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The slip boundary conditions for the compressible Navier–Stokes equations for a polyatomic gas are derived from kinetic theory using the ellipsoidal statistical model of the Boltzmann equation for a polyatomic gas. The analysis, which follows the previous work by the present authors and others for a monatomic gas [K. Aoki *et al.*, J. Stat. Phys. **169**, 744–781 (2017)], is based on the Chapman–Enskog expansion and the analysis of the Knudsen layer adjacent to the boundary. The resulting slip boundary conditions are presented with explicit slip coefficients for some typical polyatomic gases.

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I. INTRODUCTION

In the present paper, we are concerned with rarefied polyatomic gas flows at small Knudsen numbers. Here, the Knudsen number is the ratio of the mean free path of gas molecules to the characteristic length of the considered system. Our aim is to establish the slip boundary conditions for the compressible Navier–Stokes equations for a polyatomic gas. The study is a continuation of the recent paper for a monatomic gas by the present authors and others [1].

For rarefied gas flows, for which the Knudsen number takes an arbitrary value, we need, in principle, to handle the Boltzmann equation. However, because of its complexity, its application to practical gas flow problems is not an easy task though some established numerical methods, such as the direct simulation Monte Carlo (DSMC) method [2, 3], are available nowadays [4–10]. In addition, numerical solution of the Boltzmann equation becomes increasingly difficult as the Knudsen number becomes small, that is, in the vicinity of the so-called fluid-dynamic limit.

For such flows with small Knudsen numbers, an approach alternative to numerical solution of the Boltzmann equation is available. It is the so-called slip flow theory. It has long been known that the combination of the Navier–Stokes equations and appropriate boundary conditions, called the slip boundary conditions, reproduces the correct overall solutions of the corresponding boundary value problems of the Boltzmann equation. A complete slip-flow theory had been established by Sone by a formal but systematic asymptotic analysis of the boundary value problem of the Boltzmann equation for small Knudsen numbers [11–16]. The reader is also referred to his two books [17, 18]. Sone's theory, which we may call the generalized slip-flow theory, provides appropriate combinations of fluid-dynamic-type equations and their slip boundary conditions, which are different depending on the considered physical situations (see Introduction of Ref. [1]). However, for the reason of theoretical rigor, the compressible Navier–Stokes equations never appear in this theory. To be more specific, the latter equations are replaced by the combination of the Euler-type and the viscous-boundary-layer-type equations. Nevertheless, the compressible Navier–Stokes equations are general equations that contain most of the relevant fluid equations, such as the incompressible Euler, Navier–Stokes, Prandtl's boundary-layer equations, as special cases. Therefore, for the convenience of practical applications, it is useful to have the correct slip boundary conditions for the compressible Navier–Stokes equations.

The slip boundary conditions for the compressible Navier–Stokes equations are a classical subject, and some descriptions are found in standard textbooks (see, e.g., Refs. [19, 20]). However, it is hard to find the correct formulas in the general form, with explicit numerical coefficients, that are based on correct derivation using the Boltzmann equation and can be applied immediately to practical problems. The paper by Coron [21] would be the exception that provides the outline of the correct derivation under the assumption that the boundary is at rest. However,

it also does not give numerical values of the coefficients, so that its application to practical problems is not straightforward. This is the reason why Ref. [1] revisited this classical problem and provided the detailed derivation of the correct slip boundary conditions for the compressible Navier–Stokes equations for general time-dependent problems that may include moving boundaries.

Although Ref. [1] is based on the full Boltzmann equation, it restricted itself to the case of a monatomic gas. Therefore, the associated compressible Navier–Stokes equations do not contain the bulk viscosity. In the present study, we try to extend the analysis of Ref. [1] to the case of a polyatomic gas. However, handling the Boltzmann equation for a polyatomic gas is a complicated problem and is not an easy task. Therefore, we employ the ellipsoidal statistical (ES) model of the Boltzmann equation for a polyatomic gas, which was proposed in Ref. [22] and re-derived in a systematic manner in Ref. [23]. On the basis of this model, we will derive the slip boundary conditions for the compressible Navier–Stokes equations for a polyatomic gas. The analysis here tightly follows that in Ref. [1]. Therefore, we let the present paper have a similar structure as that of Ref. [1] on purpose in order to increase the readability.

It should be mentioned that some fluid type (or macroscopic) equations beyond the Navier–Stokes equations have been proposed also for polyatomic gases [24–27] for the purpose of extending the macroscopic theory to larger Knudsen numbers. In the present paper, however, we adhere to the compressible Navier–Stokes equations and do not enter discussions on these approaches.

The structure of the paper is as follows. After this introduction, the problem and the assumptions are stated in Sec. II. Section III is devoted to the formulation of the problem, which contains the detailed description of the basic equations and boundary conditions. In Sec. IV, the first-order Chapman–Enskog solution, together with the associated compressible Navier–Stokes equations, is summarized. The corresponding slip boundary conditions are derived by the Knudsen-layer analysis in Sec. V, which is the main part of the paper. In Sec. VI, the compressible Navier–Stokes equations and their slip boundary conditions are presented in the dimensional form. Some concluding remarks are given in Sec. VII.

II. PROBLEM AND ASSUMPTIONS

We consider a polyatomic ideal gas in contact with solid boundaries of arbitrary but smooth shape. The gas may extend to infinity, and no external force acts on the gas molecules. We investigate the unsteady motion of the gas under the following assumptions:

(i) The behavior of the gas is described by the ES model of the Boltzmann equation for a polyatomic gas [22, 23].

(ii) The boundaries do not deform and undergo a rigid-body motion, and the gas-surface interaction is described by the Maxwell-type diffuse-specular reflection [17, 18].

(iii) The mean free path (or the mean free time) of the gas molecules at the reference equilibrium state at rest is sufficiently small compared to the characteristic length (or the characteristic time) of the system.

(iv) At the initial time, the boundaries are at rest and have a uniform temperature, and the gas is in the equilibrium state at rest with the same temperature. After the initial time, the boundaries may start moving smoothly, and their temperature may change smoothly in time and position. (For the problems including infinities, the corresponding initial state and slow variations should be assumed at infinities.)

We put assumption (iv) for the same reason as in Ref. [1]. That is, we want to avoid the occurrence of the initial layer and that of the interaction between the initial layer and the Knudsen layer during the initial stage for the sake of theoretical rigor. However, assumption (iv) can be released if we admit the inaccuracy during the initial stage with the duration of the order of the mean free time.

III. FORMULATION OF THE PROBLEM

A. Basic equations

Let us consider a polyatomic gas with internal degrees of freedom δ ($\delta \geq 2$). Let t be the time variable, $\boldsymbol{X}$ (or X_i) the position vector in the physical space, $\boldsymbol{\xi}$ (or ξ_i) the molecular velocity, and $\mathcal{E}$ the energy per unit mass associated with the internal modes. We denote the number of the gas molecules contained in an infinitesimal volume $d\boldsymbol{X}d\boldsymbol{\xi}d\mathcal{E}$ around a point $(\boldsymbol{X}, \boldsymbol{\xi}, \mathcal{E})$ in the seven-dimensional space consisting of $\boldsymbol{X}$, $\boldsymbol{\xi}$, and $\mathcal{E}$ by

$$\frac{1}{m} f(t, \boldsymbol{X}, \boldsymbol{\xi}, \mathcal{E}) d\boldsymbol{X} d\boldsymbol{\xi} d\mathcal{E}, \tag{1}$$

where m is the mass of a molecule. We call $f(t, \boldsymbol{X}, \boldsymbol{\xi}, \mathcal{E})$ the velocity/energy distribution function of the gas molecules. It is governed by the ES model of the Boltzmann equation for a polyatomic gas [22, 23], which can be written in the following form:

$$\frac{\partial f}{\partial t} + \xi_i \frac{\partial f}{\partial X_i} = Q(f), \tag{2}$$

where

$$Q(f) = A_c(T)\rho(\mathcal{G} - f), \tag{3a}$$

$$\mathcal{G} = \frac{\rho \mathcal{E}^{\delta/2-1}}{(2\pi)^{3/2}(\det \mathsf{T})^{1/2}(RT_{\mathrm{rel}})^{\delta/2}\Gamma(\delta/2)} \exp\left(-\frac{1}{2}(\xi_i - v_i)(\mathsf{T}^{-1})_{ij}(\xi_j - v_j) - \frac{\mathcal{E}}{RT_{\mathrm{rel}}}\right), \tag{3b}$$

$$(\mathsf{T})_{ij} = (1-\theta)[(1-\nu)RT_{\mathrm{tr}}\delta_{ij} + \nu p_{ij}/\rho] + \theta RT\delta_{ij}, \tag{3c}$$

$$\rho = \iint_0^\infty f d\mathcal{E} d\boldsymbol{\xi}, \tag{3d}$$

$$v_i = \frac{1}{\rho} \iint_0^\infty \xi_i f d\mathcal{E} d\boldsymbol{\xi}, \tag{3e}$$

$$p_{ij} = \iint_0^\infty (\xi_i - v_i)(\xi_j - v_j) f d\mathcal{E} d\boldsymbol{\xi}, \tag{3f}$$

$$T_{\mathrm{tr}} = \frac{1}{3\rho R} \iint_0^\infty |\boldsymbol{\xi} - \boldsymbol{v}|^2 f d\mathcal{E} d\boldsymbol{\xi}, \tag{3g}$$

$$T_{\mathrm{int}} = \frac{2}{\delta \rho R} \iint_0^\infty \mathcal{E} f d\mathcal{E} d\boldsymbol{\xi}, \tag{3h}$$

$$T = \frac{3T_{\mathrm{tr}} + \delta T_{\mathrm{int}}}{3+\delta}, \tag{3i}$$

$$T_{\mathrm{rel}} = \theta T + (1-\theta) T_{\mathrm{int}}. \tag{3j}$$

Here, R is the gas constant per unit mass (i.e., the Boltzmann constant k_{B} divided by m), ρ is the density, $\boldsymbol{v}$ (or v_i) the flow velocity, p_{ij} the stress tensor, T_{tr} the temperature associated with the translational motion, T_{int} the temperature associated with the energy of the internal modes, T the temperature, $d\boldsymbol{\xi} = d\xi_1 d\xi_2 d\xi_3$, and the domain of integration with respect to $\boldsymbol{\xi}$ is the whole space of $\boldsymbol{\xi}$. The symbol δ_{ij} indicates the Kronecker delta, and $\nu \in [-1/2, 1)$ and $\theta \in (0, 1]$ are the constants that adjust the Prandtl number and the bulk viscosity. In addition, $A_c(T)$ is a function of T such that $A_c(T)\rho$ is the collision frequency of the gas molecules, $\Gamma(z)$ is the gamma function defined by

$$\Gamma(z) = \int_0^\infty s^{z-1} e^{-s} ds, \tag{4}$$

T is the 3×3 matrix the (i, j) component of which is defined by Eq. (3c), and $\det \mathsf{T}$ and T^{-1} are, respectively, its determinant and inverse. Here and in what follows, we basically use the summation convention, i.e., $a_i b_i = \sum_{i=1}^3 a_i b_i$, $a_i^2 = \sum_{i=1}^3 a_i^2$, $a_i b_j c_{ij} = \sum_{i,j=1}^3 a_i b_j c_{ij}$, etc.

We should note that in Ref. [22], the variable I, which is related to our $\mathcal{E}$ as $\mathcal{E} = I^{2/\delta}$, is used as an independent variable instead of $\mathcal{E}$. See Ref. [28] or Appendix A in Ref. [29] for the relation between the notation in Ref. [22] and that of the present paper.

The vanishing of the collision term $Q(f) = 0$ is equivalent to the fact that f is the following local equilibrium distribution [22]:

$$f_{\mathrm{eq}} = \frac{\rho \mathcal{E}^{\delta/2-1}}{(2\pi RT)^{3/2}(RT)^{\delta/2}\Gamma(\delta/2)} \exp\left(-\frac{|\boldsymbol{\xi}-\boldsymbol{v}|^2}{2RT} - \frac{\mathcal{E}}{RT}\right). \tag{5}$$

In addition, for an arbitrary function $g(t,\, \boldsymbol{X},\, \boldsymbol{\xi},\, \mathcal{E})$, the following relation holds:

$$\iint_0^\infty \varphi_r Q(g) d\mathcal{E} d\boldsymbol{\xi} = 0, \tag{6}$$

where φ_r ($r = 0,\, ...,\, 4$) are the collision invariants, i.e.,

$$\varphi_0 = 1, \qquad \varphi_i = \xi_i \quad (i = 1,\, 2,\, 3), \qquad \varphi_4 = \frac{1}{2}|\boldsymbol{\xi}|^2 + \mathcal{E}. \tag{7}$$

It should also be mentioned that the mean free path l_0 of the gas molecules in the equilibrium state at rest at density ρ_0 and temperature T_0 is given by

$$l_0 = \frac{2}{\sqrt{\pi}} \frac{(2RT_0)^{1/2}}{A_c(T_0)\rho_0}, \tag{8}$$

for Eq. (2), since $A_c(T_0)\rho_0$ is the collision frequency at this equilibrium state.

The initial condition for f [cf. assumption (iv)] is given at time $t = 0$ by

$$f(0,\, \boldsymbol{X},\, \boldsymbol{\xi},\, \mathcal{E}) = f_0, \tag{9}$$

where f_0 indicates the equilibrium state at rest with density ρ_0 (reference density) and temperature T_0 (reference temperature), i.e.,

$$f_0 = \frac{\rho_0 \mathcal{E}^{\delta/2-1}}{(2\pi RT_0)^{3/2}(RT_0)^{\delta/2}\Gamma(\delta/2)} \exp\left(-\frac{|\boldsymbol{\xi}|^2}{2RT_0} - \frac{\mathcal{E}}{RT_0}\right). \tag{10}$$

The boundary condition for f [cf. assumption (ii)] is written in the following form:

$$\begin{aligned} f(t,\, \boldsymbol{X}_{\mathrm{w}},\, \boldsymbol{\xi},\, \mathcal{E}) &= (1-\alpha)\mathcal{R} f(t,\, \boldsymbol{X}_{\mathrm{w}},\, \boldsymbol{\xi},\, \mathcal{E}) \\ &\quad + \alpha \frac{\rho_{\mathrm{w}} \mathcal{E}^{\delta/2-1}}{(2\pi RT_{\mathrm{w}})^{3/2}(RT_{\mathrm{w}})^{\delta/2}\Gamma(\delta/2)} \exp\left(-\frac{|\boldsymbol{\xi}-\boldsymbol{v}_{\mathrm{w}}|^2}{2RT_{\mathrm{w}}} - \frac{\mathcal{E}}{RT_{\mathrm{w}}}\right), \\ &\qquad\qquad \text{for} \quad (\boldsymbol{\xi}-\boldsymbol{v}_{\mathrm{w}})\cdot\boldsymbol{n} > 0, \end{aligned} \tag{11a}$$

$$\rho_{\mathrm{w}} = -\left(\frac{2\pi}{RT_{\mathrm{w}}}\right)^{1/2} \int_{(\boldsymbol{\xi}-\boldsymbol{v}_{\mathrm{w}})\cdot\boldsymbol{n}<0} \int_0^\infty (\boldsymbol{\xi}-\boldsymbol{v}_{\mathrm{w}})\cdot\boldsymbol{n} f(t,\, \boldsymbol{X}_{\mathrm{w}},\, \boldsymbol{\xi},\, \mathcal{E}) d\mathcal{E} d\boldsymbol{\xi}, \tag{11b}$$

where $\boldsymbol{X}_{\mathrm{w}}$ (or $X_{\mathrm{w}i}$) is the position of a point on the boundary, $\boldsymbol{v}_{\mathrm{w}}$ (or $v_{\mathrm{w}i}$) and T_{w} are the velocity and temperature of the boundary at the point $\boldsymbol{X}_{\mathrm{w}}$, and $\boldsymbol{n}$ is the unit normal vector to the boundary, pointing into the gas, at $\boldsymbol{X}_{\mathrm{w}}$. In general, $\boldsymbol{X}_{\mathrm{w}}$ is a function of t, $\boldsymbol{v}_{\mathrm{w}}$ is the time derivative of $\boldsymbol{X}_{\mathrm{w}}$, and the arguments of T_{w} and $\boldsymbol{n}$ are $(t,\, \boldsymbol{X}_{\mathrm{w}})$. To be consistent with assumption (iv), $\boldsymbol{v}_{\mathrm{w}} = 0$ and $T_{\mathrm{w}} = T_0$ should hold at $t = 0$, and $\boldsymbol{X}_{\mathrm{w}}$ (thus, $\boldsymbol{v}_{\mathrm{w}}$), T_{w}, and $\boldsymbol{n}$ are assumed to change smoothly with t. In Eq. (11a), the symbol $\mathcal{R}$ indicates the reflection operator defined by

$$\mathcal{R} g(\xi_i) = g(\xi_i - 2(\xi_j - v_{\mathrm{w}j})n_j n_i), \tag{12}$$

with an arbitrary function $g(\boldsymbol{\xi})$ of $\boldsymbol{\xi}$, and α ($0 \le \alpha \le 1$) is the so-called accommodation coefficient, giving the specular reflection when $\alpha = 0$ and the diffuse reflection when $\alpha = 1$. In the present paper, we exclude the case of specular reflection assuming that α is strictly positive. Note that this boundary condition satisfies the condition that there is no instantaneous mass flow across the boundary, i.e.,

$$\iint_0^\infty (\boldsymbol{\xi}-\boldsymbol{v}_{\mathrm{w}})\cdot\boldsymbol{n} f(t,\, \boldsymbol{X}_{\mathrm{w}},\, \boldsymbol{\xi},\, \mathcal{E}) d\mathcal{E} d\boldsymbol{\xi} = 0. \tag{13}$$

Finally, we should mention that the pressure p and the heat-flow vector q_i are given by

$$p = R\rho T, \tag{14}$$

$$q_i = \iint_0^\infty (\xi_i - v_i)\left(\frac{1}{2}|\boldsymbol{\xi} - \boldsymbol{v}|^2 + \mathcal{E}\right) f d\mathcal{E} d\boldsymbol{\xi}, \tag{15}$$

where Eq. (14) is the equation of state.

B. Dimensionless system

In this subsection we introduce dimensionless variables and present our basic system in dimensionless form. Let us denote by L the reference length, t_0 the reference time, and $p_0 = R\rho_0 T_0$ the reference pressure, where ρ_0 and T_0 are the reference density and temperature appeared in the initial state, Eq. (10). In the present study, we choose t_0 as

$$t_0 = L/(2RT_0)^{1/2}, \tag{16}$$

which corresponds to the so-called fluid-dynamic scaling. Now we introduce the dimensionless quantities ($\hat{t}$, x_i, ζ_i, $\hat{\mathcal{E}}$, $\hat{f}$, $\hat{\mathcal{G}}$, $\hat{\rho}$, $\hat{v}_i$, $\hat{T}_{\rm tr}$, $\hat{T}_{\rm int}$, $\hat{T}$, $\hat{T}_{\rm rel}$, $\hat{p}_{ij}$, $\hat{p}$, $\hat{q}_i$, $\hat{A}_c(\hat{T})$, $x_{{\rm w}i}$, $\hat{v}_{{\rm w}i}$, $\hat{T}_{\rm w}$), which correspond to the original dimensional quantities (t, X_i, ξ_i, $\mathcal{E}$, f, $\mathcal{G}$, ρ, v_i, $T_{\rm tr}$, $T_{\rm int}$, T, $T_{\rm rel}$, p_{ij}, p, q_i, $A_c(T)$, $X_{{\rm w}i}$, $v_{{\rm w}i}$, $T_{\rm w}$), by the following relations:

$$\begin{aligned}
&\hat{t} = t/t_0, \quad x_i = X_i/L, \quad \zeta_i = \xi_i/(2RT_0)^{1/2}, \quad \hat{\mathcal{E}} = \mathcal{E}/RT_0, \\
&(\hat{f}, \hat{\mathcal{G}}) = (f, \mathcal{G})/2\rho_0(2RT_0)^{-5/2}, \quad \hat{\rho} = \rho/\rho_0, \quad \hat{v}_i = v_i/(2RT_0)^{1/2}, \\
&(\hat{T}_{\rm tr}, \hat{T}_{\rm int}, \hat{T}, \hat{T}_{\rm rel}) = (T_{\rm tr}, T_{\rm int}, T, T_{\rm rel})/T_0, \quad \hat{p}_{ij} = p_{ij}/p_0, \quad \hat{p} = p/p_0, \quad \hat{q}_i = q_i/p_0(2RT_0)^{1/2}, \\
&\hat{A}_c(\hat{T}) = A_c(T)/A_c(T_0), \quad x_{{\rm w}i} = X_{{\rm w}i}/L, \quad \hat{v}_{{\rm w}i} = v_{{\rm w}i}/(2RT_0)^{1/2}, \quad \hat{T}_{\rm w} = T_{\rm w}/T_0.
\end{aligned} \tag{17}$$

We occasionally use the bold-faced letters $\boldsymbol{x}$, $\boldsymbol{\zeta}$, $\hat{\boldsymbol{v}}$, $\hat{\boldsymbol{q}}$, $\boldsymbol{x}_{\rm w}$, and $\hat{\boldsymbol{v}}_{\rm w}$ for x_i, ζ_i, $\hat{v}_i$, $\hat{q}_i$, $x_{{\rm w}i}$, and $\hat{v}_{{\rm w}i}$, respectively.

Then, we obtain the dimensionless form of the ES model (2) as follows:

$$\frac{\partial \hat{f}}{\partial \hat{t}} + \zeta_i \frac{\partial \hat{f}}{\partial x_i} = \frac{1}{\epsilon}\hat{Q}(\hat{f}), \tag{18}$$

where

$$\hat{Q}(\hat{f}) = \hat{A}_c(\hat{T})\hat{\rho}(\hat{\mathcal{G}} - \hat{f}), \tag{19a}$$

$$\hat{\mathcal{G}} = \frac{\hat{\rho}}{\pi^{3/2}(\det\hat{\mathsf{T}})^{1/2}\,\hat{T}_{\rm rel}^{\delta/2}\Gamma(\delta/2)}\,\hat{\mathcal{E}}^{\delta/2-1}\exp\left(-(\zeta_i - \hat{v}_i)(\hat{\mathsf{T}}^{-1})_{ij}(\zeta_j - \hat{v}_j) - \frac{\hat{\mathcal{E}}}{\hat{T}_{\rm rel}}\right), \tag{19b}$$

$$(\hat{\mathsf{T}})_{ij} = (1-\theta)[(1-\nu)\hat{T}_{\rm tr}\delta_{ij} + \nu\hat{p}_{ij}/\hat{\rho}] + \theta\hat{T}\delta_{ij}, \tag{19c}$$

$$\hat{\rho} = \iint_0^\infty \hat{f} d\hat{\mathcal{E}} d\boldsymbol{\zeta}, \tag{19d}$$

$$\hat{v}_i = \frac{1}{\hat{\rho}}\iint_0^\infty \zeta_i \hat{f} d\hat{\mathcal{E}} d\boldsymbol{\zeta}, \tag{19e}$$

$$\hat{p}_{ij} = 2\iint_0^\infty (\zeta_i - \hat{v}_i)(\zeta_j - \hat{v}_j)\hat{f} d\hat{\mathcal{E}} d\boldsymbol{\zeta}, \tag{19f}$$

$$\hat{T}_{\rm tr} = \frac{2}{3\hat{\rho}}\iint_0^\infty (\zeta_k - \hat{v}_k)^2 \hat{f} d\hat{\mathcal{E}} d\boldsymbol{\zeta}, \tag{19g}$$

$$\hat{T}_{\rm int} = \frac{2}{\delta\hat{\rho}}\iint_0^\infty \hat{\mathcal{E}}\hat{f} d\hat{\mathcal{E}} d\boldsymbol{\zeta}, \tag{19h}$$

$$\hat{T} = \frac{3\hat{T}_{\rm tr} + \delta\hat{T}_{\rm int}}{3+\delta}, \tag{19i}$$

$$\hat{T}_{\rm rel} = \theta\hat{T} + (1-\theta)\hat{T}_{\rm int}. \tag{19j}$$

Here, ϵ is a quantity of the order of the Knudsen number Kn defined by

$$\epsilon = \frac{\sqrt{\pi}}{2}{\rm Kn} = \frac{\sqrt{\pi}}{2}\frac{l_0}{L}, \tag{20}$$

$d\boldsymbol{\zeta} = d\zeta_1 d\zeta_2 d\zeta_3$, and the domain of integration with respect to $\boldsymbol{\zeta}$ is the whole space of $\boldsymbol{\zeta}$. The (dimensionless) pressure $\hat{p}$ and heat-flow vector $\hat{q}_i$ are given by

$$\hat{p} = \hat{\rho}\hat{T}, \tag{21}$$

$$\hat{q}_i = \iint_0^\infty (\zeta_i - \hat{v}_i)(|\boldsymbol{\zeta} - \hat{\boldsymbol{v}}|^2 + \hat{\mathcal{E}})\hat{f} d\hat{\mathcal{E}} d\boldsymbol{\zeta}. \tag{22}$$

Corresponding to the statement including Eq. (5), $\hat{Q}(\hat{f}) = 0$ is equivalent to the fact that $\hat{f}$ is the dimensionless local equilibrium given by

$$\hat{f}_{\rm eq} = \frac{\hat{\rho}\hat{\mathcal{E}}^{\delta/2-1}}{(\pi\hat{T})^{3/2}\hat{T}^{\delta/2}\Gamma(\delta/2)} \exp\left(-\frac{|\boldsymbol{\zeta} - \hat{\boldsymbol{v}}|^2}{\hat{T}} - \frac{\hat{\mathcal{E}}}{\hat{T}}\right). \tag{23}$$

In addition, the dimensionless version of the statement containing Eqs. (6) and (7) reads as follows: For an arbitrary function $\hat{g}(\hat{t}, \boldsymbol{x}, \boldsymbol{\zeta}, \hat{\mathcal{E}})$, the relation

$$\iint_0^\infty \hat{\varphi}_r \hat{Q}(\hat{g}) d\hat{\mathcal{E}} d\boldsymbol{\zeta} = 0 \tag{24}$$

holds, where $\hat{\varphi}_r$ ($r = 0, ..., 4$) are the dimensionless collision invariants, i.e.,

$$\hat{\varphi}_0 = 1, \qquad \hat{\varphi}_i = \zeta_i \quad (i = 1, 2, 3), \qquad \hat{\varphi}_4 = |\boldsymbol{\zeta}|^2 + \hat{\mathcal{E}}. \tag{25}$$

The dimensionless form of the initial condition (9) is written as

$$\hat{f}(0, \boldsymbol{x}, \boldsymbol{\zeta}, \hat{\mathcal{E}}) = \hat{f}_0, \tag{26}$$

where

$$\hat{f}_0 = [\Gamma(\delta/2)]^{-1} E(\zeta)\hat{\mathcal{E}}^{\delta/2-1} e^{-\hat{\mathcal{E}}}, \qquad \zeta = |\boldsymbol{\zeta}| = (\zeta_i^2)^{1/2}, \qquad E(\zeta) = \pi^{-3/2}\exp(-\zeta^2). \tag{27}$$

The boundary condition (11) is non-dimensionalized as follows:

$$\begin{aligned}\hat{f}(\hat{t}, \boldsymbol{x}_{\rm w}, \boldsymbol{\zeta}, \hat{\mathcal{E}}) &= (1-\alpha)\hat{\mathcal{R}}\hat{f}(\hat{t}, \boldsymbol{x}_{\rm w}, \boldsymbol{\zeta}, \hat{\mathcal{E}}) \\ &\quad + \alpha\frac{\hat{\rho}_{\rm w}\hat{\mathcal{E}}^{\delta/2-1}}{(\pi\hat{T}_{\rm w})^{3/2}\hat{T}_{\rm w}^{\delta/2}\Gamma(\delta/2)} \exp\left(-\frac{|\boldsymbol{\zeta} - \hat{\boldsymbol{v}}_{\rm w}|^2}{\hat{T}_{\rm w}} - \frac{\hat{\mathcal{E}}}{\hat{T}_{\rm w}}\right), \\ &\qquad\qquad \text{for} \quad (\boldsymbol{\zeta} - \hat{\boldsymbol{v}}_{\rm w})\cdot\boldsymbol{n} > 0,\end{aligned} \tag{28a}$$

$$\hat{\rho}_{\rm w} = -2\left(\frac{\pi}{\hat{T}_{\rm w}}\right)^{1/2} \int_{(\boldsymbol{\zeta}-\hat{\boldsymbol{v}}_{\rm w})\cdot\boldsymbol{n}<0} \int_0^\infty (\boldsymbol{\zeta} - \hat{\boldsymbol{v}}_{\rm w})\cdot\boldsymbol{n}\hat{f}(\hat{t}, \boldsymbol{x}_{\rm w}, \boldsymbol{\zeta}, \hat{\mathcal{E}}) d\hat{\mathcal{E}} d\boldsymbol{\zeta}, \tag{28b}$$

where $\hat{\mathcal{R}}$ is the dimensionless reflection operator, corresponding to (12), acting on any function $\hat{g}$ of ζ_i, i.e.,

$$\hat{\mathcal{R}}\hat{g}(\zeta_i) = \hat{g}(\zeta_i - 2(\zeta_j - \hat{v}_{{\rm w}j})n_j n_i). \tag{29}$$

We note that $\hat{\boldsymbol{v}}_{\rm w} = 0$ and $\hat{T}_{\rm w} = 1$ at $\hat{t} = 0$, and $\boldsymbol{x}_{\rm w}$ (thus $\hat{\boldsymbol{v}}_{\rm w}$), $\hat{T}_{\rm w}$, and $\boldsymbol{n}$ are assumed to change smoothly in $\hat{t}$. Corresponding to Eq. (13), the following condition holds on the boundary:

$$\iint_0^\infty (\boldsymbol{\zeta} - \hat{\boldsymbol{v}}_{\rm w})\cdot\boldsymbol{n}\hat{f}(\hat{t}, \boldsymbol{x}_{\rm w}, \boldsymbol{\zeta}, \hat{\mathcal{E}}) d\hat{\mathcal{E}} d\boldsymbol{\zeta} = 0. \tag{30}$$

We will analyze the initial- and boundary-value problem, Eqs. (18), (26), and (28), for small values of the Knudsen number Kn, i.e., for $\epsilon \ll 1$. Since the reference time is $t_0 = L/(2RT_0)^{1/2} = 1/\epsilon\overline{\nu_c}$, where $\overline{\nu_c} = \rho_0 A_c(T_0)$ is the mean collision frequency at the reference equilibrium state, it is much longer than the mean free time $1/\overline{\nu_c}$.

