{m}^\alpha \zeta^2), \quad (A7d)$$

$$\zeta_i^{\beta\alpha} = \zeta_i + (\hat{\mu}^{\beta\alpha} / \hat{m}^\alpha) (e_j V_j) e_i, \quad (A7e)$$

$$\zeta_{*i}^{\beta\alpha} = \zeta_{*i} - (\hat{\mu}^{\beta\alpha} / \hat{m}^\alpha) (e_j V_j) e_i, \quad (A7f)$$

$$V_i = \zeta_{*i} - \zeta_i, \quad (A7g)$$

$$\hat{K}^{\beta\alpha} = [(\hat{d}^\beta + \hat{d}^\alpha)/2]^2, \quad (A7h)$$

$$\hat{\mu}^{\beta\alpha} = 2\hat{m}^\beta \hat{m}^\alpha / (\hat{m}^\beta + \hat{m}^\alpha), \quad (A7i)$$

$$d^3 \zeta_* = d\zeta_{*1} d\zeta_{*2} d\zeta_{*3}. \quad (A7j)$$

In Eq. (A7b), which is the collision integral of the Boltzmann equation for a binary gas mixture, ζ_{*i} is the integration variable for ζ_i , e_i is the unit vector, $d\Omega(e_i)$ is the solid-angle element in the direction of e_i , and the domain of integration is all the directions of e_i and the whole space of ζ_{*i} . The $\tilde{L}^{\beta\alpha}$ is the linearized collision operator. Note that $\hat{\rho}_{(0)} = (\hat{m}^A X^A + \hat{m}^B X^B) \hat{n}_{(0)}$ and $\hat{n}_{(0)}^\alpha = X^\alpha \hat{n}_{(0)}$. We should also recall that X^A and X^B are not independent ($X^A + X^B = 1$) and note that A^α , B^α , and $D^{(\beta)\alpha}$ depend on X^A (or X^B), $\hat{m}^\alpha$, and $\hat{d}^\alpha$.

We then define the functions $A_1^\alpha(\zeta)$, $A_2^\alpha(\zeta)$, $D_1^{(\gamma,\kappa)\alpha}(\zeta)$, $D_2^{(\gamma,\kappa)\alpha}(\zeta)$, $D_{A1}^{(\gamma)\alpha}(\zeta)$, and $D_{A2}^{(\gamma)\alpha}(\zeta)$, which also depend on X^A (or X^B), $\hat{m}^\alpha$, and $\hat{d}^\alpha$, by the following integrals:

$$\zeta_i \zeta_j A_1^\alpha + A_2^\alpha \delta_{ij} = \sum_{\beta=A,B} \hat{K}^{\beta\alpha} X^\beta \tilde{J}^{\beta\alpha}(\zeta_i A^\beta, \zeta_j A^\alpha), \quad (A8)$$

$$\zeta_i \zeta_j D_1^{(\gamma,\kappa)\alpha} + D_2^{(\gamma,\kappa)\alpha} \delta_{ij} = \sum_{\beta=A,B} \hat{K}^{\beta\alpha} X^\beta \tilde{J}^{\beta\alpha}(\zeta_i D^{(\gamma)\beta}, \zeta_j D^{(\kappa)\alpha}), \quad (A9)$$

$$\begin{aligned} \zeta_i \zeta_j D_{A1}^{(\gamma)\alpha} + D_{A2}^{(\gamma)\alpha} \delta_{ij} = \sum_{\beta=A,B} \hat{K}^{\beta\alpha} X^\beta \tilde{J}^{\beta\alpha}(\zeta_i A^\beta, \zeta_j D^{(\gamma)\alpha}) \\ + \tilde{J}^{\beta\alpha}(\zeta_i D^{(\gamma)\beta}, \zeta_j A^\alpha), \end{aligned} \quad (A10)$$

where

$$\tilde{J}^{\beta\alpha}(f, g) = \hat{J}^{\beta\alpha}(f E^\beta, g E^\alpha) (E^\alpha)^{-1}. \quad (A11)$$