IV. CHAPMAN–ENSKOG EXPANSION AND THE COMPRESSIBLE NAVIER–STOKES EQUATIONS

As is well known, the compressible Navier–Stokes equations are formally obtained from the Boltzmann equation by the Chapman–Enskog expansion [18, 20, 30, 31]. For the present ES model for a polyatomic gas, the compressible Navier–Stokes equations are derived in Ref. [22]. In this section, we just summarize the first-order Chapman–Enskog solution and the resulting Navier–Stokes equations. The Chapman–Enskog solution is based on the assumption that the length scale of variation is of $O(1)$ [or $O(L)$ in the dimensional space] and the initial and boundary conditions are not considered. Therefore, the solution has a specific property, so that it should be distinguished from the correct solution f for the initial and boundary value problem of the ES model by an appropriate subscript, such as f_{CE}. However, in order to avoid cumbersome notation, we denote it just by f in this and following sections except in some places that need clarification.

A. Linearized collision operator

In this subsection, we summarize the linearized collision operator of the ES model. Let us consider the case where the deviation from the equilibrium state at rest with density ρ_0 and temperature T_0 is small and put $\hat{f} = \hat{f}_0(1+\phi)$ [cf. Eq. (27)], where $|\phi| \ll 1$. If we insert this $\hat{f}$ in $\hat{Q}(\hat{f})$ [cf. Eq. (19a)] and neglect the terms of the order of ϕ^2 and higher, then we obtain

$$\hat{Q}(\hat{f}) = \hat{f}_0 \mathcal{L}(\phi) = [\Gamma(\delta/2)]^{-1} E(\zeta) \hat{\mathcal{E}}^{\delta/2-1} e^{-\hat{\mathcal{E}}} \mathcal{L}(\phi), \tag{31}$$

where

$$\mathcal{L}[\phi(\hat{t}, \boldsymbol{x}, \boldsymbol{\zeta}, \hat{\mathcal{E}})](\hat{t}, \boldsymbol{x}, \boldsymbol{\zeta}, \hat{\mathcal{E}}) = \omega + 2\zeta_i u_i + \left(\hat{\mathcal{E}} - \frac{\delta}{2}\right)\tau_{\mathrm{rel}} + \left(\zeta_i\zeta_j - \frac{\delta_{ij}}{2}\right) d_{ij} - \phi, \tag{32a}$$

$$\omega = \langle \phi \rangle, \qquad u_i = \langle \zeta_i \phi \rangle, \tag{32b}$$

$$\tau_{\mathrm{rel}} = \theta\tau + (1-\theta)\tau_{\mathrm{int}}, \qquad \tau = \frac{3\tau_{\mathrm{tr}} + \delta\tau_{\mathrm{int}}}{3+\delta}, \tag{32c}$$

$$\tau_{\mathrm{tr}} = \frac{2}{3}\left\langle \left(\zeta^2 - \frac{3}{2}\right)\phi \right\rangle, \qquad \tau_{\mathrm{int}} = \frac{2}{\delta}\left\langle \left(\hat{\mathcal{E}} - \frac{\delta}{2}\right)\phi \right\rangle, \tag{32d}$$

$$d_{ij} = [(1-\theta)\tau_{\mathrm{tr}} + \theta\tau]\delta_{ij} + (1-\theta)\nu[P_{ij} - (\omega + \tau_{\mathrm{tr}})\delta_{ij}], \qquad P_{ij} = 2\langle \zeta_i\zeta_j\phi \rangle, \tag{32e}$$

and $\langle\,\cdot\,\rangle$ is defined, with an arbitrary function $\hat{g}(\boldsymbol{\zeta}, \hat{\mathcal{E}})$ of $\boldsymbol{\zeta}$ and $\hat{\mathcal{E}}$, as

$$\langle\, \hat{g}(\boldsymbol{\zeta}, \hat{\mathcal{E}})\,\rangle = \iint_0^\infty \hat{g}(\boldsymbol{\zeta}, \hat{\mathcal{E}}) \hat{f}_0(\zeta, \hat{\mathcal{E}}) d\hat{\mathcal{E}} d\boldsymbol{\zeta} = \iint_0^\infty \hat{g}(\boldsymbol{\zeta}, \hat{\mathcal{E}}) [\Gamma(\delta/2)]^{-1} E(\zeta) \hat{\mathcal{E}}^{\delta/2-1} e^{-\hat{\mathcal{E}}} d\hat{\mathcal{E}} d\boldsymbol{\zeta}. \tag{33}$$

In Eq. (32a), the argument of ϕ and that of $\mathcal{L}(\phi)$ are shown explicitly on the left-hand side. The operator $\mathcal{L}(\,\cdot\,)$ is the linearized collision operator of the ES collision operator $Q(\,\cdot\,)$ in Eq. (3a) or $\hat{Q}(\,\cdot\,)$ in (19a). It satisfies the relation

$$\langle \hat{\varphi}_r \mathcal{L}(\hat{g}) \rangle = 0, \tag{34}$$

where $\hat{\varphi}_r$ ($r = 0, ..., 4$) are given in Eq. (25). In addition, we introduce the following modified operator $\mathcal{L}_a(\phi)$:

$$\mathcal{L}_a(\phi) = \hat{A}_c(a)\, a^{-1/2} \mathcal{L}(\phi). \tag{35}$$

B. Chapman–Enskog solution and Navier–Stokes equations

As is well known, the Navier–Stokes equations correspond to the first-order Chapman–Enskog solution, which can be expressed as

$$\hat{f} = \hat{f}^{(0)} + \hat{f}^{(1)}\epsilon + O(\epsilon^2). \tag{36}$$

Here, the leading-order term $\hat{f}^{(0)}$ is a local equilibrium distribution

$$\hat{f}^{(0)} = \frac{\hat{\rho}\hat{\mathcal{E}}^{\delta/2-1}}{(\pi\hat{T})^{3/2}\hat{T}^{\delta/2}\Gamma(\delta/2)} \exp\left(-\frac{|\boldsymbol{\zeta}-\hat{\boldsymbol{v}}|^2}{\hat{T}} - \frac{\hat{\mathcal{E}}}{\hat{T}}\right), \tag{37}$$

and the first-order term $\hat{f}^{(1)}$ is given by the following form:

$$\hat{f}^{(1)} = \hat{f}^{(0)}\Psi, \tag{38a}$$

$$\Psi = -\frac{1}{\hat{\rho}\hat{T}}\mathcal{C}_j\mathcal{A}(\mathcal{C},\,\bar{\mathcal{E}},\,\hat{T})\frac{\partial\hat{T}}{\partial x_j} - \frac{1}{2\hat{\rho}\hat{T}^{1/2}}\left(\mathcal{C}_j\mathcal{C}_k - \frac{1}{3}\mathcal{C}^2\delta_{jk}\right)\mathcal{B}(\hat{T})\left(\frac{\partial\hat{v}_k}{\partial x_j} + \frac{\partial\hat{v}_j}{\partial x_k}\right) - \frac{1}{\hat{\rho}\hat{T}^{1/2}}\mathcal{B}_b(\mathcal{C},\,\bar{\mathcal{E}},\,\hat{T})\frac{\partial\hat{v}_j}{\partial x_j}, \tag{38b}$$

where

$$\mathcal{C}_i = \frac{\zeta_i - \hat{v}_i}{\hat{T}^{1/2}}, \qquad \mathcal{C} = |\boldsymbol{\mathcal{C}}| = (\mathcal{C}_j^2)^{1/2}, \qquad \bar{\mathcal{E}} = \frac{\hat{\mathcal{E}}}{\hat{T}}, \tag{39}$$

and $\mathcal{A}(\mathcal{C},\,\bar{\mathcal{E}},\,\hat{T})$, $\mathcal{B}(\hat{T})$, and $\mathcal{B}_b(\mathcal{C},\,\bar{\mathcal{E}},\,\hat{T})$ are the functions defined by

$$\mathcal{A}(\mathcal{C},\,\bar{\mathcal{E}},\,\hat{T}) = \frac{\hat{T}^{1/2}}{\hat{A}_c(\hat{T})}\left(\mathcal{C}^2 - \frac{5+\delta}{2} + \bar{\mathcal{E}}\right), \tag{40a}$$

$$\mathcal{B}(\hat{T}) = \frac{2}{1-\nu+\theta\nu}\frac{\hat{T}^{1/2}}{\hat{A}_c(\hat{T})}, \tag{40b}$$

$$\mathcal{B}_b(\mathcal{C},\,\bar{\mathcal{E}},\,\hat{T}) = \frac{1}{\theta}\frac{2}{3+\delta}\frac{\hat{T}^{1/2}}{\hat{A}_c(\hat{T})}\left(\frac{1}{3}\delta\,\mathcal{C}^2 - \bar{\mathcal{E}}\right). \tag{40c}$$

More specifically, they are the solutions of the following integral equations:

$$\mathcal{L}_{\hat{T}}(\mathcal{C}_i\mathcal{A}) = -\mathcal{C}_i\left(\mathcal{C}^2 - \frac{5+\delta}{2} + \bar{\mathcal{E}}\right), \text{ with subsidiary condition } \langle\mathcal{C}^2\mathcal{A}\rangle = 0, \tag{41a}$$

$$\mathcal{L}_{\hat{T}}\left(\left(\mathcal{C}_j\mathcal{C}_k - \frac{1}{3}\mathcal{C}^2\delta_{jk}\right)\mathcal{B}\right) = -2\left(\mathcal{C}_j\mathcal{C}_k - \frac{1}{3}\mathcal{C}^2\delta_{jk}\right), \tag{41b}$$

$$\mathcal{L}_{\hat{T}}(\mathcal{B}_b) = -\frac{2}{3+\delta}\left(\frac{1}{3}\delta\mathcal{C}^2 - \bar{\mathcal{E}}\right), \text{ with subsidiary condition } \langle\mathcal{B}_b\rangle = \langle(\mathcal{C}^2+\bar{\mathcal{E}})\mathcal{B}_b\rangle = 0. \tag{41c}$$

Note that the independent variables in $\mathcal{L}_{\hat{T}}(\,\cdot\,)$ are $\boldsymbol{\mathcal{C}}$ and $\bar{\mathcal{E}}$, and the integration variables in $\langle\,\cdot\,\rangle$ [thus in $\mathcal{L}_{\hat{T}}(\,\cdot\,)$] are also $\boldsymbol{\mathcal{C}}$ and $\bar{\mathcal{E}}$.

The macroscopic quantities associated with the Chapman–Enskog expansion are also given by Eqs. (19d)–(19j), (21), and (22). However, the expansion (36) is designed in such a way that $\hat{\rho}$, $\hat{\boldsymbol{v}}$, and $\hat{T}$ in Eq. (37) are, respectively, the density, flow velocity, and temperature associated with $\hat{f}$. Therefore, the corresponding moments of the first and higher-order terms should vanish. That is, we construct these terms in such a way that

$$\iint_0^\infty \hat{\varphi}_r\hat{f}^{(1)}d\hat{\mathcal{E}}d\boldsymbol{\zeta} = 0, \tag{42}$$

holds for $\hat{f}^{(1)}$ and the same is true for the $O(\epsilon^2)$ terms in Eq. (36). Here, $\hat{\varphi}_r$ ($r = 0, ..., 4$) are the dimensionless collision invariants given in Eq. (25). One can directly confirm that Eq. (38) fulfills this requirement.

Inserting the expansion (36) with Eqs. (37) and (38) into Eqs. (19g) and (19h) leads to the following dimensionless translational and internal temperatures $\hat{T}_{\rm tr}$ and $\hat{T}_{\rm int}$:

$$\hat{T}_{\rm tr} = \hat{T} - \epsilon\frac{2}{3}\frac{\delta}{\theta(3+\delta)}\frac{1}{\hat{\rho}}\frac{\hat{T}}{\hat{A}_c(\hat{T})}\frac{\partial\hat{v}_j}{\partial x_j} + O(\epsilon^2), \tag{43a}$$

$$\hat{T}_{\rm int} = \hat{T} + \epsilon\frac{2}{\theta(3+\delta)}\frac{1}{\hat{\rho}}\frac{\hat{T}}{\hat{A}_c(\hat{T})}\frac{\partial\hat{v}_j}{\partial x_j} + O(\epsilon^2). \tag{43b}$$

It also gives, from Eqs. (19f) and (22), the following expressions of the dimensionless stress tensor $\hat{p}_{ij}$ and heat-flow vector $\hat{q}_i$:

$$\hat{p}_{ij} = \hat{p}\delta_{ij} - \epsilon\,\Gamma_1(\hat{T})\left(\frac{\partial \hat{v}_i}{\partial x_j} + \frac{\partial \hat{v}_j}{\partial x_i} - \frac{2}{3}\frac{\partial \hat{v}_k}{\partial x_k}\delta_{ij}\right) - \epsilon\Gamma_b(\hat{T})\frac{\partial \hat{v}_k}{\partial x_k}\delta_{ij} + O(\epsilon^2), \tag{44a}$$

$$\hat{q}_i = -\frac{5}{4}\epsilon\,\Gamma_2(\hat{T})\frac{\partial \hat{T}}{\partial x_i} + O(\epsilon^2), \tag{44b}$$

where

$$\begin{aligned}\Gamma_1(\hat{T}) =& \frac{8}{15\sqrt{\pi}}\hat{T}^{1/2}\int_0^\infty\int_0^\infty \mathcal{C}^6\mathcal{B}(\hat{T})\exp(-\mathcal{C}^2)\frac{\bar{\mathcal{E}}^{\delta/2-1}}{\Gamma(\delta/2)}e^{-\bar{\mathcal{E}}}d\bar{\mathcal{E}}d\mathcal{C}\\ =& \frac{1}{1-\nu+\theta\nu}\frac{\hat{T}}{\hat{A}_c(\hat{T})},\end{aligned} \tag{45a}$$

$$\begin{aligned}\Gamma_2(\hat{T}) =& \frac{16}{15\sqrt{\pi}}\hat{T}^{1/2}\int_0^\infty\int_0^\infty \mathcal{C}^4(\mathcal{C}^2+\bar{\mathcal{E}})\mathcal{A}(\mathcal{C},\,\bar{\mathcal{E}},\,\hat{T})\exp(-\mathcal{C}^2)\frac{\bar{\mathcal{E}}^{\delta/2-1}}{\Gamma(\delta/2)}e^{-\bar{\mathcal{E}}}d\bar{\mathcal{E}}d\mathcal{C}\\ =& \left(1+\frac{\delta}{5}\right)\frac{\hat{T}}{\hat{A}_c(\hat{T})},\end{aligned} \tag{45b}$$

$$\begin{aligned}\Gamma_b(\hat{T}) =& \frac{8}{3\sqrt{\pi}}\hat{T}^{1/2}\int_0^\infty\int_0^\infty \mathcal{C}^4\mathcal{B}_b(\mathcal{C},\,\bar{\mathcal{E}},\,\hat{T})\exp(-\mathcal{C}^2)\frac{\bar{\mathcal{E}}^{\delta/2-1}}{\Gamma(\delta/2)}e^{-\bar{\mathcal{E}}}d\bar{\mathcal{E}}d\mathcal{C}\\ =& \frac{1}{\theta}\frac{2\delta}{3(3+\delta)}\frac{\hat{T}}{\hat{A}_c(\hat{T})}.\end{aligned} \tag{45c}$$

As shown in Sec. VI, $\epsilon\Gamma_1$, $\epsilon\Gamma_2$, and $\epsilon\Gamma_b$ are related to the viscosity, the thermal conductivity, and the bulk viscosity, respectively [see Eq. (134)].

If we use Eq. (44) in the Maxwell transport equations, which are derived by integrating Eq. (18) times $\hat{\varphi}_r$ ($r = 0, ..., 4$) [Eq. (25)] over the whole space of ζ_i and whole range of $\hat{\mathcal{E}}$, and neglect the terms of $O(\epsilon^2)$, we obtain the Navier–Stokes equations for compressible fluids, i.e.,

$$\frac{\partial \hat{\rho}}{\partial \hat{t}} + \frac{\partial \hat{\rho}\hat{v}_j}{\partial x_j} = 0, \tag{46a}$$

$$\begin{aligned}\frac{\partial \hat{\rho}\hat{v}_i}{\partial \hat{t}} + \frac{\partial \hat{\rho}\hat{v}_i\hat{v}_j}{\partial x_j} =& -\frac{1}{2}\frac{\partial \hat{p}}{\partial x_i} + \frac{\epsilon}{2}\frac{\partial}{\partial x_j}\left[\Gamma_1(\hat{T})\left(\frac{\partial \hat{v}_j}{\partial x_i} + \frac{\partial \hat{v}_i}{\partial x_j} - \frac{2}{3}\frac{\partial \hat{v}_k}{\partial x_k}\delta_{ij}\right)\right]\\ &+ \frac{\epsilon}{2}\frac{\partial}{\partial x_i}\left[\Gamma_b(\hat{T})\frac{\partial \hat{v}_j}{\partial x_j}\right],\end{aligned} \tag{46b}$$

$$\begin{aligned}&\frac{\partial}{\partial \hat{t}}\left[\hat{\rho}\left(\frac{3+\delta}{2}\hat{T} + \hat{v}_k^2\right)\right] + \frac{\partial}{\partial x_j}\left[\hat{\rho}\hat{v}_j\left(\frac{5+\delta}{2}\hat{T} + \hat{v}_k^2\right)\right]\\ &\quad= \frac{5}{4}\epsilon\frac{\partial}{\partial x_j}\left[\Gamma_2(\hat{T})\frac{\partial \hat{T}}{\partial x_j}\right] + \epsilon\frac{\partial}{\partial x_j}\left[\Gamma_1(\hat{T})\hat{v}_i\left(\frac{\partial \hat{v}_j}{\partial x_i} + \frac{\partial \hat{v}_i}{\partial x_j} - \frac{2}{3}\frac{\partial \hat{v}_k}{\partial x_k}\delta_{ij}\right)\right]\\ &\quad\quad+ \epsilon\frac{\partial}{\partial x_j}\left[\Gamma_b(\hat{T})\hat{v}_j\frac{\partial \hat{v}_k}{\partial x_k}\right],\end{aligned} \tag{46c}$$

where $\hat{p} = \hat{\rho}\hat{T}$. If we set $\Gamma_b(\hat{T}) = 0$ and $\delta = 0$ (since $\delta \geq 2$, this setting is just formal), Eq. (46) reduces to the (dimensionless) compressible Navier–Stokes equations for a monatomic gas [cf. Eq. (50) in Ref. [1]]. The dimensional form of Eq. (46) will be given in Sec. VI.

V. DERIVATION OF THE SLIP BOUNDARY CONDITIONS

In this section, we derive the slip boundary conditions for the compressible Navier–Stokes equations (46). The procedure, which is based on the analysis of the Knudsen layer established by Sone in the framework of his generalized slip-flow theory [11–18], is basically the same as that in the case of a monatomic gas [1] though the full Boltzmann equation is considered in this reference. Therefore, we will make a concise description referring to this reference occasionally.

A. Knudsen layer

1. Introduction of Knudsen layer

In the first-order Chapman–Enskog solution, which corresponds to the Navier–Stokes equations (46), the initial and boundary conditions (26) and (28) are not taken into account. To be consistent with the fact that the term up to $O(\epsilon)$ is considered in Eq. (36), the initial and boundary conditions should be satisfied up to the order of ϵ.

If we assume

$$\hat{\rho} = 1, \qquad \hat{\boldsymbol{v}} = 0, \qquad \hat{T} = 1, \qquad \text{at } \hat{t} = 0, \tag{47}$$

then the Chapman–Enskog solution (36) satisfies Eq. (26) up to $O(\epsilon)$ because $\partial \hat{v}_i/\partial x_j = 0$ and $\partial \hat{T}/\partial x_i = 0$ hold. Therefore, under assumption (iv) in Sec. II, Eq. (47) is the correct initial condition for Eq. (46).

Next, we consider the boundary condition (28). Since the leading-order term $\hat{f}^{(0)}$ of the Chapman–Enskog solution is a local equilibrium distribution [Eq. (37)], it can be made to satisfy Eq. (28) by assuming that

$$\hat{\boldsymbol{v}} = \hat{\boldsymbol{v}}_{\mathrm{w}}, \qquad \hat{T} = \hat{T}_{\mathrm{w}}, \qquad \text{at } \boldsymbol{x} = \boldsymbol{x}_{\mathrm{w}}. \tag{48}$$

However, as discussed in Ref. [1], if we try to satisfy the boundary condition (28) up to $O(\epsilon)$ with the first-order Chapman–Enskog solution $\hat{f}^{(0)} + \hat{f}^{(1)}\epsilon$, we encounter a contradiction.

In order to obtain the solution satisfying the boundary condition, one has to introduce the kinetic boundary layer, the so-called Knudsen layer, with thickness of the order of ϵ (with thickness of the order of the mean free path in the dimensional physical space) adjacent to the boundary [17, 18]. Let us denote the Chapman–Enskog solution (36) by $\hat{f}_{\mathrm{CE}}$, the correction term inside the Knudsen layer by $\hat{f}_{\mathrm{K}}$, and the total solution that satisfies the boundary condition by $\hat{f}_{\mathrm{tot}}$. Then, we write

$$\hat{f}_{\mathrm{tot}} = \hat{f}_{\mathrm{CE}} + \hat{f}_{\mathrm{K}}. \tag{49}$$

Correspondingly, we denote the macroscopic quantities by

$$\hat{h}_{\mathrm{tot}} = \hat{h}_{\mathrm{CE}} + \hat{h}_{\mathrm{K}}, \tag{50}$$

where $\hat{h}$ stands for any of the dimensionless macroscopic quantities, $\hat{\rho}$, $\hat{v}_i$, $\hat{p}_{ij}$, $\hat{T}_{\mathrm{tr}}$, etc., appeared in Eqs. (19d)–(19j), (21), and (22), and $\hat{h}_{\mathrm{CE}}$ and $\hat{h}_{\mathrm{K}}$ indicate these macroscopic quantities associated with the Chapman–Enskog solution and the Knudsen-layer correction, respectively. Note that the macroscopic quantities appeared in Sec. IV belong to $\hat{h}_{\mathrm{CE}}$ although the subscript "CE" was not used there.

We assume the following properties for the correction term $\hat{f}_{\mathrm{K}}$:

(a) $\hat{f}_{\mathrm{K}}$ is appreciable only in the Knudsen layer and vanishes rapidly away from the boundary.

(b) $\hat{f}_{\mathrm{K}}$ has the length scale of variation of the order of ϵ (i.e., of the order of the mean free path l_0 in the dimensional physical space) in the direction normal to the boundary, that is, $n_j \partial \hat{f}_{\mathrm{K}}/\partial x_j = O(\hat{f}_{\mathrm{K}}/\epsilon)$.

(c) $\hat{f}_{\mathrm{K}}$ has the length scale of variation of the order of 1 (i.e., of the order of the reference length L in the dimensional physical space) in the direction along the boundary.

(d) $\hat{f}_{\mathrm{K}}$ has the time scale of variation of the order of 1 [i.e., of the order of $t_0 = L/(2RT_0)^{1/2}$ in the dimensional time], i.e., $\partial \hat{f}_{\mathrm{K}}/\partial \hat{t} = O(\hat{f}_{\mathrm{K}})$.

These assumptions can be justified if such a solution is obtained actually.

If we substitute Eqs. (49) and (50) into the definitions of $\hat{h}$, i.e., Eqs. (19d)–(19j), (21), and (22) (with $\hat{f} = \hat{f}_{\mathrm{tot}}$ and $\hat{h} = \hat{h}_{\mathrm{tot}}$) and use the fact that $\hat{f}_{\mathrm{CE}}$ and $\hat{h}_{\mathrm{CE}}$ also satisfy the same

relations as Eqs. (19d)–(19j), (21), and (22) (with $\hat{f} = \hat{f}_{\rm CE}$ and $\hat{h} = \hat{h}_{\rm CE}$) (cf. Sec. IV B), we obtain the expressions of the corrections $\hat{h}_{\rm K}$ inside the Knudsen layer in terms of $\hat{f}_{\rm K}$ and $\hat{h}_{\rm CE}$. Further, if we substitute Eq. (49) into the ES model, Eq. (18), and take into account the fact that $\hat{f}_{\rm CE}$ is the solution of the same equation, we obtain the equation for the Knudsen-layer correction $\hat{f}_{\rm K}$. We also obtain the initial and boundary conditions for $\hat{f}_{\rm K}$ by inserting Eq. (49) in Eqs. (26) and (28). These procedures will be explained more specifically in the following subsections.

2. *Preliminaries*

The fact that the Chapman–Enskog solution (36) can be made to satisfy the boundary condition (28) at the leading order in ϵ by the choice (48) indicates that the differences $\hat{\boldsymbol{v}} - \hat{\boldsymbol{v}}_{\rm w}$ and $\hat{T} - \hat{T}_{\rm w}$ are small and of the order of ϵ on the boundary. Therefore, we put

$$\hat{\boldsymbol{v}} - \hat{\boldsymbol{v}}_{\rm w} = \bar{\hat{\boldsymbol{v}}}\epsilon, \qquad \hat{T} - \hat{T}_{\rm w} = \bar{\hat{T}}\epsilon, \qquad \text{at } \boldsymbol{x} = \boldsymbol{x}_{\rm w}, \tag{51}$$

where $\bar{\hat{\boldsymbol{v}}}$ and $\bar{\hat{T}}$ are the quantities of $O(1)$. The above fact also indicates that $\hat{f}_{\rm K}$ starts at the order of ϵ, so that we let

$$\hat{f}_{\rm K} = \hat{f}_{\rm K}^{(1)}\epsilon + R_f\epsilon^2, \tag{52}$$

where $R_f\epsilon^2$ is the remainder, and R_f is of $O(1)$ and has the properties (a)–(d). Correspondingly, we put

$$\hat{h}_{\rm K} = \hat{h}_{\rm K}^{(1)}\epsilon + R_h\epsilon^2, \tag{53}$$

where $R_h\epsilon^2$ is the remainder corresponding to $R_f\epsilon^2$.

We insert Eqs. (49) and (50) with Eqs. (52) and (53) into Eqs. (19d)–(19j), (21), and (22) (with $\hat{f} = \hat{f}_{\rm tot}$ and $\hat{h} = \hat{h}_{\rm tot}$) and note that $\hat{f}_{\rm CE}$ and $\hat{h}_{\rm CE}$ satisfy the same relations as Eqs. (19d)–(19j), (21), and (22) (with $\hat{f} = \hat{f}_{\rm CE}$ and $\hat{h} = \hat{h}_{\rm CE}$). Then, picking up the terms of $O(\epsilon)$ for $\hat{h}_{\rm K}^{(1)}$ and putting the $O(\epsilon^2)$ terms in $R_h\epsilon^2$, we obtain the following expressions of $\hat{h}_{\rm K}^{(1)}$:

$$\hat{\rho}_{\rm K}^{(1)} = \iint_0^\infty \hat{f}_{\rm K}^{(1)} d\hat{\mathcal{E}} d\boldsymbol{\zeta}, \tag{54a}$$

$$\hat{v}_{{\rm K}i}^{(1)} = \frac{1}{\hat{\rho}} \iint_0^\infty (\zeta_i - \hat{v}_i)\hat{f}_{\rm K}^{(1)} d\hat{\mathcal{E}} d\boldsymbol{\zeta}, \tag{54b}$$

$$\hat{p}_{{\rm K}ij}^{(1)} = 2\iint_0^\infty (\zeta_i - \hat{v}_i)(\zeta_j - \hat{v}_j)\hat{f}_{\rm K}^{(1)} d\hat{\mathcal{E}} d\boldsymbol{\zeta}, \tag{54c}$$

$$\hat{T}_{\rm trK}^{(1)} = \frac{2}{3\hat{\rho}} \iint_0^\infty \left[(\zeta_k - \hat{v}_k)^2 - \frac{3}{2}\hat{T}\right] \hat{f}_{\rm K}^{(1)} d\hat{\mathcal{E}} d\boldsymbol{\zeta}, \tag{54d}$$

$$\hat{T}_{\rm intK}^{(1)} = \frac{2}{\delta\hat{\rho}} \iint_0^\infty \left(\hat{\mathcal{E}} - \frac{\delta}{2}\hat{T}\right) \hat{f}_{\rm K}^{(1)} d\hat{\mathcal{E}} d\boldsymbol{\zeta}, \tag{54e}$$

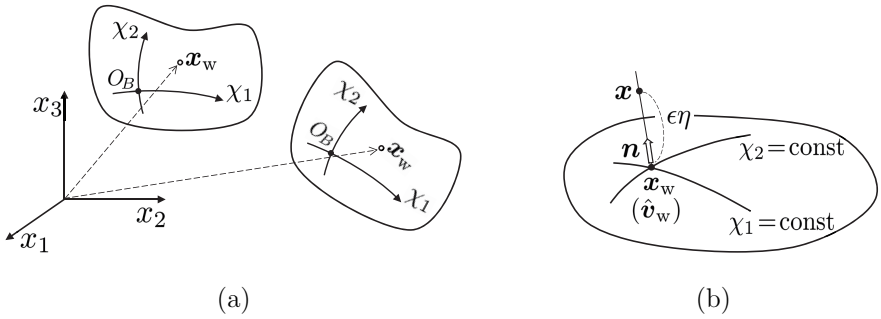
$$\hat{T}_{\rm K}^{(1)} = \frac{3\hat{T}_{\rm trK}^{(1)} + \delta\hat{T}_{\rm intK}^{(1)}}{3+\delta}, \tag{54f}$$

$$\hat{T}_{\rm relK}^{(1)} = \theta\hat{T}_{\rm K}^{(1)} + (1-\theta)\hat{T}_{\rm intK}^{(1)}, \tag{54g}$$

$$\hat{p}_{\rm K}^{(1)} = \hat{\rho}\hat{T}_{\rm K}^{(1)} + \hat{\rho}_{\rm K}^{(1)}\hat{T}, \tag{54h}$$

$$\hat{q}_{{\rm K}i}^{(1)} = \iint_0^\infty (\zeta_i - \hat{v}_i)\left[(\zeta_k - \hat{v}_k)^2 + \hat{\mathcal{E}} - \frac{5+\delta}{2}\hat{T}\right] \hat{f}_{\rm K}^{(1)} d\hat{\mathcal{E}} d\boldsymbol{\zeta}. \tag{54i}$$

Note again that $\hat{\rho}$, $\hat{v}_i$, and $\hat{T}$ here are the macroscopic quantities associated with the Chapman–Enskog solution though the subscript CE is not attached. It should also be noted that use has been made of the fact that $\hat{T}_{\rm tr} = \hat{T} + O(\epsilon)$, $\hat{T}_{\rm int} = \hat{T} + O(\epsilon)$, $\hat{T}_{\rm rel} = \hat{T} + O(\epsilon)$, and $\hat{p}_{ij} = \hat{p}\delta_{ij} + O(\epsilon)$ in the derivation of Eq. (54).



(a) (b)

FIG. 1: Coordinate systems. (a) Coordinate system on the boundary, (b) coordinate system for the Knudsen layer.

Substituting Eq. (49) with Eq. (52) into Eq. (18) and noting that $\hat{f}_{\mathrm{CE}}$ is also the solution of Eq. (18), we obtain the following equation for $\hat{f}_{\mathrm{K}}^{(1)}$ (see Appendix A for the outline of the derivation):

$$\epsilon \frac{\partial \hat{f}_{\mathrm{K}}^{(1)}}{\partial \hat{t}} + \epsilon \zeta_i \frac{\partial \hat{f}_{\mathrm{K}}^{(1)}}{\partial x_i} = \hat{A}_c(\hat{T})\hat{\rho}(\hat{\mathcal{G}}_{\mathrm{K}}^{(1)} - \hat{f}_{\mathrm{K}}^{(1)}) + O(\epsilon R_f), \tag{55}$$

where

$$\hat{\mathcal{G}}_{\mathrm{K}}^{(1)} = \hat{f}^{(0)} \left\{ \frac{\hat{\rho}_{\mathrm{K}}^{(1)}}{\hat{\rho}} + 2\frac{\hat{v}_{\mathrm{K}k}^{(1)}(\zeta_k - \hat{v}_k)}{\hat{T}} + \left[\frac{(\zeta_i - \hat{v}_i)(\zeta_j - \hat{v}_j)}{\hat{T}} - \frac{\delta_{ij}}{2} \right] d_{\mathrm{K}ij} + \left(\frac{\hat{\mathcal{E}}}{\hat{T}} - \frac{\delta}{2} \right) \frac{\hat{T}_{\mathrm{relK}}^{(1)}}{\hat{T}} \right\}, \tag{56a}$$

$$d_{\mathrm{K}ij} = \left[(1-\theta)\frac{\hat{T}_{\mathrm{trK}}^{(1)}}{\hat{T}} + \theta \frac{\hat{T}_{\mathrm{K}}^{(1)}}{\hat{T}} \right] \delta_{ij} + (1-\theta)\nu \left[\frac{\hat{p}_{\mathrm{K}ij}^{(1)}}{\hat{\rho}\hat{T}} - \left(\frac{\hat{\rho}_{\mathrm{K}}^{(1)}}{\hat{\rho}} + \frac{\hat{T}_{\mathrm{trK}}^{(1)}}{\hat{T}} \right) \delta_{ij} \right]. \tag{56b}$$

This equation will be elaborated further below.

3. *Knudsen-layer equation*

We first express a point $\boldsymbol{x}_{\mathrm{w}}$ on the boundary as a function of coordinates χ_1 and χ_2 fixed on the surface of the boundary and of time $\hat{t}$, i.e.,

$$\boldsymbol{x}_{\mathrm{w}} = \boldsymbol{x}_{\mathrm{w}}(\hat{t},\, \chi_1,\, \chi_2). \tag{57}$$

[See Fig. 1(a).] When χ_1 and χ_2 are fixed, the function $\boldsymbol{x}_{\mathrm{w}}(\hat{t},\, \chi_1,\, \chi_2)$ of $\hat{t}$ gives the trajectory of a fixed point on the boundary, and when $\hat{t}$ is fixed, the function $\boldsymbol{x}_{\mathrm{w}}(\hat{t},\, \chi_1,\, \chi_2)$ of χ_1 and χ_2 gives the parameter representation of the boundary surface at time $\hat{t}$. The velocity of the boundary $\hat{\boldsymbol{v}}_{\mathrm{w}}$ and the unit normal vector to the boundary $\boldsymbol{n}$, which are also the functions of $\hat{t}$, χ_1, and χ_2, are expressed as

$$\hat{\boldsymbol{v}}_{\mathrm{w}}(\hat{t},\, \chi_1,\, \chi_2) = \frac{\partial \boldsymbol{x}_{\mathrm{w}}}{\partial \hat{t}}, \tag{58a}$$

$$\boldsymbol{n}(\hat{t},\, \chi_1,\, \chi_2) = \pm \left(\frac{\partial \boldsymbol{x}_{\mathrm{w}}}{\partial \chi_1} \times \frac{\partial \boldsymbol{x}_{\mathrm{w}}}{\partial \chi_2} \right) \left| \frac{\partial \boldsymbol{x}_{\mathrm{w}}}{\partial \chi_1} \times \frac{\partial \boldsymbol{x}_{\mathrm{w}}}{\partial \chi_2} \right|^{-1}, \tag{58b}$$

where $\times$ indicates the vector product, and $+$ sign or $-$ sign is chosen in such a way that $\boldsymbol{n}$ points into gas region.

In order to analyze the Knudsen layer, we introduce a new coordinate system that is local near the boundary and appropriate to describe the rapid change of the physical quantities in the direction normal to the boundary. We introduce the new variables $\tilde{t}$, η, and $\boldsymbol{\zeta}_{\mathrm{w}}$ by the following relations [see Fig. 1(b)]:

$$\hat{t} = \tilde{t}, \tag{59a}$$

$$\boldsymbol{x} = \epsilon\,\eta\,\boldsymbol{n}(\tilde{t},\,\chi_1,\,\chi_2) + \boldsymbol{x}_{\mathrm{w}}(\tilde{t},\,\chi_1,\,\chi_2), \tag{59b}$$

$$\boldsymbol{\zeta} = \boldsymbol{\zeta}_{\mathrm{w}} + \hat{\boldsymbol{v}}_{\mathrm{w}}(\tilde{t},\,\chi_1,\,\chi_2). \tag{59c}$$

Here, η is a stretched normal coordinate, and $\boldsymbol{\zeta}_{\mathrm{w}}$ is the molecular velocity relative to the velocity of the boundary. In accordance with the properties (a)–(d) in Sec. V A 1, we assume that $\hat{f}_{\mathrm{K}}$ is a function of $(\tilde{t},\,\eta,\,\chi_1,\,\chi_2,\,\boldsymbol{\zeta}_{\mathrm{w}},\,\hat{\mathcal{E}})$ and vanishes rapidly as $\eta \to \infty$:

$$\hat{f}_{\mathrm{K}} = \hat{f}_{\mathrm{K}}(\tilde{t},\,\eta,\,\chi_1,\,\chi_2,\,\boldsymbol{\zeta}_{\mathrm{w}},\,\hat{\mathcal{E}}), \tag{60a}$$

$$\hat{f}_{\mathrm{K}} \to 0, \qquad \text{as } \eta \to \infty. \tag{60b}$$

Therefore, Eq. (60) also holds for $\hat{f}_{\mathrm{K}}^{(1)}$ and R_f in Eq. (52).

We now consider Eq. (55) inside the Knudsen layer, i.e., $\eta = O(1)$ or $(\boldsymbol{x} - \boldsymbol{x}_{\mathrm{w}}) \cdot \boldsymbol{n} = O(\epsilon)$. The $\boldsymbol{x}$-dependence of $\hat{f}^{(0)}$ is through $\hat{\rho}$, $\hat{\boldsymbol{v}}$, and $\hat{T}$, the length scale of which is $O(1)$. Therefore, inside the Knudsen layer, they can be Taylor expanded around $\boldsymbol{x} = \boldsymbol{x}_{\mathrm{w}}$, that is,

$$\hat{\rho} = \hat{\rho}_{\mathrm{B}} + O(\epsilon\eta), \qquad \hat{\boldsymbol{v}} = \hat{\boldsymbol{v}}_{\mathrm{B}} + O(\epsilon\eta), \qquad \hat{T} = \hat{T}_{\mathrm{B}} + O(\epsilon\eta), \tag{61}$$

where the subscript B indicates the value on the boundary $\boldsymbol{x} = \boldsymbol{x}_{\mathrm{w}}$ or $\eta = 0$. Because $\hat{\boldsymbol{v}}_{\mathrm{B}} = \hat{\boldsymbol{v}}_{\mathrm{w}} + O(\epsilon)$ and $\hat{T}_{\mathrm{B}} = \hat{T}_{\mathrm{w}} + O(\epsilon)$ [Eq. (51)], we can write

$$\hat{\rho} = \hat{\rho}_{\mathrm{B}} + O(\epsilon\eta), \qquad \hat{\boldsymbol{v}} = \hat{\boldsymbol{v}}_{\mathrm{w}} + O(\epsilon(\eta+1)), \qquad \hat{T} = \hat{T}_{\mathrm{w}} + O(\epsilon(\eta+1)). \tag{62}$$

If we substitute Eq. (62) into Eq. (54), the $O(\epsilon\eta)$ and $O(\epsilon(\eta+1))$ terms in Eq. (62) produce the terms of the order of $\epsilon(\eta+1)$ times a moment of $\hat{f}_{\mathrm{K}}^{(1)}$, which vanish rapidly as $\eta \to \infty$. Therefore, if we put these terms (times ϵ) into $R_h\epsilon^2$ in Eq. (53), we can change the expressions of $\hat{h}_{\mathrm{K}}^{(1)}$ from Eq. (54) to the following:

$$\hat{\rho}_{\mathrm{K}}^{(1)} = \iint_0^\infty \hat{f}_{\mathrm{K}}^{(1)} d\hat{\mathcal{E}} d\boldsymbol{\zeta}, \tag{63a}$$

$$\hat{v}_{\mathrm{K}i}^{(1)} = \frac{1}{\hat{\rho}_{\mathrm{B}}} \iint_0^\infty (\zeta_i - \hat{v}_{\mathrm{w}i}) \hat{f}_{\mathrm{K}}^{(1)} d\hat{\mathcal{E}} d\boldsymbol{\zeta}, \tag{63b}$$

$$\hat{p}_{\mathrm{K}ij}^{(1)} = 2 \iint_0^\infty (\zeta_i - \hat{v}_{\mathrm{w}i})(\zeta_j - \hat{v}_{\mathrm{w}j}) \hat{f}_{\mathrm{K}}^{(1)} d\hat{\mathcal{E}} d\boldsymbol{\zeta}, \tag{63c}$$

$$\hat{T}_{\mathrm{trK}}^{(1)} = \frac{2}{3\hat{\rho}_{\mathrm{B}}} \iint_0^\infty \left[(\zeta_k - \hat{v}_{\mathrm{w}k})^2 - \frac{3}{2}\hat{T}_{\mathrm{w}} \right] \hat{f}_{\mathrm{K}}^{(1)} d\hat{\mathcal{E}} d\boldsymbol{\zeta}, \tag{63d}$$

$$\hat{T}_{\mathrm{intK}}^{(1)} = \frac{2}{\delta\hat{\rho}_{\mathrm{B}}} \iint_0^\infty \left(\hat{\mathcal{E}} - \frac{\delta}{2}\hat{T}_{\mathrm{w}} \right) \hat{f}_{\mathrm{K}}^{(1)} d\hat{\mathcal{E}} d\boldsymbol{\zeta}, \tag{63e}$$

$$\hat{T}_{\mathrm{K}}^{(1)} = \frac{3\hat{T}_{\mathrm{trK}}^{(1)} + \delta\hat{T}_{\mathrm{intK}}^{(1)}}{3+\delta}, \tag{63f}$$

$$\hat{T}_{\mathrm{relK}}^{(1)} = \theta\hat{T}_{\mathrm{K}}^{(1)} + (1-\theta)\hat{T}_{\mathrm{intK}}^{(1)}, \tag{63g}$$

$$\hat{p}_{\mathrm{K}}^{(1)} = \hat{\rho}_{\mathrm{B}}\hat{T}_{\mathrm{K}}^{(1)} + \hat{\rho}_{\mathrm{K}}^{(1)}\hat{T}_{\mathrm{w}}, \tag{63h}$$

$$\hat{q}_{\mathrm{K}i}^{(1)} = \iint_0^\infty (\zeta_i - \hat{v}_{\mathrm{w}i}) \left[(\zeta_k - \hat{v}_{\mathrm{w}k})^2 + \hat{\mathcal{E}} - \frac{5+\delta}{2}\hat{T}_{\mathrm{w}} \right] \hat{f}_{\mathrm{K}}^{(1)} d\hat{\mathcal{E}} d\boldsymbol{\zeta}. \tag{63i}$$

Incidentally, with Eq. (62), $\hat{f}^{(0)}$ in Eq. (37) inside the Knudsen layer is expanded as

$$\hat{f}^{(0)} = \hat{f}_{\mathrm{w}}[1 + O(\epsilon(\eta+1))], \tag{64}$$

where

$$\hat{f}_{\mathrm{w}} = \frac{\hat{\rho}_{\mathrm{B}}\hat{\mathcal{E}}^{\delta/2-1}}{(\pi\hat{T}_{\mathrm{w}})^{3/2}\hat{T}_{\mathrm{w}}^{\delta/2}\Gamma(\delta/2)} \exp\left(-\frac{(\zeta_j - \hat{v}_{\mathrm{w}j})^2}{\hat{T}_{\mathrm{w}}} - \frac{\hat{\mathcal{E}}}{\hat{T}_{\mathrm{w}}} \right). \tag{65}$$

If we use Eqs. (62) and (64) in Eqs. (55) and (56), the $O(\epsilon\eta)$ and $O(\epsilon(\eta+1))$ terms in Eqs. (62) and (64) create the terms of the order of $\epsilon(\eta+1)$ times $\hat{f}_{\mathrm{K}}^{(1)}$ or its moment, which vanish rapidly

as $\eta \to \infty$. Therefore, we can put these terms into the remainder ϵR_f in Eq. (55). If we do so, the right-hand side of Eq. (55), $\hat{\mathcal{G}}_{\rm K}^{(1)}$ in Eq. (56a), and $d_{{\rm K}ij}$ in Eq. (56b) are, respectively, replaced by

$$\hat{A}_c(\hat{T}_{\rm w})\hat{\rho}_{\rm B}(\hat{\mathcal{G}}_{\rm K}^{(1)} - \hat{f}_{\rm K}^{(1)}) + O(\epsilon R_f), \tag{66a}$$

$$\hat{\mathcal{G}}_{\rm K}^{(1)} = \hat{f}_{\rm w}\left\{\frac{\hat{\rho}_{\rm K}^{(1)}}{\hat{\rho}_{\rm B}} + 2\frac{\hat{v}_{{\rm K}k}^{(1)}(\zeta_k - \hat{v}_{{\rm w}k})}{\hat{T}_{\rm w}} + \left[\frac{(\zeta_i - \hat{v}_{{\rm w}i})(\zeta_j - \hat{v}_{{\rm w}j})}{\hat{T}_{\rm w}} - \frac{\delta_{ij}}{2}\right]d_{{\rm K}ij} + \left(\frac{\hat{\mathcal{E}}}{\hat{T}_{\rm w}} - \frac{\delta}{2}\right)\frac{\hat{T}_{\rm relK}^{(1)}}{\hat{T}_{\rm w}}\right\}, \tag{66b}$$

$$d_{{\rm K}ij} = \left[(1-\theta)\frac{\hat{T}_{\rm trK}^{(1)}}{\hat{T}_{\rm w}} + \theta\frac{\hat{T}_{\rm K}^{(1)}}{\hat{T}_{\rm w}}\right]\delta_{ij} + (1-\theta)\nu\left[\frac{\hat{p}_{{\rm K}ij}^{(1)}}{\hat{\rho}_{\rm B}\hat{T}_{\rm w}} - \left(\frac{\hat{\rho}_{\rm K}^{(1)}}{\hat{\rho}_{\rm B}} + \frac{\hat{T}_{\rm trK}^{(1)}}{\hat{T}_{\rm w}}\right)\delta_{ij}\right]. \tag{66c}$$

On the other hand, if we express the left-hand side of Eq. (55) in terms of the new variables $(\tilde{t},\, \eta,\, \chi_1,\, \chi_2,\, \boldsymbol{\zeta}_{\rm w})$, it reduces to

$$\zeta_{{\rm w}i}n_i\frac{\partial \hat{f}_{\rm K}^{(1)}}{\partial \eta} + O(\epsilon R_f), \tag{67}$$

where $O(\epsilon R_f)$ is the remainder. Since this remainder has the same properties as that on the right-hand side, Eq. (66a), the same symbol is used. The process of the derivation of the form (67) is exactly the same as in Ref. [1] (see Sec. 5.2.2 in Ref. [1]), so that it is omitted here. However, we note the following. As mentioned in Ref. [1], we have assumed that the terms containing $\partial\hat{f}_{\rm K}^{(1)}/\partial\zeta_{{\rm w}i}$ are of $O(\epsilon R_f)$ in Eq. (67) in this process. However, $\hat{f}_{\rm K}^{(1)}$ may have a singularity at $\zeta_{{\rm w}i}n_i = 0$, so that the derivatives may diverge there [32–34]. In the present analysis, we adhere to a formal analysis putting aside the mathematical subtlety as in Ref. [1].

From Eqs. (66) and (67), we obtain the following equation for $\hat{f}_{\rm K}^{(1)}$:

$$\zeta_{{\rm w}i}n_i\frac{\partial \hat{f}_{\rm K}^{(1)}}{\partial \eta} = \hat{A}_c(\hat{T}_{\rm w})\hat{\rho}_{\rm B}(\hat{\mathcal{G}}_{\rm K}^{(1)} - \hat{f}_{\rm K}^{(1)}) + O(\epsilon R_f), \tag{68}$$

where $\hat{\mathcal{G}}_{\rm K}^{(1)}$ is given by Eqs. (66b) and (66c). Recall that R_f is a quantity of $O(1)$ that has the properties (a)–(d) in Sec. V A 1. We note that R_f vanishes rapidly as $\eta \to \infty$, $|\boldsymbol{\zeta}_{\rm w}| \to \infty$, or $\hat{\mathcal{E}} \to \infty$ in the current notation.

Here, we introduce new variables $\boldsymbol{\mathcal{C}}_{\rm w}$ and $\bar{\mathcal{E}}_{\rm w}$ by setting

$$\boldsymbol{\mathcal{C}}_{\rm w} = \frac{\boldsymbol{\zeta}_{\rm w}}{\hat{T}_{\rm w}^{1/2}} = \frac{\boldsymbol{\zeta} - \hat{\boldsymbol{v}}_{\rm w}}{\hat{T}_{\rm w}^{1/2}}, \qquad \bar{\mathcal{E}}_{\rm w} = \frac{\hat{\mathcal{E}}}{\hat{T}_{\rm w}}, \tag{69}$$

and denote the normal component and magnitude of $\boldsymbol{\mathcal{C}}_{\rm w}$ by $\mathcal{C}_{\rm wn}$ and $\mathcal{C}_{\rm w}$, respectively, i.e.,

$$\mathcal{C}_{\rm wn} = \mathcal{C}_{{\rm w}j}n_j = \boldsymbol{\mathcal{C}}_{\rm w}\cdot\boldsymbol{n}, \qquad \mathcal{C}_{\rm w} = (\mathcal{C}_{{\rm w}j}^2)^{1/2} = |\boldsymbol{\mathcal{C}}_{\rm w}|. \tag{70}$$

Then, $\hat{f}_{\rm w}$ can be expressed, by the use of the function E defined in Eq. (27), as

$$\hat{f}_{\rm w} = \frac{\hat{\rho}_{\rm B}}{\hat{T}_{\rm w}^{5/2}\Gamma(\delta/2)}E(\mathcal{C}_{\rm w})\bar{\mathcal{E}}_{\rm w}^{\delta/2-1}e^{-\bar{\mathcal{E}}_{\rm w}}. \tag{71}$$

It should be noted that $\hat{\rho}_{\rm B}$ and $\hat{T}_{\rm w}$ are functions of $(\tilde{t},\, \chi_1,\, \chi_2)$.