The transport coefficients are defined with the aid of the functions introduced above. The $\hat{\mu}$, $\hat{D}_{AB}$, k_T , and $\hat{\lambda}$ are defined as follows:

$$\hat{\mu} = \sum_{\beta=A,B} \hat{m}^\beta X^\beta I_6^\beta(B^\beta), \quad (A12a)$$

$$\hat{D}_{AB} = X^A X^B (\hat{\Delta}_{AA} + \hat{\Delta}_{BB} - \hat{\Delta}_{AB} - \hat{\Delta}_{BA}), \quad (A12b)$$

$$k_T = \hat{D}_T / \hat{D}_{AB}, \quad (A12c)$$

$$\hat{\lambda} = \hat{\lambda}' - k_T \hat{D}_T / X^A X^B, \quad (A12d)$$

where

$$\hat{\Delta}_{\alpha\beta} = \frac{5}{2} I_4^\alpha(D^{(\beta)\alpha}), \quad (A13a)$$

$$\hat{D}_T = \frac{5}{2} X^A X^B [I_4^A(A^A) - I_4^B(A^B)], \quad (A13b)$$

$$\hat{\lambda}' = \frac{5}{2} \sum_{\beta=A,B} X^\beta I_4^\beta \left(\left(\hat{m}^\beta \zeta^2 - \frac{5}{2} \right) A^\beta \right). \quad (\text{A13c})$$

As mentioned in the second paragraph in Sec. III A, $\hat{\mu}$, $\hat{\lambda}$, and $\hat{D}_{AB}$ correspond to the viscosity μ , thermal conductivity λ , and mutual-diffusion coefficient D_{AB} , respectively; i.e., they are related as $\mu = (\sqrt{\pi}/2)(2kT_0/m_0)^{-1/2} p_0 l_0 \hat{T}_{(0)}^{1/2} \hat{\mu}$, $\lambda = (\sqrt{\pi}k/m_0)(2kT_0/m_0)^{-1/2} p_0 l_0 \hat{T}_{(0)}^{1/2} \hat{\lambda}$, and $D_{AB} = (\sqrt{\pi}/2) \times (2kT_0/m_0)^{1/2} l_0 (\hat{T}_{(0)}^{1/2}/\hat{n}_{(0)}) \hat{D}_{AB}$. The $\hat{D}_T$ corresponds to the thermal-diffusion coefficient D_T ; i.e., $D_T = (\sqrt{\pi}/2) \times (2kT_0/m_0)^{1/2} l_0 (\hat{T}_{(0)}^{1/2}/\hat{n}_{(0)}) \hat{D}_T$. The $\hat{Y}_1$, $\hat{Y}_2$, $\hat{Y}_3$, $\hat{Y}_4$, and $\hat{Y}_5$ are defined by

$$\hat{Y}_1 = \frac{1}{2} \sum_{\beta=A,B} X^\beta I_6^\beta \left(B^\beta \left[A_1^\beta + (\hat{m}^\beta \zeta^2 - 3) A^\beta - \frac{\zeta}{2} \frac{\partial A^\beta}{\partial \zeta} \right] \right), \quad (\text{A14a})$$

$$\hat{Y}_2 = \frac{1}{2} \sum_{\beta=A,B} X^\beta I_6^\beta (A^\beta B^\beta), \quad (\text{A14b})$$

$$\hat{Y}_3 = \hat{Y}_3^{(A,A)} + \hat{Y}_3^{(B,B)} - \hat{Y}_3^{(A,B)} - \hat{Y}_3^{(B,A)}, \quad (\text{A14c})$$

$$\hat{Y}_4 = \hat{Y}_4^{(A)} - \hat{Y}_4^{(B)}, \quad (\text{A14d})$$

$$\hat{Y}_5 = \hat{Y}_5^{(A)} - \hat{Y}_5^{(B)}, \quad (\text{A14e})$$

where

$$\hat{Y}_3^{(\alpha,\gamma)} = \frac{1}{2} \sum_{\beta=A,B} X^\beta I_6^\beta \left(B^\beta D_1^{(\alpha,\gamma)\beta} - D^{(\alpha)\beta} \frac{\partial B^\beta}{\partial X^\gamma} \right), \quad (\text{A15a})$$