Now we let

$$\hat{f}_{\rm K}^{(1)}(\tilde{t},\, \eta,\, \chi_1,\, \chi_2,\, \hat{T}_{\rm w}^{1/2}\boldsymbol{\mathcal{C}}_{\rm w},\, \hat{T}_{\rm w}\bar{\mathcal{E}}_{\rm w}) = \hat{f}_{\rm w}\Phi(\tilde{t},\, \eta,\, \chi_1,\, \chi_2,\, \boldsymbol{\mathcal{C}}_{\rm w},\, \bar{\mathcal{E}}_{\rm w}), \tag{72}$$

and change the velocity and energy variables from $(\boldsymbol{\zeta}_{\rm w},\, \hat{\mathcal{E}})$ to $(\boldsymbol{\mathcal{C}}_{\rm w},\, \bar{\mathcal{E}}_{\rm w})$. Then, by the use of the angle brackets $\langle\cdot\rangle$ defined by Eq. (33), the macroscopic quantities $\hat{\rho}_{\rm K}^{(1)}$, $\hat{v}_{{\rm K}i}^{(1)}$, $\hat{p}_{{\rm K}ij}^{(1)}$, $\hat{T}_{\rm trK}^{(1)}$, $\hat{T}_{\rm intK}^{(1)}$,

and $\hat{q}_{\mathrm{K}i}^{(1)}$ in Eq. (63) are expressed as follows:

$$\frac{\hat{\rho}_{\mathrm{K}}^{(1)}}{\hat{\rho}_{\mathrm{B}}} = \langle\, \Phi(\tilde{t},\, \eta,\, \chi_1,\, \chi_2,\, \boldsymbol{\mathcal{C}}_{\mathrm{w}},\, \bar{\mathcal{E}}_{\mathrm{w}})\,\rangle, \tag{73a}$$

$$\frac{\hat{v}_{\mathrm{K}i}^{(1)}}{\hat{T}_{\mathrm{w}}^{1/2}} = \langle\, \mathcal{C}_{\mathrm{w}i}\Phi(\tilde{t},\, \eta,\, \chi_1,\, \chi_2,\, \boldsymbol{\mathcal{C}}_{\mathrm{w}},\, \bar{\mathcal{E}}_{\mathrm{w}})\,\rangle, \tag{73b}$$

$$\frac{\hat{p}_{\mathrm{K}ij}^{(1)}}{\hat{\rho}_{\mathrm{B}}\hat{T}_{\mathrm{w}}} = 2\langle\, \mathcal{C}_{\mathrm{w}i}\mathcal{C}_{\mathrm{w}j}\Phi(\tilde{t},\, \eta,\, \chi_1,\, \chi_2,\, \boldsymbol{\mathcal{C}}_{\mathrm{w}},\, \bar{\mathcal{E}}_{\mathrm{w}})\,\rangle, \tag{73c}$$

$$\frac{\hat{T}_{\mathrm{trK}}^{(1)}}{\hat{T}_{\mathrm{w}}} = \frac{2}{3}\left\langle \left(\mathcal{C}_{\mathrm{w}}^2 - \frac{3}{2}\right)\Phi(\tilde{t},\, \eta,\, \chi_1,\, \chi_2,\, \boldsymbol{\mathcal{C}}_{\mathrm{w}},\, \bar{\mathcal{E}}_{\mathrm{w}})\right\rangle, \tag{73d}$$

$$\frac{\hat{T}_{\mathrm{intK}}^{(1)}}{\hat{T}_{\mathrm{w}}} = \frac{2}{\delta}\left\langle \left(\bar{\mathcal{E}}_{\mathrm{w}} - \frac{\delta}{2}\right)\Phi(\tilde{t},\, \eta,\, \chi_1,\, \chi_2,\, \boldsymbol{\mathcal{C}}_{\mathrm{w}},\, \bar{\mathcal{E}}_{\mathrm{w}})\right\rangle, \tag{73e}$$

$$\frac{\hat{q}_{\mathrm{K}i}^{(1)}}{\rho_{\mathrm{B}}\hat{T}_{\mathrm{w}}^{3/2}} = \left\langle \mathcal{C}_{\mathrm{w}i}\left(\mathcal{C}_{\mathrm{w}}^2 + \bar{\mathcal{E}}_{\mathrm{w}} - \frac{5+\delta}{2}\right)\Phi(\tilde{t},\, \eta,\, \chi_1,\, \chi_2,\, \boldsymbol{\mathcal{C}}_{\mathrm{w}},\, \bar{\mathcal{E}}_{\mathrm{w}})\right\rangle. \tag{73f}$$

Note that the integration variables $(\boldsymbol{\zeta},\, \hat{\mathcal{E}})$ in the definition of $\langle\cdot\rangle$ [Eq. (33)] should be replaced by $(\boldsymbol{\mathcal{C}}_{\mathrm{w}},\, \bar{\mathcal{E}}_{\mathrm{w}})$ in the above equations, i.e.,

$$\langle\, \hat{g}(\boldsymbol{\mathcal{C}}_{\mathrm{w}},\, \bar{\mathcal{E}}_{\mathrm{w}})\,\rangle = \iint_0^\infty \hat{g}(\boldsymbol{\mathcal{C}}_{\mathrm{w}},\, \bar{\mathcal{E}}_{\mathrm{w}})[\Gamma(\delta/2)]^{-1}E(\mathcal{C}_{\mathrm{w}})\bar{\mathcal{E}}_{\mathrm{w}}^{\delta/2-1}e^{-\bar{\mathcal{E}}_{\mathrm{w}}}d\bar{\mathcal{E}}_{\mathrm{w}}d\boldsymbol{\mathcal{C}}_{\mathrm{w}}. \tag{74}$$

We use Eq. (73), the resulting expressions of $\hat{T}_{\mathrm{K}}^{(1)}$ and $\hat{T}_{\mathrm{relK}}^{(1)}$, and the new variables $\boldsymbol{\mathcal{C}}_{\mathrm{w}}$ and $\bar{\mathcal{E}}_{\mathrm{w}}$ [Eq. (69)] in Eq. (66). Then, recalling the definition of the linearized collision operator, Eq. (32), we have the following expression of the right-hand side of Eq. (68), i.e., Eq. (66):

$$\begin{aligned}&\hat{A}_c(\hat{T}_{\mathrm{w}})\hat{\rho}_{\mathrm{B}}(\hat{\mathcal{G}}_{\mathrm{K}}^{(1)} - \hat{f}_{\mathrm{K}}^{(1)}) + O(\epsilon R_f)\\ &\quad = \hat{A}_{\mathrm{c}}(\hat{T}_{\mathrm{w}})\hat{\rho}_{\mathrm{B}}\hat{f}_{\mathrm{w}}\mathcal{L}\big[\Phi(\tilde{t},\, \eta,\, \chi_1,\, \chi_2,\, \boldsymbol{\mathcal{C}}_{\mathrm{w}},\, \bar{\mathcal{E}}_{\mathrm{w}})\big](\tilde{t},\, \eta,\, \chi_1,\, \chi_2,\, \boldsymbol{\mathcal{C}}_{\mathrm{w}},\, \bar{\mathcal{E}}_{\mathrm{w}}) + O(\epsilon R_f).\end{aligned} \tag{75}$$

Here, the arguments of Φ and $\mathcal{L}(\Phi)$ are shown explicitly. With Eq. (75), Eq. (68) is rewritten as

$$\mathcal{C}_{\mathrm{wn}}\frac{\partial\Phi}{\partial\eta} = \hat{\rho}_{\mathrm{B}}\frac{\hat{A}_c(\hat{T}_{\mathrm{w}})}{\hat{T}_{\mathrm{w}}^{1/2}}\mathcal{L}(\Phi) + O(\epsilon R_f/\hat{f}_{\mathrm{w}}). \tag{76}$$

In order to get rid of the coefficient $\hat{\rho}_{\mathrm{B}}\hat{A}_c(\hat{T}_{\mathrm{w}})/\hat{T}_{\mathrm{w}}^{1/2}$ in Eq. (76), we further introduce the new normal coordinate y in place of η,

$$y = \hat{\rho}_{\mathrm{B}}\frac{\hat{A}_c(\hat{T}_{\mathrm{w}})}{\hat{T}_{\mathrm{w}}^{1/2}}\eta, \tag{77}$$

and let

$$\Phi\left(\tilde{t},\, \left[\hat{\rho}_{\mathrm{B}}\hat{A}_c(\hat{T}_{\mathrm{w}})\right]^{-1}\hat{T}_{\mathrm{w}}^{1/2}y,\, \chi_1,\, \chi_2,\, \boldsymbol{\mathcal{C}}_{\mathrm{w}},\, \bar{\mathcal{E}}_{\mathrm{w}}\right) = \phi(\tilde{t},\, y,\, \chi_1,\, \chi_2,\, \boldsymbol{\mathcal{C}}_{\mathrm{w}},\, \bar{\mathcal{E}}_{\mathrm{w}}). \tag{78}$$

Then, Eq. (76) reduces to

$$\mathcal{C}_{\mathrm{wn}}\frac{\partial\phi}{\partial y} = \mathcal{L}(\phi) + O(\epsilon R_f/\hat{f}_{\mathrm{w}}). \tag{79}$$

If we neglect the terms of $O(\epsilon R_f/\hat{f}_{\mathrm{w}})$, we obtain the equation for ϕ, i.e., that for $\hat{f}_{\mathrm{K}}^{(1)}$.

4. Knudsen-layer boundary condition

Now we consider the boundary condition. We impose the boundary condition (28) to the total solution $\hat{f}_{\rm tot}$ [Eq. (49)]. If we use Eq. (49) with $\hat{f}_{\rm CE}$ given by Eq. (36) and with $\hat{f}_{\rm K}$ given by Eq. (52) in Eq. (28), we obtain the following relation at $\eta=0$ (or $\boldsymbol{x}=\boldsymbol{x}_{\rm w}$):

$$\epsilon\hat{f}_{\rm K}^{(1)}=(1-\alpha)\epsilon\hat{\mathcal{R}}\hat{f}_{\rm K}^{(1)}-\hat{f}^{(0)}-\epsilon\hat{f}^{(1)}+(1-\alpha)\hat{\mathcal{R}}(\hat{f}^{(0)}+\epsilon\hat{f}^{(1)})+\alpha\frac{\hat{\rho}_{\rm w}}{\hat{\rho}_{\rm B}}\hat{f}_{\rm w}+O(\epsilon^2R_{\rm w}),\quad \text{for}\quad (\boldsymbol{\zeta}-\hat{\boldsymbol{v}}_{\rm w})\cdot\boldsymbol{n}>0, \tag{80a}$$

$$\hat{\rho}_{\rm w}=-2\left(\frac{\pi}{\hat{T}_{\rm w}}\right)^{1/2}\int_{(\boldsymbol{\zeta}-\hat{\boldsymbol{v}}_{\rm w})\cdot\boldsymbol{n}<0}\int_0^\infty(\boldsymbol{\zeta}-\hat{\boldsymbol{v}}_{\rm w})\cdot\boldsymbol{n}(\hat{f}^{(0)}+\epsilon\hat{f}^{(1)}+\epsilon\hat{f}_{\rm K}^{(1)})d\hat{\mathcal{E}}d\boldsymbol{\zeta}+O(\epsilon^2), \tag{80b}$$

where $R_{\rm w}$ is a remainder of $O(1)$ vanishing rapidly as $|\boldsymbol{\zeta}|$ (or $|\boldsymbol{\mathcal{C}}_{\rm w}|$) $\to\infty$ or $\hat{\mathcal{E}}$ (or $\bar{\mathcal{E}}_{\rm w}$) $\to\infty$. For instance, $\hat{f}_{\rm w}$ [Eq. (65)] belongs to the class of $R_{\rm w}$.

A slight modification of the corresponding calculation in the case of a monatomic gas (see Appendix B in Ref. [1]) shows that $\hat{f}^{(0)}$, $\hat{f}^{(1)}$, and $\hat{\rho}_{\rm w}$ contained in Eq. (80) can be expressed in the following form:

$$\hat{f}^{(0)}=\hat{f}_{\rm w}\left\{1+\epsilon\left[2\mathcal{C}_{{\rm w}j}\frac{\bar{\bar{v}}_j}{\hat{T}_{\rm w}^{1/2}}+\left(\mathcal{C}_{\rm w}^2-\frac{3+\delta}{2}+\bar{\mathcal{E}}_{\rm w}\right)\frac{\bar{\bar{T}}}{\hat{T}_{\rm w}}\right]+O(\epsilon^2)\right\}, \tag{81a}$$

$$\hat{f}^{(1)}=\hat{f}_{\rm w}[\Psi_{\rm w}+O(\epsilon)], \tag{81b}$$

$$\begin{aligned}\frac{\hat{\rho}_{\rm w}}{\hat{\rho}_{\rm B}}=&1+\epsilon\Bigg\{-\sqrt{\pi}\frac{\bar{\bar{v}}_i}{\hat{T}_{\rm w}^{1/2}}n_i+\frac{1}{2}\frac{\bar{\bar{T}}}{\hat{T}_{\rm w}}\\&-\frac{1}{6}\mathcal{I}_{\mathcal{B}}(\hat{T}_{\rm w})\frac{1}{\hat{\rho}_{\rm B}\hat{T}_{\rm w}^{1/2}}\left[\left(\frac{\partial\hat{v}_j}{\partial x_i}\right)_{\rm B}+\left(\frac{\partial\hat{v}_i}{\partial x_j}\right)_{\rm B}\right]\left[n_in_j-\frac{1}{2}(\delta_{ij}-n_in_j)\right]\\&-2\mathcal{I}_{\mathcal{B}_b}(\hat{T}_{\rm w})\frac{1}{\hat{\rho}_{\rm B}\hat{T}_{\rm w}^{1/2}}\left(\frac{\partial\hat{v}_j}{\partial x_j}\right)_{\rm B}\\&-\frac{2}{\hat{\rho}_{\rm B}}\left(\frac{\pi}{\hat{T}_{\rm w}}\right)^{1/2}\int_{(\boldsymbol{\zeta}-\hat{\boldsymbol{v}}_{\rm w})\cdot\boldsymbol{n}<0}\int_0^\infty(\boldsymbol{\zeta}-\hat{\boldsymbol{v}}_{\rm w})\cdot\boldsymbol{n}\hat{f}_{\rm K}^{(1)}d\hat{\mathcal{E}}d\boldsymbol{\zeta}\Bigg\}+O(\epsilon^2),\end{aligned} \tag{81c}$$

where

$$\begin{aligned}\Psi_{\rm w}=&-\frac{1}{\hat{\rho}_{\rm B}\hat{T}_{\rm w}}\mathcal{C}_{{\rm w}i}\mathcal{A}(\mathcal{C}_{\rm w},\,\bar{\mathcal{E}}_{\rm w},\,\hat{T}_{\rm w})\left(\frac{\partial\hat{T}}{\partial x_i}\right)_{\rm B}\\&-\frac{1}{2\hat{\rho}_{\rm B}\hat{T}_{\rm w}^{1/2}}\left(\mathcal{C}_{{\rm w}i}\mathcal{C}_{{\rm w}j}-\frac{1}{3}\mathcal{C}_{\rm w}^2\delta_{ij}\right)\mathcal{B}(\hat{T}_{\rm w})\left[\left(\frac{\partial\hat{v}_j}{\partial x_i}\right)_{\rm B}+\left(\frac{\partial\hat{v}_i}{\partial x_j}\right)_{\rm B}\right]\\&-\frac{1}{\hat{\rho}_{\rm B}\hat{T}_{\rm w}^{1/2}}\mathcal{B}_b(\mathcal{C}_{\rm w},\,\bar{\mathcal{E}}_{\rm w},\,\hat{T}_{\rm w})\left(\frac{\partial\hat{v}_j}{\partial x_j}\right)_{\rm B},\end{aligned} \tag{82}$$

$$\mathcal{I}_{\mathcal{B}}(\hat{T}_{\rm w})=\frac{1}{\Gamma(\delta/2)}\int_0^\infty\int_0^\infty\mathcal{C}_{\rm w}^5\mathcal{B}(\hat{T}_{\rm w})e^{-\mathcal{C}_{\rm w}^2}\bar{\mathcal{E}}_{\rm w}^{\delta/2-1}e^{-\bar{\mathcal{E}}_{\rm w}}d\bar{\mathcal{E}}_{\rm w}d\mathcal{C}_{\rm w}=\mathcal{B}(\hat{T}_{\rm w})=\frac{2}{1-\nu+\theta\nu}\frac{\hat{T}_{\rm w}^{1/2}}{\hat{A}_c(\hat{T}_{\rm w})}, \tag{83a}$$

$$\mathcal{I}_{\mathcal{B}_b}(\hat{T}_{\rm w})=\frac{1}{\Gamma(\delta/2)}\int_0^\infty\int_0^\infty\mathcal{C}_{\rm w}^3\mathcal{B}_b(\mathcal{C}_{\rm w},\,\bar{\mathcal{E}}_{\rm w},\,\hat{T}_{\rm w})e^{-\mathcal{C}_{\rm w}^2}\bar{\mathcal{E}}_{\rm w}^{\delta/2-1}e^{-\bar{\mathcal{E}}_{\rm w}}d\bar{\mathcal{E}}_{\rm w}d\mathcal{C}_{\rm w}=\frac{\delta}{6\theta(3+\delta)}\frac{\hat{T}_{\rm w}^{1/2}}{\hat{A}_c(\hat{T}_{\rm w})}. \tag{83b}$$

In Eqs. (81a), (82), and (83), use has been made of the new variables $\boldsymbol{\mathcal{C}}_{\rm w}$ and $\bar{\mathcal{E}}_{\rm w}$ and the notation $\mathcal{C}_{\rm w}$ introduced in Eqs. (69) and (70). For the new velocity variable $\boldsymbol{\mathcal{C}}_{\rm w}$, the reflection operator (29) is replaced by the following $\widetilde{\mathcal{R}}$:

$$\widetilde{\mathcal{R}}\hat{g}(\mathcal{C}_{{\rm w}i})=\hat{g}(\mathcal{C}_{{\rm w}i}-2\mathcal{C}_{{\rm w}j}n_jn_i), \tag{84}$$

where $\hat{g}(\mathcal{C}_{\mathrm{w}i})$ is a function of $\mathcal{C}_{\mathrm{w}i}$. It should be noted that $\widetilde{\mathcal{R}}\hat{f}_{\mathrm{w}} = \hat{f}_{\mathrm{w}}$ holds. Taking into account Eqs. (81) and (84) in Eq. (80), we can transform Eq. (80) to the following form:

$$\hat{f}_{\mathrm{K}}^{(1)} = (1-\alpha)\hat{\mathcal{R}}\hat{f}_{\mathrm{K}}^{(1)} + \hat{f}_{\mathrm{w}}\hat{\mathcal{F}} + O(\epsilon R_{\mathrm{w}}), \quad \text{at } \eta = 0, \text{ for } (\boldsymbol{\zeta} - \hat{\boldsymbol{v}}_{\mathrm{w}})\cdot\boldsymbol{n} > 0, \tag{85}$$

where

$$\begin{aligned}\hat{\mathcal{F}} = &-2[\mathcal{C}_{\mathrm{w}j} - (1-\alpha)\widetilde{\mathcal{R}}\mathcal{C}_{\mathrm{w}j}]\frac{\bar{\bar{v}}_j}{\hat{T}_{\mathrm{w}}^{1/2}} - \alpha\sqrt{\pi}\frac{\bar{\bar{v}}_j}{\hat{T}_{\mathrm{w}}^{1/2}}n_j - \alpha\left(\mathcal{C}_{\mathrm{w}}^2 - \frac{4+\delta}{2} + \bar{\mathcal{E}}_{\mathrm{w}}\right)\frac{\bar{\bar{T}}}{\hat{T}_{\mathrm{w}}} \\ &- \Psi_{\mathrm{w}} + (1-\alpha)\widetilde{\mathcal{R}}\Psi_{\mathrm{w}} \\ &- \alpha\Bigg\{\frac{1}{6}\mathcal{I}_{\mathcal{B}}(\hat{T}_{\mathrm{w}})\frac{1}{\hat{\rho}_{\mathrm{B}}\hat{T}_{\mathrm{w}}^{1/2}}\left[\left(\frac{\partial\hat{v}_j}{\partial x_i}\right)_{\mathrm{B}} + \left(\frac{\partial\hat{v}_i}{\partial x_j}\right)_{\mathrm{B}}\right]\left[n_in_j - \frac{1}{2}(\delta_{ij} - n_in_j)\right] \\ &\quad + 2\mathcal{I}_{\mathcal{B}_b}(\hat{T}_{\mathrm{w}})\frac{1}{\hat{\rho}_{\mathrm{B}}\hat{T}_{\mathrm{w}}^{1/2}}\left(\frac{\partial\hat{v}_j}{\partial x_j}\right)_{\mathrm{B}} \\ &\quad + \frac{2}{\hat{\rho}_{\mathrm{B}}}\left(\frac{\pi}{\hat{T}_{\mathrm{w}}}\right)^{1/2}\int_{(\boldsymbol{\zeta}-\hat{\boldsymbol{v}}_{\mathrm{w}})\cdot\boldsymbol{n}<0}\int_0^\infty(\boldsymbol{\zeta}-\hat{\boldsymbol{v}}_{\mathrm{w}})\cdot\boldsymbol{n}\hat{f}_{\mathrm{K}}^{(1)}d\hat{\mathcal{E}}d\boldsymbol{\zeta}\Bigg\}.\end{aligned} \tag{86}$$

This expression can be simplified slightly more, as shown below.

First, let us integrate Eq. (68) with respect to $\boldsymbol{\zeta}_{\mathrm{w}}$ over its whole space and with respect to $\hat{\mathcal{E}}$ from 0 to ∞. Then, the integral of $\hat{\mathcal{G}}_{\mathrm{K}}^{(1)} - \hat{f}_{\mathrm{K}}^{(1)}$ vanishes, so that we have

$$\frac{\partial}{\partial\eta}\iint_0^\infty \zeta_{\mathrm{w}i}n_i\hat{f}_{\mathrm{K}}^{(1)}d\hat{\mathcal{E}}d\boldsymbol{\zeta}_{\mathrm{w}} = O\left(\epsilon\iint_0^\infty R_f d\hat{\mathcal{E}}d\boldsymbol{\zeta}_{\mathrm{w}}\right). \tag{87}$$

Since $\hat{f}_{\mathrm{K}}^{(1)}$ and R_f vanish rapidly as $\eta\to\infty$, the integration of the above equation with respect to η from 0 to ∞ gives $\iint_0^\infty \zeta_{\mathrm{w}i}n_i\hat{f}_{\mathrm{K}}^{(1)}d\hat{\mathcal{E}}d\boldsymbol{\zeta}_{\mathrm{w}} = O(\epsilon)$ at $\eta = 0$. Therefore, it follows that

$$\iint_0^\infty \zeta_{\mathrm{w}i}n_i\hat{f}_{\mathrm{K}}^{(1)}d\hat{\mathcal{E}}d\boldsymbol{\zeta}_{\mathrm{w}} = O(\epsilon), \quad \text{for any } \eta. \tag{88}$$

On the other hand, the total solution $\hat{f}_{\mathrm{tot}}$ of Eq. (49) has to satisfy the condition of no net mass flow on the boundary, Eq. (30). If we insert Eq. (49) in Eq. (30) and consider the properties of $\hat{f}_{\mathrm{CE}}$, we obtain the relation $\hat{\rho}_{\mathrm{B}}(\hat{\boldsymbol{v}}_{\mathrm{B}} - \hat{\boldsymbol{v}}_{\mathrm{w}})\cdot\boldsymbol{n} + \int\int_0^\infty(\boldsymbol{\zeta}-\hat{\boldsymbol{v}}_{\mathrm{w}})\cdot\boldsymbol{n}\hat{f}_{\mathrm{K}}(\eta=0)d\hat{\mathcal{E}}d\boldsymbol{\zeta} = 0$. Then, with the help of Eqs. (51), (52), (59c), and (88), we can show that

$$\hat{\rho}_{\mathrm{B}}\epsilon\bar{\bar{\boldsymbol{v}}}\cdot\boldsymbol{n} = -\iint_0^\infty \boldsymbol{\zeta}_{\mathrm{w}}\cdot\boldsymbol{n}[\epsilon\hat{f}_{\mathrm{K}}^{(1)} + O(\epsilon^2 R_f)](\eta=0)d\hat{\mathcal{E}}d\boldsymbol{\zeta}_{\mathrm{w}} = O(\epsilon^2), \tag{89}$$

that is,

$$\bar{\bar{\boldsymbol{v}}}\cdot\boldsymbol{n} = O(\epsilon). \tag{90}$$

Next, we should mention that, as shown in Ref. [1], the following relations hold:

$$\left[\left(\frac{\partial\hat{v}_i}{\partial x_j}\right)_{\mathrm{B}} + \left(\frac{\partial\hat{v}_j}{\partial x_i}\right)_{\mathrm{B}}\right](\delta_{ij} - n_in_j) = O(\epsilon), \tag{91a}$$

$$\begin{aligned}&\left[\left(\frac{\partial\hat{v}_i}{\partial x_j}\right)_{\mathrm{B}} + \left(\frac{\partial\hat{v}_j}{\partial x_i}\right)_{\mathrm{B}}\right](\delta_{ik} - n_in_k)(\delta_{jl} - n_jn_l) \\ &\qquad = \epsilon\left(\frac{\partial\bar{\bar{v}}_i}{\partial x_j} + \frac{\partial\bar{\bar{v}}_j}{\partial x_i}\right)(\delta_{ik} - n_in_k)(\delta_{jl} - n_jn_l) = O(\epsilon),\end{aligned} \tag{91b}$$

$$\begin{aligned}&\left(\mathcal{C}_{\mathrm{w}i}\mathcal{C}_{\mathrm{w}j} - \frac{1}{3}\mathcal{C}_{\mathrm{w}}^2\delta_{ij}\right)\left[\left(\frac{\partial\hat{v}_j}{\partial x_i}\right)_{\mathrm{B}} + \left(\frac{\partial\hat{v}_i}{\partial x_j}\right)_{\mathrm{B}}\right] \\ &\qquad = 2\left(\mathcal{C}_{\mathrm{wn}}^2 - \frac{1}{3}\mathcal{C}_{\mathrm{w}}^2\right)\left(\frac{\partial\hat{v}_i}{\partial x_j}\right)_{\mathrm{B}}n_in_j\end{aligned}$$

$$+ 2\mathcal{C}_{\mathrm{wn}}\mathcal{C}_{\mathrm{w}i}n_l(\delta_{ij} - n_in_j)\left[\left(\frac{\partial \hat{v}_j}{\partial x_l}\right)_{\mathrm{B}} + \left(\frac{\partial \hat{v}_l}{\partial x_j}\right)_{\mathrm{B}}\right] + O(\epsilon). \tag{91c}$$

The relations (91a) and (91b) are due to the rigid-body motion of the boundary, and Eq. (91c) is a consequence of Eq. (91b). In addition, it follows from Eq. (91a) that

$$\begin{aligned}\left(\frac{\partial \hat{v}_j}{\partial x_j}\right)_{\mathrm{B}} &= \left(\frac{\partial \hat{v}_i}{\partial x_j}\right)_{\mathrm{B}} \delta_{ij} \\ &= \left(\frac{\partial \hat{v}_i}{\partial x_j}\right)_{\mathrm{B}} n_in_j + \frac{1}{2}\left[\left(\frac{\partial \hat{v}_i}{\partial x_j}\right)_{\mathrm{B}} + \left(\frac{\partial \hat{v}_j}{\partial x_i}\right)_{\mathrm{B}}\right](\delta_{ij} - n_in_j) \\ &= \left(\frac{\partial \hat{v}_i}{\partial x_j}\right)_{\mathrm{B}} n_in_j + O(\epsilon).\end{aligned} \tag{92}$$

Now we make use of Eqs. (72) and (78) in Eq. (85) to derive the boundary condition for ϕ. To be more specific, we change the integration variables from $(\boldsymbol{\zeta},\, \hat{\mathcal{E}})$ to $(\boldsymbol{\mathcal{C}}_{\mathrm{w}},\, \bar{\mathcal{E}}_{\mathrm{w}})$ in the integral in Eq. (86) with the help of Eqs. (69) and (71). Then, we use Eqs. (90)–(92) and the relations $\mathcal{C}_{\mathrm{w}i} = \mathcal{C}_{\mathrm{wn}}n_i + \mathcal{C}_{\mathrm{w}j}(\delta_{ij} - n_in_j)$ and $\widetilde{\mathcal{R}}\mathcal{C}_{\mathrm{w}i} = -\mathcal{C}_{\mathrm{wn}}n_i + \mathcal{C}_{\mathrm{w}j}(\delta_{ij} - n_in_j)$. As the consequence, Eq. (85) reduces to the following form:

$$\begin{aligned}\phi = {} & (1-\alpha)\widetilde{\mathcal{R}}\phi - \alpha\left(\mathcal{C}_{\mathrm{w}}^2 - \frac{4+\delta}{2} + \bar{\mathcal{E}}_{\mathrm{w}}\right)\frac{\bar{\bar{T}}}{\hat{T}_{\mathrm{w}}} - 2\alpha\mathcal{C}_{\mathrm{w}i}(\delta_{ij} - n_in_j)\frac{\bar{\bar{v}}_j}{\hat{T}_{\mathrm{w}}^{1/2}} \\ & - 2\alpha\sqrt{\pi}\int_{\mathcal{C}_{\mathrm{wn}}<0}\int_0^\infty \mathcal{C}_{\mathrm{wn}}\phi E(\mathcal{C}_{\mathrm{w}})\frac{\bar{\mathcal{E}}_{\mathrm{w}}^{\delta/2-1}}{\Gamma(\delta/2)}e^{-\bar{\mathcal{E}}_{\mathrm{w}}}d\bar{\mathcal{E}}_{\mathrm{w}}d\boldsymbol{\mathcal{C}}_{\mathrm{w}} \\ & + (2-\alpha)\frac{1}{\hat{\rho}_{\mathrm{B}}\hat{T}_{\mathrm{w}}}\mathcal{C}_{\mathrm{wn}}\mathcal{A}(\mathcal{C}_{\mathrm{w}},\, \bar{\mathcal{E}}_{\mathrm{w}},\, \hat{T}_{\mathrm{w}})\left(\frac{\partial \hat{T}}{\partial x_i}\right)_{\mathrm{B}} n_i \\ & + \alpha\left[\left(\mathcal{C}_{\mathrm{wn}}^2 - \frac{1}{3}\mathcal{C}_{\mathrm{w}}^2\right)\mathcal{B}(\hat{T}_{\mathrm{w}}) + \mathcal{B}_b(\mathcal{C}_{\mathrm{w}},\, \bar{\mathcal{E}}_{\mathrm{w}},\, \hat{T}_{\mathrm{w}}) - \frac{1}{3}\mathcal{I}_{\mathcal{B}}(\hat{T}_{\mathrm{w}}) - 2\mathcal{I}_{\mathcal{B}_b}(\hat{T}_{\mathrm{w}})\right] \\ & \qquad\qquad \times \frac{1}{\hat{\rho}_{\mathrm{B}}\hat{T}_{\mathrm{w}}^{1/2}}\left(\frac{\partial \hat{v}_i}{\partial x_j}\right)_{\mathrm{B}} n_in_j \\ & + (2-\alpha)\frac{1}{\hat{\rho}_{\mathrm{B}}\hat{T}_{\mathrm{w}}^{1/2}}\mathcal{C}_{\mathrm{wn}}\mathcal{C}_{\mathrm{w}i}n_l(\delta_{ij} - n_in_j)\mathcal{B}(\hat{T}_{\mathrm{w}})\left[\left(\frac{\partial \hat{v}_j}{\partial x_l}\right)_{\mathrm{B}} + \left(\frac{\partial \hat{v}_l}{\partial x_j}\right)_{\mathrm{B}}\right] \\ & + \alpha\frac{1}{\hat{\rho}_{\mathrm{B}}\hat{T}_{\mathrm{w}}}\mathcal{C}_{\mathrm{w}i}(\delta_{ij} - n_in_j)\mathcal{A}(\mathcal{C}_{\mathrm{w}},\, \bar{\mathcal{E}}_{\mathrm{w}},\, \hat{T}_{\mathrm{w}})\left(\frac{\partial \hat{T}}{\partial x_j}\right)_{\mathrm{B}} + O(\epsilon), \quad (y = 0,\ \mathcal{C}_{\mathrm{wn}} > 0).\end{aligned} \tag{93}$$