$$\hat{Y}_4^{(\alpha)} = \frac{1}{2} \sum_{\beta=A,B} X^\beta I_6^\beta \left(B^\beta \left(D_{A1}^{(\alpha)\beta} + (\hat{m}^\beta \zeta^2 - 2) D^{(\alpha)\beta} - \frac{\zeta}{2} \frac{\partial D^{(\alpha)\beta}}{\partial \zeta} \right) - A^\beta \frac{\partial B^\beta}{\partial X^\alpha} \right), \quad (\text{A15b})$$

$$\hat{Y}_5^{(\alpha)} = \frac{1}{2} \sum_{\beta=A,B} X^\beta I_6^\beta (B^\beta D^{(\alpha)\beta}). \quad (\text{A15c})$$

It should be noted that the partial derivatives of B^α with respect to the concentration X^A or X^B appear in Eq. (A15). Their meaning is as follows. Since Eq. (A3) is also valid for X^A and X^B that are independent of each other, the solution B^α can be regarded as functions of two independent variables X^A and X^B . We first take partial derivatives of such B^α and then introduce the restriction $X^A + X^B = 1$.

A database that gives accurate values of $\hat{\mu}$, $\hat{\lambda}$, $\hat{D}_{AB}$, k_T , $\hat{Y}_1$, $\hat{Y}_2$, $\hat{Y}_3$, $\hat{Y}_4$, and $\hat{Y}_5$ immediately for any value of X^A in the case of $d^B/d^A = 0.5, 1$, and 2 and for many values of m^B/m^A , was constructed in Ref. 24. The database is available from the present authors.

APPENDIX B: SLIP COEFFICIENTS AND THEIR DATABASE

The slip coefficients b_7 and b_9 contained in Eq. (8d) can be obtained by analyzing the two fundamental half-space boundary-value problems for the linearized Boltzmann equation for a binary gas mixture, that is, the thermal-slip (or thermal-creep) problem and the diffusion-slip problem. In Ref. 25, these problems were studied numerically on the basis of the linearized Boltzmann equation and the diffuse-reflection boundary condition. In the present study, the vapor molecules obey the boundary condition (iii) in Sec. II, which is different from the diffuse reflection. However, the values of b_7 and b_9 are unchanged. In Ref. 25, these coefficients are expressed in the following form:

$$b_7 = -b_I \text{ (Ref. 25)} = -\frac{1}{(\hat{m}^A - \hat{m}^B)X^A + \hat{m}^B} \sum_{n=0}^N b_I^{(n)} T_n(2X^A - 1), \quad (\text{B1})$$

$$b_9 = -b_{II} \text{ (Ref. 25)} = -\frac{1}{(\hat{m}^A - \hat{m}^B)X^A + \hat{m}^B} \sum_{n=0}^N b_{II}^{(n)} T_n(2X^A - 1), \quad (\text{B2})$$

where $T_n(x)$ is the Chebyshev polynomial defined by

$$T_n(\cos \theta) = \cos n\theta, \quad (\text{B3})$$

for $0 \leq \theta \leq \pi$. The numerical values of $b_I^{(n)}$ and $b_{II}^{(n)}$ are tabulated for $m^B/m^A = 2, 4, 5$, and 10 and for $d^B/d^A = 1$ in Tables I and II in Ref. 25. For $m^B/m^A = 1/2, 1/4, 1/5$, and $1/10$ in the case of $d^B/d^A = 1$, the corresponding b_7 and b_9 are obtained from these tables with the help of the following simple relation derived by interchanging the roles of A and B components: when $d^B/d^A = 1$,

$$b_7 \left(X^A, \frac{m^B}{m^A} \right) = b_7 \left(1 - X^A, \left(\frac{m^B}{m^A} \right)^{-1} \right) \left(\frac{m^B}{m^A} \right)^{-1/2}, \quad (\text{B4a})$$

$$b_9 \left(X^A, \frac{m^B}{m^A} \right) = -b_9 \left(1 - X^A, \left(\frac{m^B}{m^A} \right)^{-1} \right) \left(\frac{m^B}{m^A} \right)^{-1/2}. \quad (\text{B4b})$$

With Eqs. (B1) and (B2), we can obtain accurate values of b_7 and b_9 instantaneously for any X^A . The corresponding database is available from the authors.

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