5. *Summary*

If we omit the terms of $O(\epsilon)$ in Eqs. (79) and (93) and take into account Eq. (60b), then we obtain the problem for ϕ. In order to avoid cumbersome notations and to match the variables with those in the definition of the linearized collision operator in Eq. (32), we change the names of the variables from $(\boldsymbol{\mathcal{C}}_{\mathrm{w}},\, \bar{\mathcal{E}}_{\mathrm{w}})$ to $(\boldsymbol{\zeta},\, \hat{\mathcal{E}})$ and denote ϕ as a function of $(\tilde{t},\, y,\, \chi_1,\, \chi_2,\, \boldsymbol{\zeta},\, \hat{\mathcal{E}})$, that is,

$$\boldsymbol{\mathcal{C}}_{\mathrm{w}} \to \boldsymbol{\zeta}, \qquad \bar{\mathcal{E}}_{\mathrm{w}} \to \hat{\mathcal{E}}, \qquad \phi(\tilde{t},\, y,\, \chi_1,\, \chi_2,\, \boldsymbol{\mathcal{C}}_{\mathrm{w}},\, \bar{\mathcal{E}}_{\mathrm{w}}) \to \phi(\tilde{t},\, y,\, \chi_1,\, \chi_2,\, \boldsymbol{\zeta},\, \hat{\mathcal{E}}). \tag{94}$$

Then, the equation and the boundary condition for ϕ become as follows.

$$\zeta_{\mathrm{n}}\frac{\partial \phi}{\partial y} = \mathcal{L}(\phi), \qquad (y > 0), \tag{95a}$$

$$\begin{aligned}\phi = {} & (1-\alpha)\widetilde{\mathcal{R}}\phi - \alpha\left(\zeta^2 - \frac{4+\delta}{2} + \hat{\mathcal{E}}\right)\frac{\bar{\bar{T}}}{\hat{T}_{\mathrm{w}}} - 2\alpha\zeta_i(\delta_{ij} - n_in_j)\frac{\bar{\bar{v}}_j}{\hat{T}_{\mathrm{w}}^{1/2}} \\ & - 2\alpha\sqrt{\pi}\int_{\zeta_{\mathrm{n}}<0}\int_0^\infty \zeta_{\mathrm{n}}\phi E(\zeta)\frac{\hat{\mathcal{E}}^{\delta/2-1}}{\Gamma(\delta/2)}e^{-\hat{\mathcal{E}}}d\hat{\mathcal{E}}d\boldsymbol{\zeta}\end{aligned}$$

$$
\begin{aligned}
&+(2-\alpha)\frac{1}{\hat{\rho}_{\mathrm{B}}\hat{T}_{\mathrm{w}}}\zeta_{\mathrm{n}}\mathcal{A}(\zeta,\,\hat{\mathcal{E}},\,\hat{T}_{\mathrm{w}})\left(\frac{\partial\hat{T}}{\partial x_i}\right)_{\mathrm{B}}n_i \\
&+\alpha\left[\left(\zeta_{\mathrm{n}}^2-\frac{1}{3}\zeta^2\right)\mathcal{B}(\hat{T}_{\mathrm{w}})+\mathcal{B}_b(\zeta,\,\hat{\mathcal{E}},\,\hat{T}_{\mathrm{w}})-\frac{1}{3}\mathcal{I}_{\mathcal{B}}(\hat{T}_{\mathrm{w}})-2\mathcal{I}_{\mathcal{B}_b}(\hat{T}_{\mathrm{w}})\right] \\
&\qquad\qquad\times\frac{1}{\hat{\rho}_{\mathrm{B}}\hat{T}_{\mathrm{w}}^{1/2}}\left(\frac{\partial\hat{v}_i}{\partial x_j}\right)_{\mathrm{B}}n_in_j \\
&+(2-\alpha)\frac{1}{\hat{\rho}_{\mathrm{B}}\hat{T}_{\mathrm{w}}^{1/2}}\zeta_{\mathrm{n}}\zeta_in_l(\delta_{ij}-n_in_j)\mathcal{B}(\hat{T}_{\mathrm{w}})\left[\left(\frac{\partial\hat{v}_j}{\partial x_l}\right)_{\mathrm{B}}+\left(\frac{\partial\hat{v}_l}{\partial x_j}\right)_{\mathrm{B}}\right] \\
&+\alpha\frac{1}{\hat{\rho}_{\mathrm{B}}\hat{T}_{\mathrm{w}}}\zeta_i(\delta_{ij}-n_in_j)\mathcal{A}(\zeta,\,\hat{\mathcal{E}},\,\hat{T}_{\mathrm{w}})\left(\frac{\partial\hat{T}}{\partial x_j}\right)_{\mathrm{B}}, \qquad (y=0,\ \zeta_{\mathrm{n}}>0), \qquad (95\mathrm{b})
\end{aligned}
$$

$$
\phi\to 0, \qquad (y\to\infty), \qquad (95\mathrm{c})
$$

where $\mathcal{A}$, $\mathcal{B}$, and $\mathcal{B}_b$ are given in Eq. (40), and $\mathcal{I}_{\mathcal{B}}$ and $\mathcal{I}_{\mathcal{B}_b}$ in Eq. (83). Here and in what follows, the reflection operator $\widetilde{\mathcal{R}}$ indicates $\widetilde{\mathcal{R}}\hat{g}(\zeta_i)=\hat{g}(\zeta_i-2\zeta_jn_jn_i)$ because of Eqs. (84) and (94).

The problem (95) is a steady boundary-value problem of the linearized ES model for a polyatomic gas in the half space $y>0$. The corresponding problem of the linearized Boltzmann equation for a monatomic gas has been studied mathematically [35–38], and its mathematical structure, such as the existence and uniqueness of the solution, has been well understood. Numerical analysis of some relevant problems can also be found in the literature (e.g., Refs. [39, 40]). In accordance with these results, we expect that the present problem (95) has the same structure. To be more specific, the problem should have a unique solution only when $\bar{\bar{T}}$ and $\bar{\bar{\boldsymbol{v}}}$ are related to $\partial\hat{T}/\partial x_j$ and $\partial\hat{v}_i/\partial x_j$ appropriately. These relations provide the desired boundary conditions for the compressible Navier–Stokes equations (46), as we will see in the following subsections.

The detailed difference between the problem (95) and the corresponding problem for a monatomic gas [cf. Eq. (100) in Ref. [1]] lies in the following points. In the former, the solution depends on the energy variable $\hat{\mathcal{E}}$ associated with the internal modes, which does not appear in the latter problem for a monatomic gas; $\hat{\mathcal{E}}$ appears explicitly in the term containing $\bar{\bar{T}}/\hat{T}_{\mathrm{w}}$ and in the functions $\mathcal{A}$ and $\mathcal{B}_b$, as well as in the integral term, in the boundary condition (95b). In addition, the quantities $\mathcal{B}_b$ and $\mathcal{I}_{\mathcal{B}_b}$, which are related to the bulk viscosity, and the parameter δ do not occur in the problem for a monatomic gas. As we will see in Secs. V B 6 and VI, however, the slip boundary conditions obtained from the problem (95) is basically of the same form as those for a monatomic gas, since the manner of appearance of the boundary values $\bar{\bar{T}}$, $\bar{\bar{\boldsymbol{v}}}$, $(\partial\hat{T}/\partial x_i)_{\mathrm{B}}$, etc. in Eq. (95b) are essentially the same as in the case of a monatomic gas.

We have not mentioned the initial condition for the Knudsen-layer equation so far. Since the time-derivative term is not contained in Eq. (95a), we cannot impose the initial condition to this equation. However, we can show that the problem (95) is consistent with the initial condition (47) for the compressible Navier–Stokes equations and assumption (iv) in Sec. II. For the detailed discussion on this point, the reader is referred to Sec. 5.2.4 in Ref. [1].

B. Slip boundary conditions

1. *Decomposition of the Knudsen-layer problem*

If the four terms containing the boundary values of the derivatives $(\partial\hat{T}/\partial x_i)_{\mathrm{B}}$ and $(\partial\hat{v}_i/\partial x_j)_{\mathrm{B}}$ in Eq. (95b) are set to be zero, then the problem (95) has a trivial solution $\phi=0$, $\bar{\bar{T}}=0$, and $\bar{\bar{v}}_i=0$, which should be unique in analogy with the case of the linearized Boltzmann equation. Therefore, these four terms are the inhomogeneous terms, and $\bar{\bar{T}}$ and $\bar{\bar{v}}_i$ are a part of the solution. That is, ϕ as well as $\bar{\bar{T}}$ and $\bar{\bar{v}}_i$ is determined depending on the inhomogeneous terms. Because of the linearity of the problem, the problem (95) can be decomposed in accordance with the form of the inhomogeneous terms.

Here, we recall that, for an arbitrary vector $\boldsymbol{a}$, $a_j(\delta_{ij} - n_i n_j) = a_i - (a_j n_j) n_i$ indicates the tangential component of $\boldsymbol{a}$, i.e., the projection of $\boldsymbol{a}$ onto the plane tangent to the boundary. Therefore, $\zeta_i(\delta_{ij} - n_i n_j)$ in the last two lines of Eq. (95b) is the tangential component of $\boldsymbol{\zeta}$. From the form of the inhomogeneous terms in Eq. (95b), we assume the solution ϕ in the following form:

$$
\begin{aligned}
&\phi(\tilde{t},\, y, \chi_1,\, \chi_2,\, \boldsymbol{\zeta},\, \hat{\mathcal{E}}) \\
&\quad = \frac{1}{\hat{\rho}_{\mathrm{B}} \hat{T}_{\mathrm{w}}^{1/2}} \frac{\hat{T}_{\mathrm{w}}^{1/2}}{\hat{A}_c(\hat{T}_{\mathrm{w}})} \left[\left(\frac{\partial \hat{v}_j}{\partial x_l} \right)_{\mathrm{B}} + \left(\frac{\partial \hat{v}_l}{\partial x_j} \right)_{\mathrm{B}} \right] \zeta_i n_l (\delta_{ij} - n_i n_j)\, \phi_v^I(y,\, \zeta_{\mathrm{n}},\, \zeta,\, \hat{\mathcal{E}}) \\
&\qquad + \frac{1}{\hat{\rho}_{\mathrm{B}} \hat{T}_{\mathrm{w}}} \frac{\hat{T}_{\mathrm{w}}^{1/2}}{\hat{A}_c(\hat{T}_{\mathrm{w}})} \left(\frac{\partial \hat{T}}{\partial x_j} \right)_{\mathrm{B}} \zeta_i (\delta_{ij} - n_i n_j)\, \phi_T^I(y,\, \zeta_{\mathrm{n}},\, \zeta,\, \hat{\mathcal{E}}) \\
&\qquad + \frac{1}{\hat{\rho}_{\mathrm{B}} \hat{T}_{\mathrm{w}}^{1/2}} \frac{\hat{T}_{\mathrm{w}}^{1/2}}{\hat{A}_c(\hat{T}_{\mathrm{w}})} \left(\frac{\partial \hat{v}_i}{\partial x_j} \right)_{\mathrm{B}} n_i n_j\, \phi_v^{II}(y,\, \zeta_{\mathrm{n}},\, \zeta,\, \hat{\mathcal{E}}) \\
&\qquad + \frac{1}{\hat{\rho}_{\mathrm{B}} \hat{T}_{\mathrm{w}}} \frac{\hat{T}_{\mathrm{w}}^{1/2}}{\hat{A}_c(\hat{T}_{\mathrm{w}})} \left(\frac{\partial \hat{T}}{\partial x_i} \right)_{\mathrm{B}} n_i \phi_T^{II}(y,\, \zeta_{\mathrm{n}},\, \zeta,\, \hat{\mathcal{E}}).
\end{aligned} \tag{96}
$$

Then, we need to set the unknown parameters $\bar{\bar{v}}_j$ and $\bar{\bar{T}}$ in accordance with the form of the macroscopic quantities in the inhomogeneous terms. Since $(\delta_{ij} - n_i n_j)\bar{\bar{v}}_j$ is a tangential vector, it should be related to the (macroscopic) tangential vectors in the inhomogeneous terms, i.e., $(\delta_{ij} - n_i n_j)[(\partial \hat{v}_j / \partial x_l)_{\mathrm{B}} + (\partial \hat{v}_l / \partial x_j)_{\mathrm{B}}] n_l$ and $(\delta_{ij} - n_i n_j)(\partial \hat{T} / \partial x_j)_{\mathrm{B}}$. On the other hand, because $\bar{\bar{T}}$ is a scalar, it should be related to the (macroscopic) scalars in the inhomogeneous terms, i.e., $(\partial \hat{T} / \partial x_i)_{\mathrm{B}} n_i$ and $(\partial \hat{v}_i / \partial x_j)_{\mathrm{B}} n_i n_j$. In summary, we let

$$
\begin{aligned}
\frac{\bar{\bar{v}}_j}{\hat{T}_{\mathrm{w}}^{1/2}} (\delta_{ij} - n_i n_j) &= c_v^I \frac{1}{\hat{\rho}_{\mathrm{B}} \hat{T}_{\mathrm{w}}^{1/2}} \frac{\hat{T}_{\mathrm{w}}^{1/2}}{\hat{A}_c(\hat{T}_{\mathrm{w}})} \left[\left(\frac{\partial \hat{v}_j}{\partial x_l} \right)_{\mathrm{B}} + \left(\frac{\partial \hat{v}_l}{\partial x_j} \right)_{\mathrm{B}} \right] n_l (\delta_{ij} - n_i n_j) \\
&\qquad + c_T^I \frac{1}{\hat{\rho}_{\mathrm{B}} \hat{T}_{\mathrm{w}}} \frac{\hat{T}_{\mathrm{w}}^{1/2}}{\hat{A}_c(\hat{T}_{\mathrm{w}})} \left(\frac{\partial \hat{T}}{\partial x_j} \right)_{\mathrm{B}} (\delta_{ij} - n_i n_j),
\end{aligned} \tag{97a}
$$

$$
\frac{\bar{\bar{T}}}{\hat{T}_{\mathrm{w}}} = c_v^{II} \frac{1}{\hat{\rho}_{\mathrm{B}} \hat{T}_{\mathrm{w}}^{1/2}} \frac{\hat{T}_{\mathrm{w}}^{1/2}}{\hat{A}_c(\hat{T}_{\mathrm{w}})} \left(\frac{\partial \hat{v}_i}{\partial x_j} \right)_{\mathrm{B}} n_i n_j + c_T^{II} \frac{1}{\hat{\rho}_{\mathrm{B}} \hat{T}_{\mathrm{w}}} \frac{\hat{T}_{\mathrm{w}}^{1/2}}{\hat{A}_c(\hat{T}_{\mathrm{w}})} \left(\frac{\partial \hat{T}}{\partial x_i} \right)_{\mathrm{B}} n_i, \tag{97b}
$$

where c_v^I, c_T^I, c_v^{II}, and c_T^{II} are undetermined constants depending on the properties of the gas and the accommodation coefficient α and are determined together with the solutions ϕ_v^I, ϕ_T^I, ϕ_v^{II}, and ϕ_T^{II}. Once they have been determined, Eq. (97) gives the desired slip boundary conditions for the compressible Navier–Stokes equations, and the constants c_v^I, c_T^I, c_v^{II}, and c_T^{II} are called the slip coefficients. If we denote by $\boldsymbol{t}$ an arbitrary unit vector on the plane tangent to the boundary and fixed to the boundary (i.e., $\boldsymbol{n} \cdot \boldsymbol{t} = 0$), Eq. (97a) is equivalent to the following form:

$$
\frac{\bar{\bar{v}}_i}{\hat{T}_{\mathrm{w}}^{1/2}} t_i = c_v^I \frac{1}{\hat{\rho}_{\mathrm{B}} \hat{T}_{\mathrm{w}}^{1/2}} \frac{\hat{T}_{\mathrm{w}}^{1/2}}{\hat{A}_c(\hat{T}_{\mathrm{w}})} \left[\left(\frac{\partial \hat{v}_i}{\partial x_j} \right)_{\mathrm{B}} + \left(\frac{\partial \hat{v}_j}{\partial x_i} \right)_{\mathrm{B}} \right] n_i t_j + c_T^I \frac{1}{\hat{\rho}_{\mathrm{B}} \hat{T}_{\mathrm{w}}} \frac{\hat{T}_{\mathrm{w}}^{1/2}}{\hat{A}_c(\hat{T}_{\mathrm{w}})} \left(\frac{\partial \hat{T}}{\partial x_i} \right)_{\mathrm{B}} t_i. \tag{98}
$$

The assumption that ϕ_v^I, ϕ_T^I, ϕ_v^{II}, and ϕ_T^{II} are all functions of y, ζ_{n}, ζ, and $\hat{\mathcal{E}}$ will turn out to be consistent.

Substituting Eqs. (96) and (97) into Eq. (95), we obtain the following four decomposed problems for ϕ_v^I, ϕ_T^I, ϕ_v^{II}, and ϕ_T^{II}:

(i) Problem for $(\phi_v^I;\, c_v^I)$:

$$
\zeta_{\mathrm{n}} \frac{\partial \phi_v^I}{\partial y} = \mathcal{L}^S(\phi_v^I), \qquad (y > 0), \tag{99a}
$$

$$
\phi_v^I = (1 - \alpha) \widetilde{\mathcal{R}} \phi_v^I - 2\alpha c_v^I + (2 - \alpha)\, \zeta_{\mathrm{n}}\, B, \qquad (y = 0,\ \zeta_{\mathrm{n}} > 0), \tag{99b}
$$

$$
\phi_v^I \to 0, \qquad (y \to \infty). \tag{99c}
$$

(ii) Problem for $(\phi_T^I;\, c_T^I)$:

$$\zeta_{\rm n}\frac{\partial\phi_T^I}{\partial y} = \mathcal{L}^S(\phi_T^I), \qquad (y>0), \tag{100a}$$

$$\phi_T^I = (1-\alpha)\widetilde{\mathcal{R}}\phi_T^I - 2\alpha c_T^I + \alpha\, A(\zeta,\, \hat{\mathcal{E}}), \qquad (y=0,\ \zeta_{\rm n}>0), \tag{100b}$$

$$\phi_T^I \to 0, \qquad (y\to\infty). \tag{100c}$$

(iii) Problem for $(\phi_v^{II};\, c_v^{II})$:

$$\zeta_{\rm n}\frac{\partial\phi_v^{II}}{\partial y} = \mathcal{L}(\phi_v^{II}), \qquad (y>0), \tag{101a}$$

$$\begin{aligned}\phi_v^{II} &= (1-\alpha)\widetilde{\mathcal{R}}\phi_v^{II} - 2\alpha\sqrt{\pi}\int_{\zeta_{\rm n}<0}\int_0^\infty \zeta_{\rm n}\phi_v^{II}E(\zeta)\frac{\hat{\mathcal{E}}^{\delta/2-1}}{\Gamma(\delta/2)}e^{-\hat{\mathcal{E}}}d\hat{\mathcal{E}}d\boldsymbol{\zeta}\\ &\quad -\alpha\left(\zeta^2-\frac{4+\delta}{2}+\hat{\mathcal{E}}\right)c_v^{II}\\ &\quad +\alpha\left[\left(\zeta_{\rm n}^2-\frac{1}{3}\zeta^2\right)B + B_b(\zeta,\,\hat{\mathcal{E}}) - \frac{1}{3}I_B - 2I_{B_b}\right], \qquad (y=0,\ \zeta_{\rm n}>0),\end{aligned} \tag{101b}$$

$$\phi_v^{II} \to 0, \qquad (y\to\infty). \tag{101c}$$

(iv) Problem for $(\phi_T^{II};\, c_T^{II})$:

$$\zeta_{\rm n}\frac{\partial\phi_T^{II}}{\partial y} = \mathcal{L}(\phi_T^{II}), \qquad (y>0), \tag{102a}$$

$$\begin{aligned}\phi_T^{II} &= (1-\alpha)\widetilde{\mathcal{R}}\phi_T^{II} - 2\alpha\sqrt{\pi}\int_{\zeta_{\rm n}<0}\int_0^\infty \zeta_{\rm n}\phi_T^{II}E(\zeta)\frac{\hat{\mathcal{E}}^{\delta/2-1}}{\Gamma(\delta/2)}e^{-\hat{\mathcal{E}}}d\hat{\mathcal{E}}d\boldsymbol{\zeta}\\ &\quad -\alpha\left(\zeta^2-\frac{4+\delta}{2}+\hat{\mathcal{E}}\right)c_T^{II} + (2-\alpha)\zeta_{\rm n}A(\zeta,\,\hat{\mathcal{E}}), \qquad (y=0,\ \zeta_{\rm n}>0),\end{aligned} \tag{102b}$$

$$\phi_T^{II} \to 0, \qquad (y\to\infty). \tag{102c}$$

In Eqs. (99a) and (100a), $\mathcal{L}^S(\,\cdot\,)$ is the linear operator defined as follows: If $\mathcal{L}$ is operated on any function of the form $\zeta_j t_j \varphi(\zeta_{\rm n},\, \zeta,\, \hat{\mathcal{E}})$, it can be shown that the resulting function is of the form $\zeta_j t_j \times$ (a function of $\zeta_{\rm n},\ \zeta,$ and $\hat{\mathcal{E}}$); $\mathcal{L}^S(\,\cdot\,)$ is defined by this resulting function of $\zeta_{\rm n}$, ζ, and $\hat{\mathcal{E}}$, that is,

$$\mathcal{L}[\zeta_j t_j \varphi(\zeta_{\rm n},\, \zeta,\, \hat{\mathcal{E}})] = \zeta_j t_j \mathcal{L}^S[\varphi(\zeta_{\rm n},\, \zeta,\, \hat{\mathcal{E}})](\zeta_{\rm n},\, \zeta,\, \hat{\mathcal{E}}), \tag{103}$$

where the last parentheses show the independent variables of $\mathcal{L}^S(\varphi)$. In the present ES model, $\mathcal{L}^S(\varphi)$ takes the following form:

$$\mathcal{L}^S(\varphi) = \left\langle(\zeta^2-\zeta_{\rm n}^2)\varphi\right\rangle + 2(1-\theta)\nu\zeta_{\rm n}\left\langle\zeta_{\rm n}(\zeta^2-\zeta_{\rm n}^2)\varphi\right\rangle - \varphi, \tag{104}$$

with $\langle\,\cdot\,\rangle$ defined in Eq. (33). The functions A and B_b and the constants B, I_B, and I_{B_b} occurring in Eqs. (99)–(102) are defined by

$$A(\zeta,\, \hat{\mathcal{E}}) = \mathcal{A}(\zeta,\, \hat{\mathcal{E}},\, \hat{T}_{\rm w})\frac{\hat{A}_c(\hat{T}_{\rm w})}{\hat{T}_{\rm w}^{1/2}} = \zeta^2 - \frac{5+\delta}{2} + \hat{\mathcal{E}}, \tag{105a}$$

$$B_b(\zeta,\, \hat{\mathcal{E}}) = \mathcal{B}_b(\zeta,\, \hat{\mathcal{E}},\, \hat{T}_{\rm w})\frac{\hat{A}_c(\hat{T}_{\rm w})}{\hat{T}_{\rm w}^{1/2}} = \frac{1}{\theta}\frac{2}{3+\delta}\left(\frac{1}{3}\delta\,\zeta^2 - \hat{\mathcal{E}}\right), \tag{105b}$$

$$B = \mathcal{B}(\hat{T}_{\rm w})\frac{\hat{A}_c(\hat{T}_{\rm w})}{\hat{T}_{\rm w}^{1/2}} = \frac{2}{1-\nu+\theta\nu}, \tag{105c}$$

$$I_B = \mathcal{I}_{\mathcal{B}}(\hat{T}_{\rm w})\frac{\hat{A}_c(\hat{T}_{\rm w})}{\hat{T}_{\rm w}^{1/2}} = \frac{2}{1-\nu+\theta\nu}, \tag{105d}$$

$$I_{B_b} = \mathcal{I}_{\mathcal{B}_b}(\hat{T}_{\rm w})\frac{\hat{A}_c(\hat{T}_{\rm w})}{\hat{T}_{\rm w}^{1/2}} = \frac{\delta}{6\theta(3+\delta)}. \tag{105e}$$

2. Further simplification of decomposed problems

Before discussing the solutions of the four problems obtained in the previous subsection, we simplify these problems further. For this purpose, we introduce a unit vector $\boldsymbol{s}$ on the plane tangent to the boundary and orthogonal to $\boldsymbol{t}$ (i.e., $\boldsymbol{n}\cdot\boldsymbol{s}=\boldsymbol{t}\cdot\boldsymbol{s}=0$). Denoting the tangential components of $\boldsymbol{\zeta}$ by $\zeta_{\rm s}=\boldsymbol{\zeta}\cdot\boldsymbol{s}$ and $\zeta_{\rm t}=\boldsymbol{\zeta}\cdot\boldsymbol{t}$, we introduce the reduced velocity distribution functions $(\varphi_v^I,\,\varphi_T^I,\,\varphi_v^{II},\,\varphi_T^{II})$, $(\psi_v^I,\,\psi_T^I,\,\psi_v^{II},\,\psi_T^{II})$, and $(\chi_v^I,\,\chi_T^I,\,\chi_v^{II},\,\chi_T^{II})$ corresponding to $(\phi_v^I,\,\phi_T^I,\,\phi_v^{II},\,\phi_T^{II})$, by the following equations:

$$\varphi_\kappa^N(y,\,\zeta_{\rm n})=\frac{1}{\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_0^{\infty}\phi_\kappa^N(y,\,\zeta_{\rm n},\,\zeta,\,\hat{\mathcal{E}})e^{-\zeta_{\rm s}^2-\zeta_{\rm t}^2}\frac{\hat{\mathcal{E}}^{\delta/2-1}}{\Gamma(\delta/2)}e^{-\hat{\mathcal{E}}}d\hat{\mathcal{E}}d\zeta_{\rm t}d\zeta_{\rm s}, \tag{106a}$$

$$\psi_\kappa^N(y,\,\zeta_{\rm n})=\frac{1}{\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_0^{\infty}(\zeta_{\rm s}^2+\zeta_{\rm t}^2)\phi_\kappa^N(y,\,\zeta_{\rm n},\,\zeta,\,\hat{\mathcal{E}})e^{-\zeta_{\rm s}^2-\zeta_{\rm t}^2}\frac{\hat{\mathcal{E}}^{\delta/2-1}}{\Gamma(\delta/2)}e^{-\hat{\mathcal{E}}}d\hat{\mathcal{E}}d\zeta_{\rm t}d\zeta_{\rm s}, \tag{106b}$$

$$\chi_\kappa^N(y,\,\zeta_{\rm n})=\frac{1}{\pi}\frac{2}{\delta}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_0^{\infty}\hat{\mathcal{E}}\phi_\kappa^N(y,\,\zeta_{\rm n},\,\zeta,\,\hat{\mathcal{E}})e^{-\zeta_{\rm s}^2-\zeta_{\rm t}^2}\frac{\hat{\mathcal{E}}^{\delta/2-1}}{\Gamma(\delta/2)}e^{-\hat{\mathcal{E}}}d\hat{\mathcal{E}}d\zeta_{\rm t}d\zeta_{\rm s}, \tag{106c}$$

$$(\kappa=v,\ T \text{ and } N=I,\ II).$$

Noting that $\zeta^2-\zeta_{\rm n}^2=\zeta_{\rm s}^2+\zeta_{\rm t}^2$, we can rewrite $\mathcal{L}^S(\phi_\kappa^I)$ $(\kappa=v,\,T)$ [cf. Eq. (104)] using ψ_κ^I as follows:

$$\mathcal{L}^S(\phi_\kappa^I)=\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty}\psi_\kappa^I e^{-\zeta_{\rm n}^2}d\zeta_{\rm n}+2(1-\theta)\nu\zeta_{\rm n}\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty}\zeta_{\rm n}\psi_\kappa^I e^{-\zeta_{\rm n}^2}d\zeta_{\rm n}-\phi_\kappa^I. \tag{107}$$

We can also rewrite $\mathcal{L}(\phi_\kappa^{II})$ $(\kappa=v,\,T)$ [cf. Eq. (32)] using φ_κ^{II}, ψ_κ^{II}, and χ_κ^{II} in the following form:

$$\mathcal{L}(\phi_\kappa^{II})=\omega+2\zeta_{\rm n}u_{\rm n}+\left(\hat{\mathcal{E}}-\frac{\delta}{2}\right)\tau_{\rm rel}+\left(\zeta_i\zeta_j-\frac{\delta_{ij}}{2}\right)d_{ij}-\phi_\kappa^{II}, \tag{108a}$$

$$\omega=\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty}\varphi_\kappa^{II}e^{-\zeta_{\rm n}^2}d\zeta_{\rm n},\qquad u_{\rm n}=\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty}\zeta_{\rm n}\varphi_\kappa^{II}e^{-\zeta_{\rm n}^2}d\zeta_{\rm n}, \tag{108b}$$

$$\tau_{\rm rel}=\theta\tau+(1-\theta)\tau_{\rm int},\qquad \tau=\frac{3\tau_{\rm tr}+\delta\tau_{\rm int}}{3+\delta}, \tag{108c}$$

$$\tau_{\rm tr}=\frac{2}{3}\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty}\left(\zeta_{\rm n}^2-\frac{3}{2}\right)\varphi_\kappa^{II}e^{-\zeta_{\rm n}^2}d\zeta_{\rm n}+\frac{2}{3}\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty}\psi_\kappa^{II}e^{-\zeta_{\rm n}^2}d\zeta_{\rm n}, \tag{108d}$$

$$\tau_{\rm int}=\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty}\chi_\kappa^{II}e^{-\zeta_{\rm n}^2}d\zeta_{\rm n}-\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty}\varphi_\kappa^{II}e^{-\zeta_{\rm n}^2}d\zeta_{\rm n}, \tag{108e}$$

$$d_{ij}=[(1-\theta)\tau_{\rm tr}+\theta\tau]\delta_{ij}+(1-\theta)\nu[P_{ij}-(\omega+\tau_{\rm tr})\delta_{ij}], \tag{108f}$$

$$P_{ij}=\frac{2}{\sqrt{\pi}}\int_{-\infty}^{\infty}\zeta_{\rm n}^2\varphi_\kappa^{II}e^{-\zeta_{\rm n}^2}d\zeta_{\rm n}\,n_in_j+\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty}\psi_\kappa^{II}e^{-\zeta_{\rm n}^2}d\zeta_{\rm n}(\delta_{ij}-n_in_j). \tag{108g}$$

Here, we have omitted the subscript κ and superscript II for the macroscopic quantities ω, $u_{\rm n}$, $\tau_{\rm rel}$, etc. to avoid cumbersome notation. With these expressions, we consider the individual problems.

(i) Problem for $(\phi_v^I;\,c_v^I)$:

If we multiply Eq. (99a) [with Eq. (107)] by $(1/\pi)(\zeta_{\rm s}^2+\zeta_{\rm t}^2)[\Gamma(\delta/2)]^{-1}e^{-\zeta_{\rm s}^2-\zeta_{\rm t}^2}\hat{\mathcal{E}}^{\delta/2-1}e^{-\hat{\mathcal{E}}}$ and integrate the resulting equation with respect to $\hat{\mathcal{E}}$ from 0 to ∞ and with respect to $\zeta_{\rm s}$ and $\zeta_{\rm t}$ from $-\infty$ to ∞ for both variables, then we have

$$\zeta_{\rm n}\frac{\partial\psi_v^I}{\partial y}=\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty}\psi_v^I e^{-\zeta_{\rm n}^2}d\zeta_{\rm n}+2(1-\theta)\nu\zeta_{\rm n}\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty}\zeta_{\rm n}\psi_v^I e^{-\zeta_{\rm n}^2}d\zeta_{\rm n}-\psi_v^I. \tag{109}$$

The integration of this equation times $e^{-\zeta_{\rm n}^2}$ with respect to $\zeta_{\rm n}$ from $-\infty$ to ∞ gives

$$\frac{d}{dy}\int_{-\infty}^{\infty}\zeta_{\rm n}\psi_v^I e^{-\zeta_{\rm n}^2}d\zeta_{\rm n}=0. \tag{110}$$

Since $\psi_v^I \to 0$ as $y \to \infty$, it follows that

$$\int_{-\infty}^{\infty} \zeta_{\rm n} \psi_v^I e^{-\zeta_{\rm n}^2} d\zeta_{\rm n} = 0. \tag{111}$$

That is, the second integral on the right-hand side in Eq. (109) vanishes. If we carry out the same operation as that led to Eq. (109) on the boundary conditions (99b) and (99c), we obtain the boundary conditions for ψ_v^I. The condition at infinity is obvious, and that on the boundary becomes

$$\psi_v^I = (1-\alpha)\widetilde{\mathcal{R}}\psi_v^I - 2\alpha c_v^I + (2-\alpha)\,\frac{2}{1-\nu+\theta\nu}\zeta_{\rm n}, \qquad (y=0,\ \zeta_{\rm n}>0). \tag{112}$$

Therefore, if we let

$$\psi_v^I = \frac{1}{1-\nu+\theta\nu}\bar{\psi}_v^I, \qquad c_v^I = \frac{1}{1-\nu+\theta\nu}\bar{c}_v^I, \tag{113}$$

the problem for ϕ_v^I reduces to the following problem for $(\bar{\psi}_v^I;\, \bar{c}_v^I)$:

$$\zeta_{\rm n}\frac{\partial \bar{\psi}_v^I}{\partial y} = \frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} \bar{\psi}_v^I e^{-\zeta_{\rm n}^2} d\zeta_{\rm n} - \bar{\psi}_v^I, \qquad (y>0), \tag{114a}$$

$$\bar{\psi}_v^I = (1-\alpha)\widetilde{\mathcal{R}}\bar{\psi}_v^I - 2\alpha\bar{c}_v^I + 2(2-\alpha)\,\zeta_{\rm n}, \qquad (y=0,\ \zeta_{\rm n}>0), \tag{114b}$$

$$\bar{\psi}_v^I \to 0, \qquad (y\to\infty). \tag{114c}$$

(ii) Problem for $(\phi_T^I;\, c_T^I)$:

With the procedure same as that was used to derive the problem for ψ_v^I, we can reduce the problem for ϕ_T^I to the following problem for $(\psi_T^I;\, c_T^I)$:

$$\zeta_{\rm n}\frac{\partial \psi_T^I}{\partial y} = \frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} \psi_T^I e^{-\zeta_{\rm n}^2} d\zeta_{\rm n} - \psi_T^I, \qquad (y>0), \tag{115a}$$

$$\psi_T^I = (1-\alpha)\widetilde{\mathcal{R}}\psi_T^I - 2\alpha c_T^I + \alpha\left(\zeta_{\rm n}^2 - \frac{1}{2}\right), \qquad (y=0,\ \zeta_{\rm n}>0), \tag{115b}$$

$$\psi_T^I \to 0, \qquad (y\to\infty). \tag{115c}$$

(iii) Problem for $(\phi_v^{II};\, c_v^{II})$:

Since Eqs. (101a) and (102a) are of the same form, we consider these equations together. Because of the property (34) and the fact that $\phi_\kappa^{II} \to 0$ as $y \to \infty$, it follows from Eqs. (101a) and (102a) that

$$\langle \zeta_{\rm n}\phi_\kappa^{II}\rangle = \langle \zeta_{\rm n}^2\phi_\kappa^{II}\rangle = \langle \zeta_{\rm n}(\zeta^2+\hat{\mathcal{E}})\phi_\kappa^{II}\rangle = 0, \qquad (\kappa = v,\, T). \tag{116}$$

These conservation relations are rewritten in terms of φ_κ^{II}, ψ_κ^{II}, and χ_κ^{II} as follows:

$$\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} \zeta_{\rm n}\varphi_\kappa^{II} e^{-\zeta_{\rm n}^2} d\zeta_{\rm n} = u_{\rm n} = 0, \tag{117a}$$

$$\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} \zeta_{\rm n}^2\varphi_\kappa^{II} e^{-\zeta_{\rm n}^2} d\zeta_{\rm n} = \frac{1}{2}P_{ij}n_i n_j = 0, \tag{117b}$$

$$\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} \zeta_{\rm n}\left(\zeta_{\rm n}^2\varphi_\kappa^{II} + \psi_\kappa^{II} + \frac{\delta}{2}\chi_\kappa^{II}\right) e^{-\zeta_{\rm n}^2} d\zeta_{\rm n} = 0. \tag{117c}$$

We multiply Eqs. (101a) and (102a) by $[1,\, \zeta_{\rm s}^2+\zeta_{\rm t}^2,\, (2/\delta)\hat{\mathcal{E}}](1/\pi)[\Gamma(\delta/2)]^{-1}e^{-\zeta_{\rm s}^2-\zeta_{\rm t}^2}\hat{\mathcal{E}}^{\delta/2-1}\times e^{-\hat{\mathcal{E}}}$ and integrate the resulting equations with respect to $\hat{\mathcal{E}}$ from 0 to ∞ and with respect to $\zeta_{\rm s}$ and $\zeta_{\rm t}$ from $-\infty$ to ∞ for both variables. If we use the explicit expression of P_{ij}, ω,

and $\tau_{\rm tr}$ [cf. Eq. (108)] in the term $P_{ij}-(\omega+\tau_{\rm tr})\delta_{ij}$ and take account of Eqs. (117a) and (117b), we have the following system of equations for φ_κ^{II}, ψ_κ^{II}, and χ_κ^{II} ($\kappa=v,\,T$):

$$\zeta_{\rm n}\frac{\partial}{\partial y}\begin{bmatrix}\varphi_\kappa^{II}\\ \psi_\kappa^{II}\\ \chi_\kappa^{II}\end{bmatrix}=\omega\begin{bmatrix}1\\1\\1\end{bmatrix}+\tau_{\rm rel}\begin{bmatrix}0\\0\\1\end{bmatrix}+[(1-\theta)\tau_{\rm tr}+\theta\tau]\begin{bmatrix}\zeta_{\rm n}^2-\frac{1}{2}\\ \zeta_{\rm n}^2+\frac{1}{2}\\ \zeta_{\rm n}^2-\frac{1}{2}\end{bmatrix}$$
$$-\frac{2}{3}(1-\theta)\nu\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty}\psi_k^{II}e^{-\zeta_{\rm n}^2}d\zeta_{\rm n}\begin{bmatrix}\zeta_{\rm n}^2-\frac{1}{2}\\ \zeta_{\rm n}^2-1\\ \zeta_{\rm n}^2-\frac{1}{2}\end{bmatrix}-\begin{bmatrix}\varphi_k^{II}\\ \psi_k^{II}\\ \chi_k^{II}\end{bmatrix}. \tag{118}$$

The corresponding boundary conditions for (φ_v^{II}, ψ_v^{II}, χ_v^{II}) are obtained by applying the same procedure, i.e., the integration after multiplying by $[1,\,\zeta_{\rm s}^2+\zeta_{\rm t}^2,\,(2/\delta)\hat{\mathcal{E}}](1/\pi)\times[\Gamma(\delta/2)]^{-1}e^{-\zeta_{\rm s}^2-\zeta_{\rm t}^2}\hat{\mathcal{E}}^{\delta/2-1}e^{-\hat{\mathcal{E}}}$, to Eqs. (101b) and (101c). The results are as follows:

$$\begin{bmatrix}\varphi_v^{II}\\ \psi_v^{II}\\ \chi_v^{II}\end{bmatrix}=(1-\alpha)\widetilde{\mathcal{R}}\begin{bmatrix}\varphi_v^{II}\\ \psi_v^{II}\\ \chi_v^{II}\end{bmatrix}-2\alpha\int_{-\infty}^{0}\zeta_{\rm n}\varphi_v^{II}e^{-\zeta_{\rm n}^2}d\zeta_{\rm n}\begin{bmatrix}1\\1\\1\end{bmatrix}-\alpha c_v^{II}\begin{bmatrix}\zeta_{\rm n}^2-1\\ \zeta_{\rm n}^2\\ \zeta_{\rm n}^2\end{bmatrix}$$
$$+\alpha\frac{2}{3}B\begin{bmatrix}\zeta_{\rm n}^2-\frac{1}{2}\\ \zeta_{\rm n}^2-1\\ \zeta_{\rm n}^2-\frac{1}{2}\end{bmatrix}+\alpha\frac{1}{\theta}\frac{2}{3+\delta}\begin{bmatrix}\frac{\delta}{3}\left(\zeta_{\rm n}^2-\frac{1}{2}\right)\\ \frac{\delta}{3}\left(\zeta_{\rm n}^2+\frac{1}{2}\right)\\ \frac{\delta}{3}\left(\zeta_{\rm n}^2-\frac{1}{2}\right)-1\end{bmatrix}$$
$$-\alpha\left(\frac{1}{3}I_B+2I_{B_b}\right)\begin{bmatrix}1\\1\\1\end{bmatrix},\qquad (y=0,\ \zeta_{\rm n}>0), \tag{119a}$$

$$\begin{bmatrix}\varphi_v^{II}\\ \psi_v^{II}\\ \chi_v^{II}\end{bmatrix}\to 0,\qquad (y\to\infty). \tag{119b}$$

In summary, Eqs. (118) (with $\kappa=v$) and (119) form the half-space problem for (φ_v^{II}, ψ_v^{II}, χ_v^{II}; c_v^{II}).

(iv) Problem for (ϕ_T^{II}; c_T^{II}):

The equation for ϕ_T^{II} is given by Eq. (118) with $\kappa=T$. The boundary conditions for (φ_T^{II}, ψ_T^{II}, χ_T^{II}) are obtained from Eqs. (102b) and (102c) in the same way as Eq. (119).

That is,

$$\begin{bmatrix} \varphi_T^{II} \\ \psi_T^{II} \\ \chi_T^{II} \end{bmatrix} = (1-\alpha)\widetilde{\mathcal{R}} \begin{bmatrix} \varphi_T^{II} \\ \psi_T^{II} \\ \chi_T^{II} \end{bmatrix} - 2\alpha \int_{-\infty}^{0} \zeta_{\mathrm{n}} \varphi_T^{II} e^{-\zeta_{\mathrm{n}}^2} d\zeta_{\mathrm{n}} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} - \alpha c_T^{II} \begin{bmatrix} \zeta_{\mathrm{n}}^2 - 1 \\ \zeta_{\mathrm{n}}^2 \\ \zeta_{\mathrm{n}}^2 \end{bmatrix}$$
$$+ (2-\alpha)\zeta_{\mathrm{n}} \begin{bmatrix} \zeta_{\mathrm{n}}^2 - \dfrac{3}{2} \\ \zeta_{\mathrm{n}}^2 - \dfrac{1}{2} \\ \zeta_{\mathrm{n}}^2 - \dfrac{1}{2} \end{bmatrix}, \qquad (y = 0,\ \zeta_{\mathrm{n}} > 0), \tag{120a}$$

$$\begin{bmatrix} \varphi_T^{II} \\ \psi_T^{II} \\ \chi_T^{II} \end{bmatrix} \to 0, \qquad (y \to \infty). \tag{120b}$$

To summarize, the half-space problem for $(\varphi_T^{II},\ \psi_T^{II},\ \chi_T^{II};\ c_T^{II})$ is given by Eqs. (118) (with $\kappa = T$) and (120).

3. *Some remarks on decomposed problems*

The problems for $(\phi_v^I;\ c_v^I)$, $(\phi_T^I;\ c_T^I)$, and $(\phi_T^{II};\ c_T^{II})$ in Sec. V B 1 are the classical half-space problems in kinetic theory formulated by the use of the linearized ES model and the Maxwell-type boundary condition for a polyatomic gas. To be more specific, the problem for $(\phi_v^I;\ c_v^I)$ is the problem of shear slip (the so-called Kramers problem), that for $(\phi_T^I;\ c_T^I)$ is the problem of thermal creep, and that for $(\phi_T^{II};\ c_T^{II})$ is the problem of temperature jump.

As we have seen in Sec. V B 2, the problem for $(\phi_v^I;\ c_v^I)$ is reduced to that for $(\bar{\psi}_v^I;\ \bar{c}_v^I)$, Eq. (114). We note here that Eq. (114) is exactly the same as the problem of the Knudsen layer for the shear slip based on the linearized Bhatnagar–Gross–Krook (BGK) model for a monatomic gas [41, 42] and the Maxwell-type boundary condition. It is one of the classical problems in kinetic theory studied by various authors [43–47] [there are some earlier results [48, 49] for $\alpha = 1$ (diffuse reflection)]. In fact, $\bar{c}_v^I$ is the slip coefficient of the problem, which is equal to κ in Ref. [44] and ζ_P in Ref. [47]. Therefore, we can easily find the value of $\bar{c}_v^I$ in the literature and can, in principle, recover the solution $\bar{\psi}_v^I$ from the data in the literature. Consequently, we can obtain the solution, i.e., the reduced distribution ψ_v^I of ϕ_v^I and c_v^I, of the original problem, Eq. (99), immediately from Eq. (113). If we rewrite $(\bar{\psi}_v^I,\ \bar{c}_v^I)$ as $(\psi_{v\mathrm{BGK}}^I,\ c_{v\mathrm{BGK}}^I)$, Eq. (113) reads

$$\psi_v^I = \frac{1}{1-\nu+\theta\nu}\psi_{v\mathrm{BGK}}^I, \qquad c_v^I = \frac{1}{1-\nu+\theta\nu}c_{v\mathrm{BGK}}^I, \tag{121}$$

where and in what follows the subscript BGK indicates the corresponding quantities for the BGK model for a monatomic gas. Then, if necessary, ϕ_v^I can be reconstructed easily by the integration of Eq. (99a) with Eqs. (99b) and (99c) because the first two terms in the right-hand side of Eq. (107) are known from ψ_v^I. It should be noted that similar reductions from the ES model for a polyatomic gas to the BGK model for a monatomic gas have been used for the Poiseuille flow and thermal transpiration between two plates and through a circular pipe [28, 29].

On the other hand, the problem for $(\phi_T^I;\ c_T^I)$ is reduced to that for $(\psi_T^I;\ c_T^I)$, Eq. (115). We note that Eq. (115) is exactly the same as the problem of the Knudsen layer for the thermal creep based on the linearized BGK model and the Maxwell-type boundary condition. Therefore, the effect of a polyatomic gas does not appear. This is also a classical problem that has been investigated in several papers [45, 47, 50, 51] (there is an earlier work [52] for $\alpha = 1$), and c_T^I corresponds to the slip coefficient of the problem, which is equal to $d/2$ in Ref. [51] and ζ_T in

Ref. [47]. Therefore, the numerical value of c_T^I is available, and the reduced distribution ψ_T^I of ϕ_T^I can, in principle, be obtained from the literature. This fact is summarized by writing

$$\psi_T^I = \psi_{T\mathrm{BGK}}^I, \qquad c_T^I = c_{T\mathrm{BGK}}^I. \tag{122}$$

The reconstruction of ϕ_T^I is also possible with the help of Eq. (100).

In this way, the problem for $(\phi_v^I;\, c_v^I)$ and that for $(\phi_T^I;\, c_T^I)$ are reduced to the case of the BGK model for a monatomic gas, so that we do not need new computations basically. On the contrary, the problem for $(\varphi_v^{II},\, \psi_v^{II},\, \chi_v^{II};\, c_v^{II})$, Eqs. (118) ($\kappa = v$) and (119), and that for $(\varphi_T^{II},\, \psi_T^{II},\, \chi_T^{II};\, c_T^{II})$, Eqs. (118) ($\kappa = T$) and (120), are new in the sense that they cannot be reduced to any known problems and require new computation. Although these problems, which are half-space boundary-value problems of three simultaneous integro-differential equations, appear to be more complicated, they are essentially of the same structure as the problems for $(\phi_v^I;\, c_v^I)$ and for $(\phi_T^I;\, c_T^I)$. Therefore, the numerical solution of these problems can be carried out without any difficulty. Some numerical results will be given in Secs. V B 5 and V B 7.

4. *Remarks on actual numerical computation*

The decomposed Knudsen-layer problems have been reduced to their simplest forms in Sec. V B 2, and some remarks on them have been made in Sec. V B 3 because they may facilitate other researchers' computation of the solution of the Knudsen-layer problems, which lead to the slip boundary conditions, for gases other than those considered in the present paper. However, in the present study, we solve the problems in intermediate forms between Eqs. (99)–(102) and Eqs. (114), (115), and (118)–(120) for the reason described below.

The intermediate forms are for the reduced distribution functions G_κ^N and H_κ^N defined by

$$G_\kappa^N(y,\, \zeta_\mathrm{n},\, \zeta) = E(\zeta) \int_0^\infty \phi_\kappa^N(y,\, \zeta_\mathrm{n},\, \zeta,\, \hat{\mathcal{E}}) \frac{\hat{\mathcal{E}}^{\delta/2-1}}{\Gamma(\delta/2)} e^{-\hat{\mathcal{E}}} d\hat{\mathcal{E}}, \tag{123a}$$

$$H_\kappa^N(y,\, \zeta_\mathrm{n},\, \zeta) = \frac{2}{\delta} E(\zeta) \int_0^\infty \hat{\mathcal{E}} \phi_\kappa^N(y,\, \zeta_\mathrm{n},\, \zeta,\, \hat{\mathcal{E}}) \frac{\hat{\mathcal{E}}^{\delta/2-1}}{\Gamma(\delta/2)} e^{-\hat{\mathcal{E}}} d\hat{\mathcal{E}}, \tag{123b}$$

where $\kappa = v,\, T$ and $N = I,\, II$. In a paper by Hattori (one of the present authors) and Takata [33], the authors analyzed numerically some Knudsen-layer problems using the linearized Boltzmann equation for a monatomic hard-sphere gas. Unlike the BGK and ES models, the problems can be reduced only to the half-space boundary value problems for functions of $(y,\, \zeta_\mathrm{n},\, \zeta)$. In Ref. [33], an accurate finite-difference scheme was devised on the basis of the integral form of the linearized Boltzmann equation. This scheme has an advantage that it captures the singularities in macroscopic quantities on the boundary ($y = 0$) precisely. The accuracy of the scheme has been checked carefully in Ref. [33]. The coupled equations for G_κ^N and H_κ^N in the present problem have essentially the same structure as the equations solved in Ref. [33]. In addition, the former equations, based on the ES model, are much simpler than the latter equations based on the real Boltzmann equation. Therefore, it is straightforward to modify and adapt the scheme in Ref. [33] to the equations for G_κ^N and H_κ^N. Since the scheme in Ref. [33] is well established, we preferred to use this approach, rather than developing a new scheme and code for Eq. (118) in spite of the fact that the independent variables of Eq. (118) are only $(y,\, \zeta_\mathrm{n})$. The descriptions of the intermediate equations for G_κ^N and H_κ^N and the numerical schemes for them are cumbersome, so that we omit them in the present paper. Leaving some remarks on the accuracy of the computation in Appendix B, we will directly jump to the numerical results.

5. *Results of numerical analysis*

In the present paper, we give the numerical results of the slip coefficients and the profiles of the macroscopic quantities inside the Knudsen layer and omit those of the velocity distribution function. In particular, we concentrate on the slip coefficients in this Sec. V B 5 leaving the macroscopic quantities in the Knudsen layer to Sec. V B 7.

We consider four kinds of gases: nitrogen (N_2), methanol (CH_3OH), water vapor (H_2O), and carbon dioxide (CO_2). To carry out computation, we need an appropriate parameter setting for each gas. The original ES model contains the three parameters δ, ν, and θ. As we will see in Sec.VI (see also Ref. [22]), they are related to the ratio μ_b/μ, where μ is the viscosity and μ_b is the bulk viscosity, and the Prandtl number Pr by Eqs. (136) and (137) appearing later. For each gas, we specify δ, μ_b/μ, and Pr according to the literature and then determine ν and θ. It is known that μ_b/μ is very large and about 1000 for CO_2 gas. However, for large values of μ_b/μ, the Knudsen layer in the problems for ϕ_v^{II} and ϕ_T^{II} decays very slowly because of the slow relaxation of the internal modes, so that the computation becomes increasingly difficult. This situation is similar to the increase of the thickness of a shock wave for large μ_b/μ [53]. For this reason, we consider a fictitious gas, called pseudo-CO_2 gas [53], that has the correct Prandtl number but smaller values of μ_b/μ ($\mu_b/\mu = 5$, 10, 20, and 50) and denote it by $CO_2(\mu_b/\mu)$ [$CO_2(5)$, $CO_2(10)$, $CO_2(20)$, and $CO_2(50)$]. For other parameters, we set $\mathrm{Pr} = 0.767$ (the value at 273K based on the data in Ref. [54]) and $\delta = 3$ (Note that $\delta = 4$ is used in Ref. [53] because it is more appropriate for the high temperature in a strong shock wave). The parameters for the four gases are summarized in Table I. The values for N_2 are taken from Ref. [28] (see Ref. [28] for the original references and the reason for these choices). The values for CH_3OH and H_2O are based on Ref. [55].

TABLE I: The values of μ_b/μ, Pr, ν, θ, and δ for the gases.

	μ_b/μ	Pr	ν	θ	δ
N_2	0.736	0.787	-0.5	0.46	2
CH_3OH	0.808	0.85	-0.49991668	0.647	6
H_2O (290K)	0.702	1.01	0.018681113	0.47	3
$CO_2(5)$	5	0.767	-0.332698715	0.086918731	3
$CO_2(10)$	10	0.767	-0.31758292	0.043459365	3
$CO_2(20)$	20	0.767	-0.31052865	0.021729683	3
$CO_2(50)$	50	0.767	-0.30644454	0.0086918731	3

TABLE II: The values of c_v^I and c_T^I for different gases.

α	c_v^I					c_T^I [47]
	BGK [47]	N_2	CH_3OH	H_2O	$CO_2(n)$	
0.1	17.10313	13.46703	14.53766	17.27416	13.11810	0.2641783
0.2	8.224902	6.476301	6.991167	8.307151	6.308500	0.2781510
0.3	5.255112	4.137883	4.466845	5.307663	4.030671	0.2919238
0.4	3.762619	2.962692	3.198226	3.800245	2.885929	0.3055019
0.5	2.861190	2.252906	2.432012	2.889802	2.194533	0.3188906
0.6	2.255410	1.775913	1.917099	2.277964	1.729899	0.3320949
0.7	1.818667	1.432021	1.545867	1.836854	1.394918	0.3451195
0.8	1.487654	1.171381	1.264506	1.502531	1.141031	0.3579692
0.9	1.227198	0.9662976	1.043118	1.239470	0.9412609	0.3706483
1.0	1.016191	0.8001504	0.8637624	1.026353	0.7794185	0.3831612

As mentioned in Sec. V B 3, the coefficient c_T^I is the same as in the case of the BGK model for a monatomic gas [cf. Eq. (122)], and the coefficient c_v^I is obtained immediately by Eq. (121) from the value $c_{v\mathrm{BGK}}^I$ for the BGK model. The numerical values of c_v^I and c_T^I are shown in Table II. Here, the values for the BGK models are taken from Ref. [47], in which the results based on different models of the Boltzmann equation, including the BGK model, are compared. For $CO_2(n)$, the value of c_v^I is independent of n because $c_v^I = \mathrm{Pr}\,\bar{c}_v^I$ [Eqs. (113) and (137)] and Pr is fixed independent of n. The values of the slip coefficients c_v^{II} and c_T^{II}, which were obtained by the present computation, are shown in Tables III and IV, respectively. For $CO_2(n)$, accurate computation becomes increasingly difficult as n becomes large. Therefore, we give only two

TABLE III: The values of c_v^{II} for different gases.

α	N_2	CH_3OH	H_2O	$CO_2(5)$	$CO_2(10)$	$CO_2(20)$	$CO_2(50)$
0.1	0.28324	0.19074	0.30749	0.7527	1.3862	2.705	6.9
0.2	0.29461	0.19928	0.32089	0.8029	1.4981	2.958	7.6
0.3	0.30572	0.20767	0.33393	0.8464	1.5879	3.143	8.1
0.4	0.31658	0.21590	0.34662	0.8848	1.6621	3.286	8.4
0.5	0.32721	0.22399	0.35898	0.9190	1.7249	3.400	8.6
0.6	0.33762	0.23194	0.37103	0.9498	1.7789	3.494	8.8
0.7	0.34783	0.23975	0.38279	0.9779	1.8262	3.574	9.0
0.8	0.35783	0.24744	0.39426	1.0036	1.8681	3.642	9.1
0.9	0.36765	0.25499	0.40547	1.0274	1.9057	3.702	9.2
1.0	0.37730	0.26243	0.41641	1.0495	1.9398	3.755	9.3

TABLE IV: The values of c_T^{II} for different gases.

α	N_2	CH_3OH	H_2O	$CO_2(5)$	$CO_2(10)$	$CO_2(20)$	$CO_2(50)$
0.1	20.0188	18.8622	19.6093	19.6187	19.6272	19.639	19.659
0.2	9.65649	9.09291	9.45850	9.46581	9.47206	9.4797	9.4919
0.3	6.18752	5.82305	6.06030	6.06604	6.07070	6.0761	6.0840
0.4	4.44218	4.17830	4.35058	4.35508	4.35858	4.3624	4.3678
0.5	3.38654	3.18379	3.31648	3.32000	3.32265	3.3255	3.3292
0.6	2.67594	2.51458	2.62039	2.62313	2.62514	2.6272	2.6299
0.7	2.16266	2.03137	2.11760	2.11972	2.12125	2.1228	2.1248
0.8	1.77283	1.66454	1.73576	1.73738	1.73854	1.7397	1.7411
0.9	1.46541	1.37539	1.43465	1.43588	1.43675	1.4376	1.4387
1.0	1.21578	1.14069	1.19016	1.19107	1.19172	1.1923	1.1931

digits for $CO_2(50)$ in Table III. According to Table IV, c_T^{II} depends weakly on the types of gases.

6. *Summary of the slip boundary conditions*

With the numerical results in Sec. V B 5, the slip boundary conditions for the compressible Navier–Stokes equations (46) follow immediately from Eqs. (51), (90), (97b), and (98). That is,

$$(\hat{v}_i - \hat{v}_{\mathrm{w}i})n_i = 0, \tag{124a}$$

$$(\hat{v}_i - \hat{v}_{\mathrm{w}i})t_i = \epsilon c_v^I \frac{\hat{T}_{\mathrm{w}}^{1/2}}{\hat{A}_c(\hat{T}_{\mathrm{w}})} \frac{1}{\hat{\rho}} \left(\frac{\partial \hat{v}_i}{\partial x_j} + \frac{\partial \hat{v}_j}{\partial x_i} \right) n_i t_j + \epsilon c_T^I \frac{1}{\hat{A}_c(\hat{T}_{\mathrm{w}})} \frac{1}{\hat{\rho}} \frac{\partial \hat{T}}{\partial x_i} t_i, \tag{124b}$$

$$\hat{T} - \hat{T}_{\mathrm{w}} = \epsilon c_v^{II} \frac{\hat{T}_{\mathrm{w}}}{\hat{A}_c(\hat{T}_{\mathrm{w}})} \frac{1}{\hat{\rho}} \frac{\partial \hat{v}_i}{\partial x_j} n_i n_j + \epsilon c_T^{II} \frac{\hat{T}_{\mathrm{w}}^{1/2}}{\hat{A}_c(\hat{T}_{\mathrm{w}})} \frac{1}{\hat{\rho}} \frac{\partial \hat{T}}{\partial x_i} n_i, \tag{124c}$$

where the quantities $\hat{\rho}$, $\hat{v}_i$, and $\hat{T}$, which belong to the Chapman–Enskog solution, as well as their derivatives are all evaluated on the boundary. The values of the slip coefficients c_v^I, c_T^I, c_v^{II}, and c_T^{II} are summarized in Sec. V B 5. As noted in Ref. [1], Eq. (124) forms two-dimensional fields on the boundary at each time and is independent of the trajectory of the points on the boundary. It should be noted that Eq. (124) is of essentially the same form as the slip boundary conditions for a monatomic gas [cf. Eq. (118) in Ref. [1]]. The effect of polyatomic gases appears through the slip coefficients.

The initial condition for Eq. (46) is given by Eq. (47) under assumption (iv) in Sec. II. However, if we are interested only in the behavior of the gas in the fluid-dynamic time scale

that is much longer than the mean free time in practical applications, we may ignore assumption (iv) in Sec. II and assume the following more general initial condition:

$$\hat{\rho} = \hat{\rho}^{\rm in}(\boldsymbol{x}), \qquad \hat{\boldsymbol{v}} = \hat{\boldsymbol{v}}^{\rm in}(\boldsymbol{x}), \qquad \hat{T} = \hat{T}^{\rm in}(\boldsymbol{x}), \qquad \text{at } \hat{t} = 0, \tag{125}$$

where $\hat{\rho}^{\rm in}(\boldsymbol{x})$, $\hat{\boldsymbol{v}}^{\rm in}(\boldsymbol{x})$, and $\hat{T}^{\rm in}(\boldsymbol{x})$ are the density, flow velocity, and temperature generated from the initial condition, which is more general than Eq. (26), for the ES model specified in the problem under consideration:

$$\hat{f}(0,\, \boldsymbol{x},\, \boldsymbol{\zeta},\, \hat{\mathcal{E}}) = \hat{f}^{\rm in}(\boldsymbol{x},\, \boldsymbol{\zeta},\, \hat{\mathcal{E}}). \tag{126}$$

The reader is referred to Sec. 5.2.4 in Ref. [1] for more detailed discussion about the initial condition.

7. *Summary of macroscopic quantities inside the Knudsen layer*

Equation (88) with Eqs. (71), (72), and (78) gives the relation

$$\langle \mathcal{C}_{\rm wn}\phi\rangle = O(\epsilon). \tag{127}$$

Here and in Eq. (128) bellow, the integration variables $(\boldsymbol{\zeta},\, \hat{\mathcal{E}})$ in the definition of $\langle\,\cdot\,\rangle$ [Eq. (33)] should be replaced by $(\boldsymbol{\mathcal{C}}_{\rm w},\, \bar{\mathcal{E}}_{\rm w})$, as in Eq. (74). Similarly, if we integrate Eq. (79) multiplied by $(\mathcal{C}_{{\rm w}i},\, \mathcal{C}_{\rm w}^2 + \bar{\mathcal{E}}_{\rm w})E(\mathcal{C}_{\rm w})\bar{\mathcal{E}}_{\rm w}^{\delta/2-1}\exp(-\bar{\mathcal{E}}_{\rm w})$ over the whole range of $(\boldsymbol{\mathcal{C}}_{\rm w},\, \bar{\mathcal{E}}_{\rm w})$ and take into account the fact that $\phi \to 0$ as $y \to \infty$, we obtain

$$\langle \mathcal{C}_{{\rm w}i}\mathcal{C}_{\rm wn}\phi\rangle = O(\epsilon), \qquad \left\langle \left(\mathcal{C}_{\rm w}^2 + \bar{\mathcal{E}}_{\rm w}\right)\mathcal{C}_{\rm wn}\phi\right\rangle = O(\epsilon). \tag{128}$$

Equations (127) and (128) mean, from Eqs. (73b), (73c), and (73f), that $\hat{v}_{{\rm K}i}^{(1)}n_i$, $\hat{p}_{{\rm K}ij}^{(1)}n_j$, and $\hat{q}_{{\rm K}i}^{(1)}n_i$ are all of $O(\epsilon)$. Other components of the macroscopic quantities $\hat{h}_{\rm K}^{(1)}$ can be obtained by using Eqs. (78) and (96) in Eq. (73) and by noting that the change of the names of the variables (94) has been made in Eq. (96). We summarize the result of the Knudsen-layer correction of the macroscopic quantities $\hat{h}_{\rm K} = \hat{h}_{\rm K}^{(1)}\epsilon + O(\epsilon^2)$ [Eq. (53)] neglecting the terms of $O(\epsilon^2)$, that is,

$$\hat{v}_{{\rm K}i}n_i = 0, \tag{129a}$$

$$\hat{v}_{{\rm K}i}t_i = \epsilon Y_v(y)\frac{\hat{T}_{\rm w}^{1/2}}{\hat{A}_c(\hat{T}_{\rm w})}\frac{1}{\hat{\rho}}\left(\frac{\partial \hat{v}_i}{\partial x_j} + \frac{\partial \hat{v}_j}{\partial x_i}\right)n_i t_j + \epsilon Y_T(y)\frac{1}{\hat{A}_c(\hat{T}_{\rm w})}\frac{1}{\hat{\rho}}\frac{\partial \hat{T}}{\partial x_i}t_i, \tag{129b}$$

$$\hat{\rho}_{\rm K} = \epsilon\Omega_v(y)\frac{1}{\hat{A}_c(\hat{T}_{\rm w})}\frac{\partial \hat{v}_i}{\partial x_j}n_i n_j + \epsilon\Omega_T(y)\frac{1}{\hat{T}_{\rm w}^{1/2}}\frac{1}{\hat{A}_c(\hat{T}_{\rm w})}\frac{\partial \hat{T}}{\partial x_i}n_i, \tag{129c}$$

$$\begin{bmatrix} \hat{T}_{\rm trK} \\ \hat{T}_{\rm intK} \\ \hat{T}_{\rm K} \end{bmatrix} = \epsilon \begin{bmatrix} \Theta_v^{\rm tr}(y) \\ \Theta_v^{\rm int}(y) \\ \Theta_v(y) \end{bmatrix} \frac{\hat{T}_{\rm w}}{\hat{A}_c(\hat{T}_{\rm w})}\frac{1}{\hat{\rho}}\frac{\partial \hat{v}_i}{\partial x_j}n_i n_j + \epsilon \begin{bmatrix} \Theta_T^{\rm tr}(y) \\ \Theta_T^{\rm int}(y) \\ \Theta_T(y) \end{bmatrix} \frac{\hat{T}_{\rm w}^{1/2}}{\hat{A}_c(\hat{T}_{\rm w})}\frac{1}{\hat{\rho}}\frac{\partial \hat{T}}{\partial x_i}n_i, \tag{129d}$$

$$\hat{p}_{{\rm K}ij}n_j = 0, \tag{129e}$$

$$\hat{p}_{{\rm K}ij}t_j = \epsilon\Pi_v(y)\frac{\hat{T}_{\rm w}}{\hat{A}_c(\hat{T}_{\rm w})}\frac{\partial \hat{v}_j}{\partial x_k}n_j n_k t_i + \epsilon\Pi_T(y)\frac{\hat{T}_{\rm w}^{1/2}}{\hat{A}_c(\hat{T}_{\rm w})}\frac{\partial \hat{T}}{\partial x_j}n_j t_i, \tag{129f}$$

$$\hat{q}_{{\rm K}i}n_i = 0, \tag{129g}$$

$$\hat{q}_{{\rm K}i}t_i = \epsilon H_v(y)\frac{\hat{T}_{\rm w}^{3/2}}{\hat{A}_c(\hat{T}_{\rm w})}\left(\frac{\partial \hat{v}_i}{\partial x_j} + \frac{\partial \hat{v}_j}{\partial x_i}\right)n_i t_j + \epsilon H_T(y)\frac{\hat{T}_{\rm w}}{\hat{A}_c(\hat{T}_{\rm w})}\frac{\partial \hat{T}}{\partial x_i}t_i, \tag{129h}$$

where, with $\kappa = v,\, T$,

$$Y_\kappa(y) = \frac{1}{2}\left\langle (\zeta^2 - \zeta_{\rm n}^2)\phi_\kappa^I\right\rangle, \tag{130a}$$

$$\Omega_\kappa(y) = \left\langle \phi_\kappa^{II} \right\rangle, \tag{130b}$$

$$\Theta_\kappa^{\rm tr}(y) = \frac{2}{3}\left\langle \left(\zeta^2 - \frac{3}{2}\right)\phi_\kappa^{II} \right\rangle, \tag{130c}$$

$$\Theta_\kappa^{\rm int}(y) = \frac{2}{\delta}\left\langle \left(\hat{\mathcal{E}} - \frac{\delta}{2}\right)\phi_\kappa^{II} \right\rangle, \tag{130d}$$

$$\Theta_\kappa(y) = \frac{3\Theta_\kappa^{\rm tr} + \delta\Theta_\kappa^{\rm int}}{3+\delta}, \tag{130e}$$

$$\Pi_\kappa(y) = \frac{3}{2}[\Omega_\kappa(y) + \Theta_\kappa^{\rm tr}(y)], \tag{130f}$$

$$H_\kappa(y) = \frac{1}{2}\left\langle (\zeta^2 - \zeta_{\rm n}^2)\left(\zeta^2 + \hat{\mathcal{E}} - \frac{5+\delta}{2}\right)\phi_\kappa^{I} \right\rangle. \tag{130g}$$

In Eq. (130), $\langle\cdot\rangle$ is defined with the variables $(\boldsymbol{\zeta}, \hat{\mathcal{E}})$ by Eq. (33).

Now we give some numerical result for the Knudsen-layer functions $Y_\kappa(y)$, $\Omega_\kappa(y)$, ..., $H_\kappa(y)$. In Sec. V B 2, we mentioned that the problem for ϕ_v^I is reduced to the problem of ψ_v^I, which is then reduced to the problem for $\bar{\psi}_v^I$ for the BGK model for a monatomic gas by Eq. (113). Similarly, the problem for ϕ_T^I is reduced to that for ψ_T^I, which is exactly the same as the corresponding problem for the BGK model. Using this fact and making some considerations (see Appendix C), we can obtain the following relations between the present ES model and the BGK model for the functions $Y_v(y)$, $H_v(y)$, $Y_T(y)$, and $H_T(y)$:

$$\begin{bmatrix} Y_v(y) \\ H_v(y) \end{bmatrix} = \frac{1}{1-\nu+\theta\nu}\begin{bmatrix} Y_{v\rm BGK}(y) \\ H_{v\rm BGK}(y) \end{bmatrix}, \tag{131a}$$

$$Y_T(y) = Y_{T\rm BGK}(y), \qquad H_T(y) = H_{T\rm BGK}(y) + \frac{\delta\alpha}{4\sqrt{\pi}}J_0(y), \tag{131b}$$

where $J_n(y)$ is the so-called Abramowitz function [56] defined by

$$J_n(y) = \int_0^\infty z^n e^{-z^2-\frac{y}{z}}dz, \qquad (y \geq 0). \tag{132}$$

We recall that we can, in principle, reconstruct the data of $Y_{v\rm BGK}(y)$, $H_{v\rm BGK}(y)$, $Y_{T\rm BGK}(y)$, and $H_{T\rm BGK}(y)$ from the information in the literature, for instance, from Refs. [44, 51]. In order to save space, we only show the basic functions $Y_{v\rm BGK}(y)$, $H_{v\rm BGK}(y)$, $Y_{T\rm BGK}(y)$, and $H_{T\rm BGK}(y)$ for $\alpha = 1.0$, 0.5, and 0.2 in Fig. 2 and the function $J_0(y)$ in Table V. We note that the results shown in Fig. 2 were newly recomputed using the schemes for (G_κ^I, H_κ^I) $(\kappa = v, T)$, not reconstructed from the data in the literature, and that the values in Table V were computed by the use of the FORTRAN subroutine provided in Ref. [57].

TABLE V: Abramowitz function $J_0(y)$.

y	$J_0(y)$	y	$J_0(y)$	y	$J_0(y)$
0.0	0.886227	0.1	0.634322	1.2	0.117823
0.01	0.838746	0.2	0.506231	1.4	0.093710
0.02	0.804956	0.3	0.417408	1.6	0.075313
0.03	0.776230	0.4	0.350797	1.8	0.061060
0.04	0.750737	0.5	0.298717	2.0	0.049876
0.05	0.727609	0.6	0.256889	2.5	0.030899
0.06	0.706336	0.7	0.222647	3.0	0.019739
0.07	0.686581	0.8	0.194206	4.0	0.008619
0.08	0.668105	0.9	0.170310	5.0	0.004022
0.09	0.650731	1.0	0.150046	6.0	0.001972

In Figs. 3–8, we show the profiles of the functions $\Omega_v(y)$, $\Omega_T(y)$, $\Theta_v^{\rm tr}(y)$, $\Theta_v^{\rm int}(y)$, $\Theta_T^{\rm tr}(y)$, and $\Theta_T^{\rm int}(y)$, respectively, in the case of $\alpha = 1.0$, 0.5, and 0.2 for nitrogen, methanol, and water

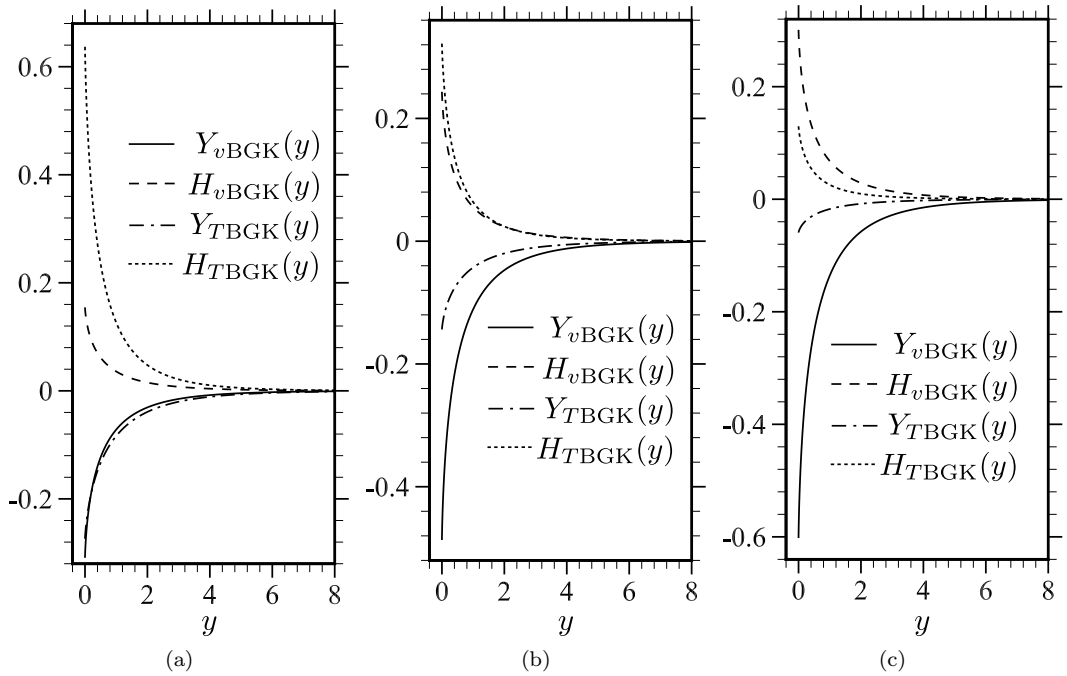


FIG. 2: Knudsen-layer functions for the BGK model. (a) $\alpha = 1.0$, (b) $\alpha = 0.5$, (c) $\alpha = 0.2$. The solid line indicates $Y_{v\mathrm{BGK}}(y)$, the dashed line $H_{v\mathrm{BGK}}(y)$, the dot-dashed line $Y_{T\mathrm{BGK}}(y)$, and the dotted line $H_{T\mathrm{BGK}}(y)$.

vapor. In Figs. 3–5 and 7, the corresponding profiles for the BGK model for a monatomic gas are also shown. Figures 9 and 10 show, respectively, the profiles of $[\Omega_v(y), \Theta_v^{\mathrm{tr}}(y), \Theta_v^{\mathrm{int}}(y)]$ and $[\Omega_T(y), \Theta_T^{\mathrm{tr}}(y), \Theta_T^{\mathrm{int}}(y)]$ in the case of $\alpha = 1$ (diffuse reflection) for $\mathrm{CO_2}(n)$ gas ($n = 5, 10, 20, 50$).

Once the solution of the compressible Navier–Stokes equations (46) with the slip boundary conditions (124) (and the initial conditions) is obtained, the profiles of corrections of the macroscopic quantities inside the Knudsen layer, $\hat{h}_{\mathrm{K}}$ in Eq. (50), are obtained from Eq. (129), and thus the profiles of the macroscopic quantities inside the Knudsen layer are given by Eq. (50).

VI. NAVIER–STOKES EQUATIONS AND SLIP BOUNDARY CONDITIONS IN DIMENSIONAL FORM

In this section, we transform the compressible Navier–Stokes equations (46) and the slip boundary conditions (124) to their original dimensional form.

We start with the stress tensor and the heat-flow vector. Using Eq. (17) in Eq. (44) and neglecting the terms of $O(\epsilon^2)$, we obtain the dimensional stress tensor p_{ij} and heat-flow vector q_i in the following form:

$$p_{ij} = p\delta_{ij} - \mu(T)\left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3}\frac{\partial v_k}{\partial X_k}\delta_{ij}\right) - \mu_b(T)\frac{\partial v_k}{\partial X_k}\delta_{ij}, \tag{133a}$$

$$q_i = -\lambda(T)\frac{\partial T}{\partial X_i}, \tag{133b}$$

where $\mu(T)$, $\mu_b(T)$, and $\lambda(T)$ are, respectively, the viscosity, the bulk viscosity, and the thermal

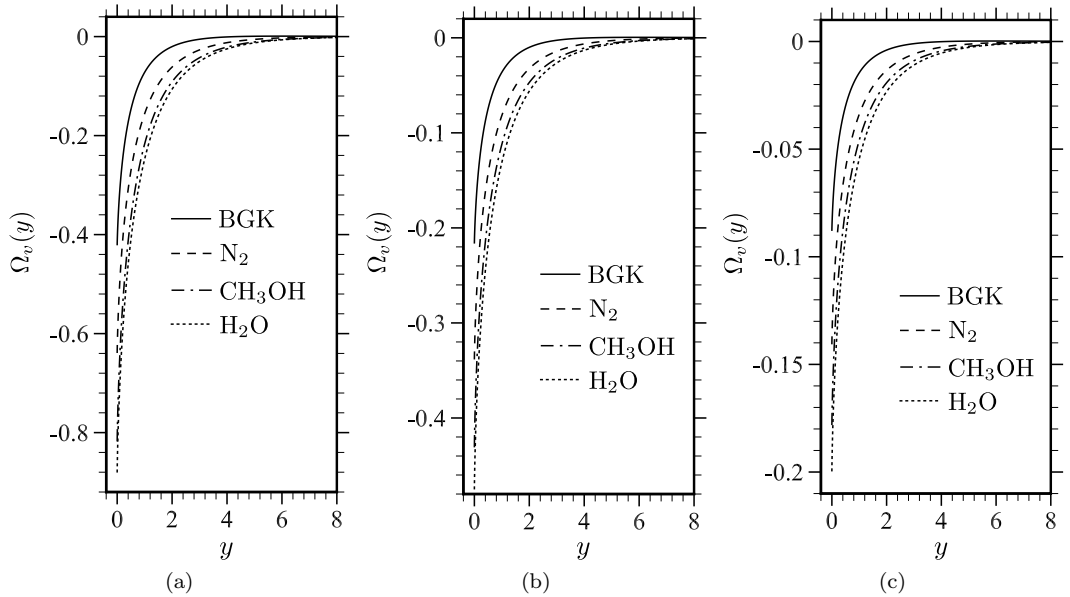


FIG. 3: Knudsen-layer function $\Omega_v(y)$. (a) $\alpha = 1.0$, (b) $\alpha = 0.5$, (c) $\alpha = 0.2$. The solid line indicates the result for the BGK model for a monatomic gas, the dashed line for nitrogen, the dot-dashed line for methanol, and the dotted line for water vapor.

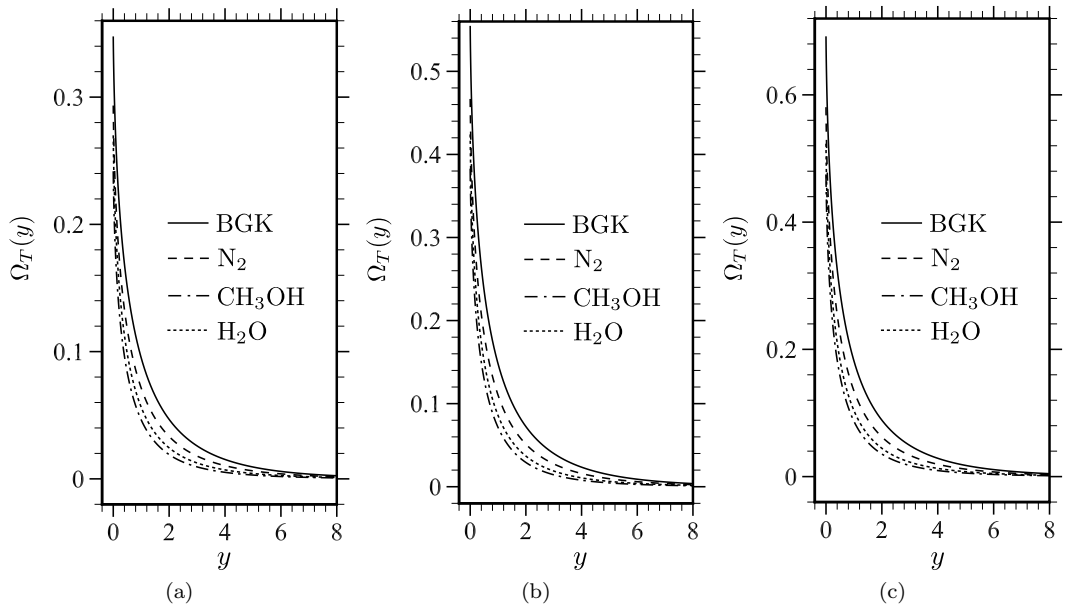


FIG. 4: Knudsen-layer function $\Omega_T(y)$. (a) $\alpha = 1.0$, (b) $\alpha = 0.5$, (c) $\alpha = 0.2$. See the caption of Fig. 3.

conductivity and are expressed as follows:

$$\mu(T) = \frac{p_0 L}{(2RT_0)^{1/2}} \epsilon \Gamma_1(\hat{T}) = \frac{1}{1-\nu+\theta\nu} \frac{RT}{A_c(T)}, \tag{134a}$$

$$\mu_b(T) = \frac{p_0 L}{(2RT_0)^{1/2}} \epsilon \Gamma_b(\hat{T}) = \frac{2}{3} \frac{\delta}{\theta(3+\delta)} \frac{RT}{A_c(T)}, \tag{134b}$$

$$\lambda(T) = \frac{5}{4} \frac{p_0 (2RT_0)^{1/2} L}{T_0} \epsilon \Gamma_2(\hat{T}) = \frac{5+\delta}{2} \frac{R^2 T}{A_c(T)}. \tag{134c}$$

In deriving the respective rightmost sides, use has been made of Eqs. (8), (20), and (45) in

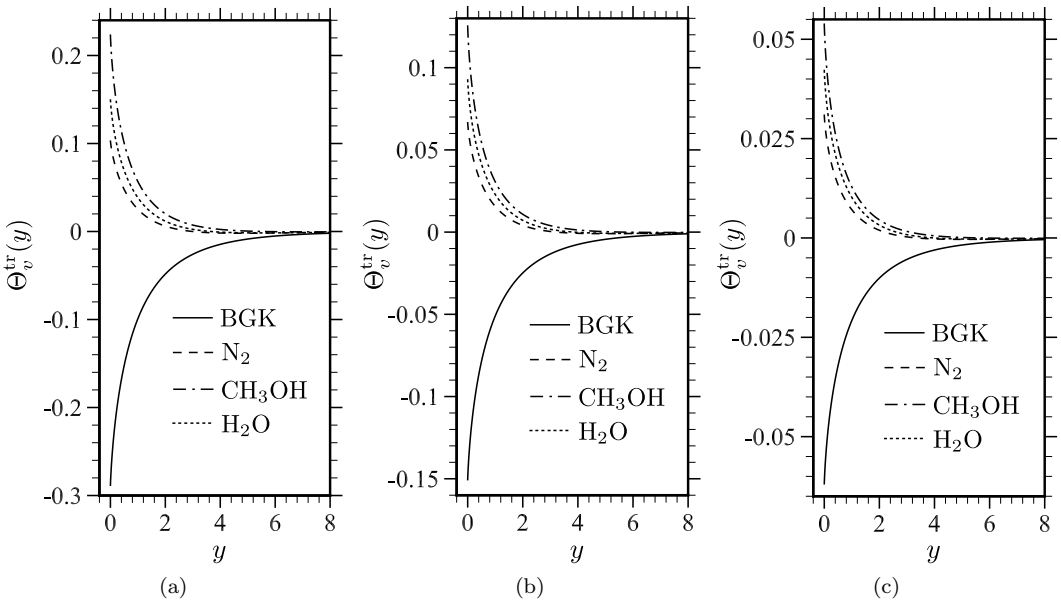


FIG. 5: Knudsen-layer function $\Theta_v^{\rm tr}(y)$. (a) $\alpha = 1.0$, (b) $\alpha = 0.5$, (c) $\alpha = 0.2$. See the caption of Fig. 3.

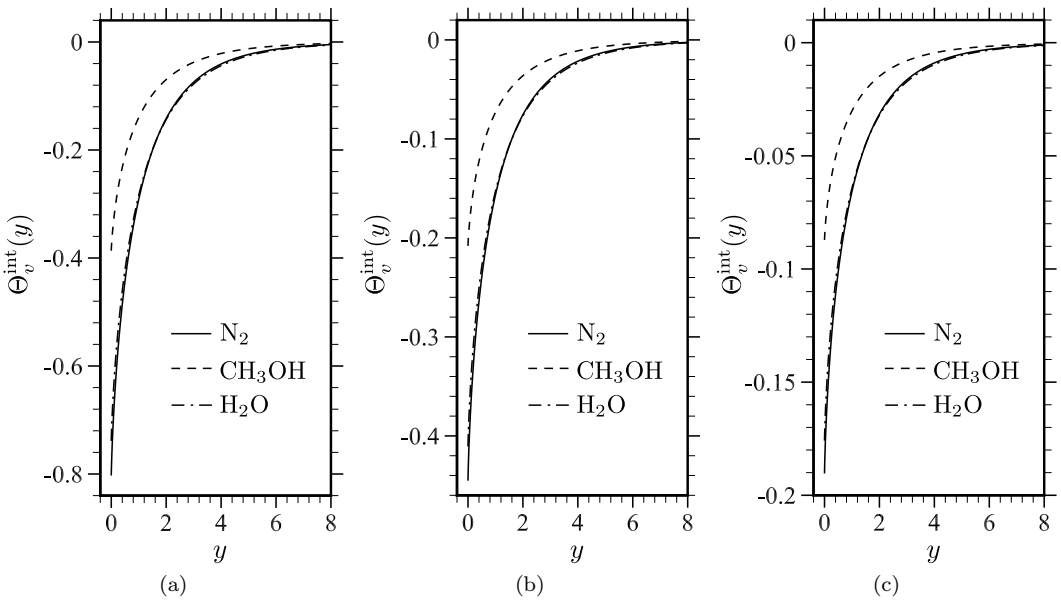


FIG. 6: Knudsen-layer function $\Theta_v^{\rm int}(y)$. (a) $\alpha = 1.0$, (b) $\alpha = 0.5$, (c) $\alpha = 0.2$. The solid line indicates the result for nitrogen, the dashed line for methanol, and the dot-dashed line for water vapor.

addition to Eq. (17).

Let us denote by γ the ratio of the specific heats, that is, $\gamma = c_p/c_v$, where c_p and c_v are the specific heat at constant pressure and that at constant volume, respectively. In this paper, we assume that c_p, c_v, and thus γ are constant (calorically perfect gas). Then, γ is expressed in terms of the internal degrees of freedom δ of a molecule as

$$\gamma = (\delta + 5)/(\delta + 3). \tag{135}$$

Therefore, μ_b and λ can also be written as

$$\mu_b(T) = \frac{5 - 3\gamma}{3\theta}\frac{\mu(T)}{\mathrm{Pr}}, \qquad \lambda(T) = \frac{R\gamma}{\gamma - 1}\frac{RT}{A_c(T)}, \tag{136}$$

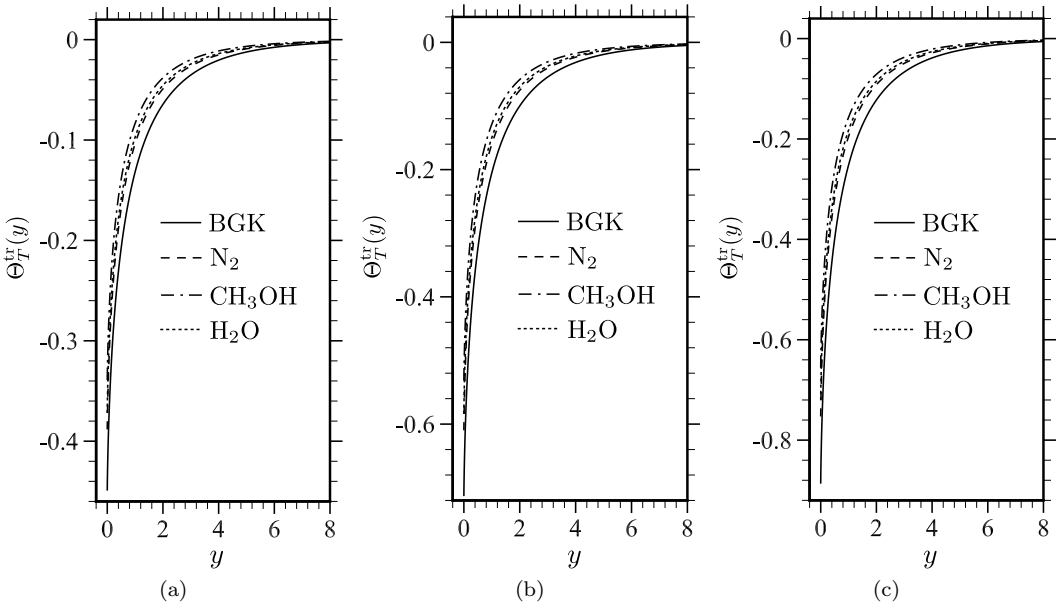


FIG. 7: Knudsen-layer function $\Theta_T^{\rm tr}(y)$. (a) $\alpha = 1.0$, (b) $\alpha = 0.5$, (c) $\alpha = 0.2$. See the caption of Fig. 3.

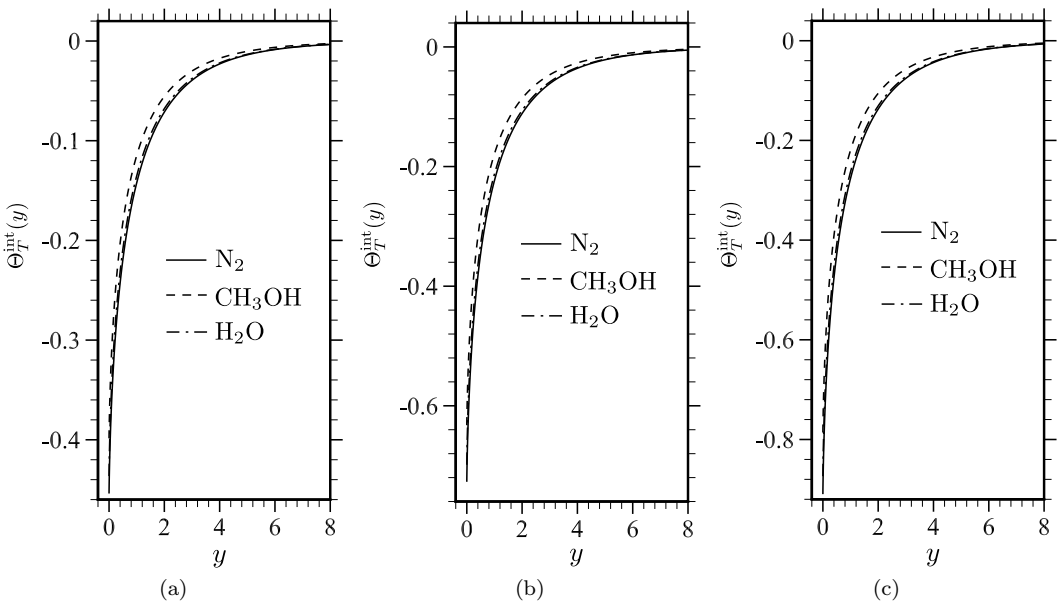


FIG. 8: Knudsen-layer function $\Theta_T^{\rm int}(y)$. (a) $\alpha = 1.0$, (b) $\alpha = 0.5$, (c) $\alpha = 0.2$. See the caption of Fig. 6.

where $\mathrm{Pr} = c_p\mu/\lambda$ is the Prandtl number and is expressed as

$$\mathrm{Pr} = 1/(1-\nu+\theta\nu), \tag{137}$$

because of the relation $c_p = R\gamma/(\gamma-1)$.

With the help of Eqs. (17) and (134), the compressible Navier–Stokes equations are transformed from the dimensionless form, Eq. (46), to the following dimensional form:

$$\frac{\partial\rho}{\partial t} + \frac{\partial\rho v_j}{\partial X_j} = 0, \tag{138a}$$

$$\frac{\partial\rho v_i}{\partial t} + \frac{\partial\rho v_i v_j}{\partial X_j} = -\frac{\partial p}{\partial X_i} + \frac{\partial}{\partial X_j}\left[\mu(T)\left(\frac{\partial v_j}{\partial X_i} + \frac{\partial v_i}{\partial X_j} - \frac{2}{3}\frac{\partial v_k}{\partial X_k}\delta_{ij}\right)\right]$$

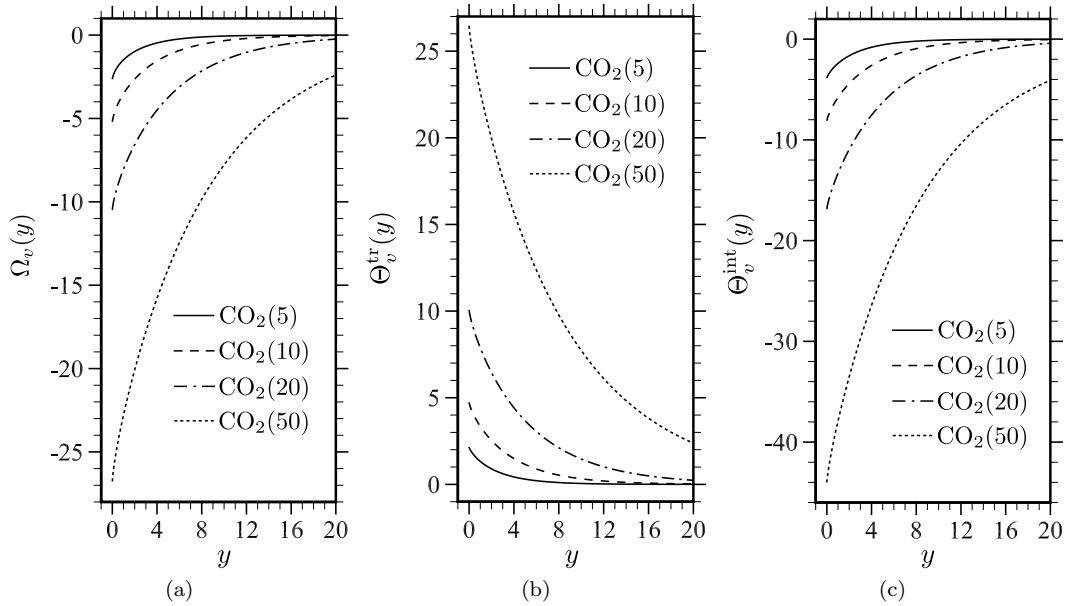


FIG. 9: Knudsen-layer functions $\Omega_v(y)$, $\Theta_v^{\rm tr}(y)$, and $\Theta_v^{\rm int}(y)$ in the case of $\alpha = 1$ for $CO_2(n)$. (a) $\Omega_v(y)$, (b) $\Theta_v^{\rm tr}(y)$, (c) $\Theta_v^{\rm int}(y)$. The solid line indicates the result for $CO_2(5)$, the dashed line for $CO_2(10)$, the dot-dashed line for $CO_2(20)$, and the dotted line for $CO_2(50)$.

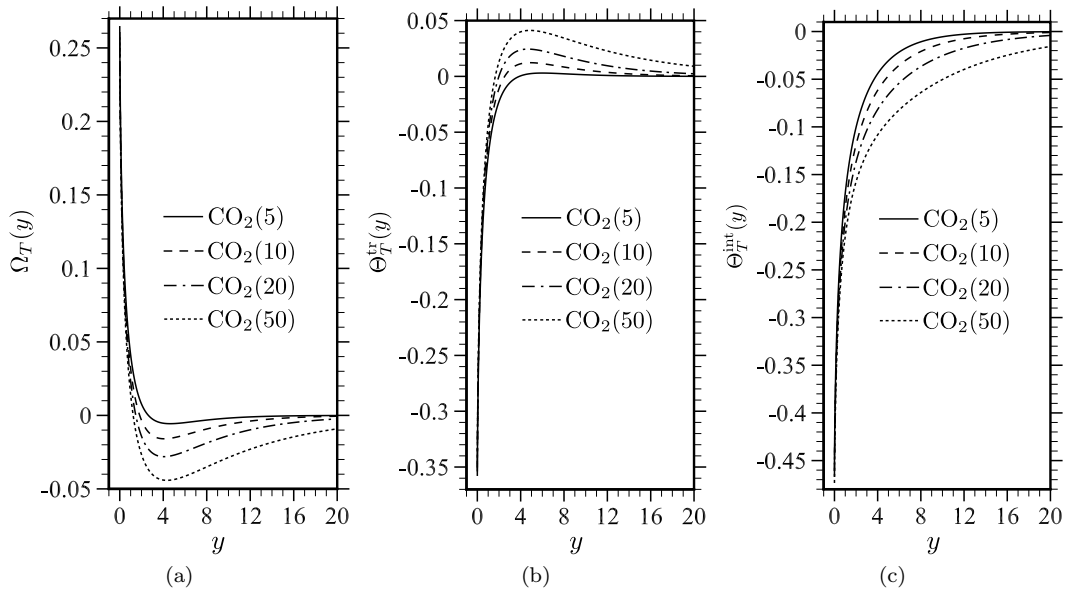


FIG. 10: Knudsen-layer functions $\Omega_T(y)$, $\Theta_T^{\rm tr}(y)$, and $\Theta_T^{\rm int}(y)$ in the case of $\alpha = 1$ for $CO_2(n)$. (a) $\Omega_T(y)$, (b) $\Theta_T^{\rm tr}(y)$, (c) $\Theta_T^{\rm int}(y)$. See the caption of Fig. 9.

$$+ \frac{\partial}{\partial X_i}\left[\mu_b(T)\frac{\partial v_j}{\partial X_j}\right], \tag{138b}$$

$$\begin{aligned}
&\frac{\partial}{\partial t}\left[\rho\left(\frac{3+\delta}{2}RT + \frac{1}{2}v_k^2\right)\right] + \frac{\partial}{\partial X_j}\left[\rho v_j\left(\frac{5+\delta}{2}RT + \frac{1}{2}v_k^2\right)\right] \\
&\quad = \frac{\partial}{\partial X_j}\left[\lambda(T)\frac{\partial T}{\partial X_j}\right] + \frac{\partial}{\partial X_j}\left[\mu(T)v_i\left(\frac{\partial v_j}{\partial X_i} + \frac{\partial v_i}{\partial X_j} - \frac{2}{3}\frac{\partial v_k}{\partial X_k}\delta_{ij}\right)\right] \\
&\quad\quad + \frac{\partial}{\partial X_j}\left[\mu_b(T)v_j\frac{\partial v_k}{\partial X_k}\right].
\end{aligned} \tag{138c}$$

By letting both of the bulk viscosity $\mu_b(T)$ and the degrees of freedom of the internal modes δ be zero, Eq. (138) reduces to the same form as the compressible Navier–Stokes equations for a monatomic gas [cf. Eq. (123) in Ref. [1]]. Therefore, the terms containing these quantities express the effect of polyatomic gases.

Next, we transform the slip boundary conditions (124) into their dimensional form. That is, if we use Eq. (17) and eliminate ϵ with the help of Eqs. (134a) and (134c) at $T = T_{\rm w}$ in Eq. (124), we obtain the following dimensional form of the slip boundary conditions:

$$(v_i - v_{{\rm w}i})n_i = 0, \tag{139a}$$

$$(v_i - v_{{\rm w}i})t_i = \frac{\sqrt{2}}{R^{1/2}} a_v^I \frac{\mu(T_{\rm w})}{\rho T_{\rm w}^{1/2}} \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} \right) n_i t_j + \frac{4}{5R} a_T^I \frac{\lambda(T_{\rm w})}{\rho T_{\rm w}} \frac{\partial T}{\partial X_i} t_i, \tag{139b}$$

$$T - T_{\rm w} = \frac{1}{R} a_v^{II} \frac{\mu(T_{\rm w})}{\rho} \frac{\partial v_i}{\partial X_j} n_i n_j + \frac{2\sqrt{2}}{5R^{3/2}} a_T^{II} \frac{\lambda(T_{\rm w})}{\rho T_{\rm w}^{1/2}} \frac{\partial T}{\partial X_i} n_i, \tag{139c}$$

where

$$a_v^I = (1 - \nu + \theta\nu) c_v^I = \bar{c}_v^I, \qquad a_T^I = (1 + \delta/5)^{-1} c_T^I, \tag{140a}$$

$$a_v^{II} = (1 - \nu + \theta\nu) c_v^{II}, \qquad a_T^{II} = (1 + \delta/5)^{-1} c_T^{II}. \tag{140b}$$

In Eqs. (139b) and (139c), μ is used in the terms containing the derivative of the flow velocity, and λ is used in those containing the derivative of the temperature. In contrast to the Navier–Stokes equations (138), the slip boundary conditions (139) are of essentially the same form as those for a monatomic gas [cf. Eq. (124) in Ref. [1]]. The effect of polyatomic gases appears indirectly via the coefficients a_v^I, a_T^I, a_v^{II}, and a_T^{II} as well as $\mu(T_{\rm w})$ and $\lambda(T_{\rm w})$.

The initial condition for Eq. (138) is given by

$$\rho = \rho_0, \qquad \boldsymbol{v} = 0, \qquad T = T_0, \qquad \text{at } t = 0, \tag{141}$$

corresponding to Eq. (47), under assumption (iv) in Sec. II, or

$$\rho = \rho^{\rm in}(\boldsymbol{X}), \qquad \boldsymbol{v} = \boldsymbol{v}^{\rm in}(\boldsymbol{X}), \qquad T = T^{\rm in}(\boldsymbol{X}), \qquad \text{at } t = 0, \tag{142}$$

corresponding to Eq. (125) in more general case without assumption (iv) and in the case when we ignore the accuracy for short time (within the scale of the mean free time). Here $\rho^{\rm in}$, $\boldsymbol{v}^{\rm in}$, and $T^{\rm in}$ are the density, flow velocity, and temperature obtained from the initial distribution $f^{\rm in}$ corresponding to Eq. (126) (see Sec. 5.2.4 in Ref. [1]).

VII. CONCLUDING REMARKS

In the present paper, we have derived the slip boundary conditions for the compressible Navier–Stokes equations for a polyatomic gas on the basis of the Chapman–Enskog solution and the Knudsen-layer analysis. It is an extension of Ref. [1], where the corresponding slip boundary conditions were derived for a monatomic gas. The full Boltzmann equation was used in Ref. [1], whereas the ES model of the Boltzmann equation was adopted in the present study because of the complexity of the Boltzmann collision integral for a polyatomic gas.

As in Ref. [1], the problem of determining the slip boundary conditions and the slip coefficients included in the conditions is reduced to the four half-space boundary-value problems for the linearized ES model, three of which are the classical problems of shear slip (the so-called Kramers problem), thermal creep, and temperature jump. For the ES model, the problem of thermal creep is the same as that for the BGK model for a monatomic gas, so that the polyatomic gas effect does not appear. The problem of shear slip is also reduced to that for the BGK model. Therefore, the values of the slip coefficients associated with these two problems for a polyatomic gas can be obtained from the data in the literature without computation. On the other hand, the other two problems, which cannot be reduced to the case of the BGK model, were solved numerically to determine the corresponding slip coefficients. In this way, the slip boundary conditions for the compressible Navier–Stokes equations for a polyatomic gas

have been established. At the same time, the profiles of the macroscopic quantities inside the Knudsen layer have been obtained.

In the present study, we adopted the ES model because the H-theorem has been proved for this model [22], and the Prandtl number is adjustable. In addition, it has the convenient property that the shear slip and thermal creep problems are reduced to those for the BGK model for a monatomic gas. Here, we should mention that many model Boltzmann equations have been proposed for a polyatomic gas since 1960's [27, 58–65], and for some of them [27, 64, 65], the H-theorem can be proved and the Prandtl number is adjustable. We also note that the shear-slip problem [corresponding to Eq. (99)] and the thermal-creep problem [corresonding to Eq. (100)] was investigated in Ref. [66] using the linearized version of the model proposed in Ref. [61], and the temperature-jump problem [corresponding to Eq. (102)] was investigated in Ref. [67] by the use of the linearized version of the model proposed in Ref. [60] (see also Ref. [68]). For instance, referring to Refs. [66, 68], we can express the slip coefficient c_T^I as $c_T^I = (3/10)f_{\rm tr}(1+0.5\alpha)({\rm Pr}/2)$, where $f_{\rm tr}$ is a parameter depending on the types of gases and set to be $f_{\rm tr} = 2.17 \sim 2.31$ for N_2 and $f_{\rm tr} = 2$ for CO_2 in Ref. [66]. This means that in contrast to our result, the values of c_T^I depends on the types of gases. However, the dependence is not large, and for N_2 with $f_{\rm tr} = 2.17$, the above formula gives $c_T^I = 0.281785$ ($\alpha = 0.2$), 0.307402 ($\alpha = 0.4$), 0.333019 ($\alpha = 0.6$), 0.358636 ($\alpha = 0.8$), and 0.384253 ($\alpha = 1$). These values are close to our c_T^I in Table II. According to Refs. [67, 68], c_T^{II} may be expressed as $c_T^{II} = (\sqrt{\pi}/2)[(\delta+5)/(\delta+4)][(2-\alpha)/\alpha+0.17]$. This formula gives, for instance, $c_T^{II} = 9.48115$ ($\alpha = 0.2$), 4.31149 ($\alpha = 0.4$), 2.58827 ($\alpha = 0.6$), 1.72667 ($\alpha = 0.8$), and 1.20970 ($\alpha = 1$) for N_2, which are close to our c_T^{II} in Table IV.

Chapman–Enskog solution has been obtained for many model equations including the Boltzmann-type model [69]. Therefore, by following the line of the present analysis, the slip boundary conditions for the compressible Navier–Stokes equations can be established for different model equations. The first-order Chapman–Enskog solutions of correct models should have essentially the same form, since they should give the correct compressible Navier–Stokes equations. Therefore, the basic form of the slip boundary conditions derived from different models should be the same as Eq. (124) or (139). However, the Chapman–Enskog solutions of different models have different dependence on the variables, which may be continuous or discrete, associated with the internal modes, so that the values of the slip coefficients naturally depend on the models. Although the numerical values shown in the preceding paragraph show weak model dependence, these examples are too few to lead a conclusion. A comprehensive investigation of the dependence of the slip boundary conditions on model equations would be an important and interesting problem.

Acknowledgments

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Appendix A: Outline of the derivation of Eqs. (55) and (56)

If we substitute Eq. (49) into Eq. (18) and consider the fact that $\hat{f}_{\rm CE}$ satisfies the same Eq. (18), we have

$$\epsilon\frac{\partial \hat{f}_{\rm K}^{(1)}}{\partial \hat{t}} + \epsilon\zeta_i\frac{\partial \hat{f}_{\rm K}^{(1)}}{\partial x_i} + O(\epsilon^2 R_f) = \frac{1}{\epsilon}[\hat{Q}(\hat{f}_{\rm CE} + \hat{f}_{\rm K}) - \hat{Q}(\hat{f}_{\rm CE})], \tag{A1}$$

where Eq. (52) has been used on the left-hand side. To calculate the right-hand side, we need some preparations.

If we use Eq. (50) with Eq. (53) in Eq. (19c) and recall that $\hat{h}_{\rm CE}$ are $\hat{h}$ appeared in Sec. IV B without the subscript CE, we obtain the following expansion of $\hat{\mathsf{T}}$ evaluated with $\hat{h} = \hat{h}_{\rm tot}$, which is denoted by $\hat{\mathsf{T}}|_{\hat{h}=\hat{h}_{\rm tot}}$:

$$\left(\hat{\mathsf{T}}|_{\hat{h}=\hat{h}_{\rm tot}}\right)_{ij} = (\mathsf{A})_{ij} + \epsilon(\mathsf{B})_{ij} + O(\epsilon^2 R_h), \tag{A2}$$

where

$$(\mathsf{A})_{ij} = (1-\theta)\left[(1-\nu)\hat{T}_{\rm tr}\delta_{ij} + \nu\frac{\hat{p}_{ij}}{\hat{\rho}}\right] + \theta\hat{T}\delta_{ij} = \left(\hat{\mathsf{T}}|_{\hat{h}=\hat{h}_{\rm CE}}\right)_{ij}, \tag{A3a}$$

$$(\mathsf{B})_{ij} = (1-\theta)\left[(1-\nu)\hat{T}^{(1)}_{\rm trK}\delta_{ij} + \nu\frac{1}{\hat{\rho}}\left(\hat{p}^{(1)}_{{\rm K}ij} - \hat{p}_{ij}\frac{\hat{\rho}^{(1)}_{\rm K}}{\hat{\rho}}\right)\right] + \theta\hat{T}^{(1)}_{\rm K}\delta_{ij}, \tag{A3b}$$

and $\hat{\mathsf{T}}|_{\hat{h}=\hat{h}_{\rm CE}}$ indicates $\hat{\mathsf{T}}$ evaluated with $\hat{h} = \hat{h}_{\rm CE}$. Note that $\hat{\rho}$, $\hat{p}_{ij}$, $\hat{T}_{\rm tr}$, and $\hat{T}$ in Eq. (A3) are the Chapman–Enskog macroscopic quantities. Then, the inverse and the determinant of $\hat{\mathsf{T}}|_{\hat{h}=\hat{h}_{\rm tot}}$ are expressed as

$$\left(\hat{\mathsf{T}}|^{-1}_{\hat{h}=\hat{h}_{\rm tot}}\right)_{ij} = (\mathsf{A}^{-1})_{ij} - (\mathsf{A}^{-1}\mathsf{B}\mathsf{A}^{-1})_{ij}\,\epsilon + O(R_h\epsilon^2), \tag{A4}$$

$$\det\hat{\mathsf{T}}|_{\hat{h}=\hat{h}_{\rm tot}} = D^{(0)} + D^{(1)}\epsilon + O(R_h\epsilon^2), \tag{A5}$$

where

$$D^{(0)} = \varepsilon_{ijk}(\mathsf{A})_{1i}(\mathsf{A})_{2j}(\mathsf{A})_{3k} = \det\hat{\mathsf{T}}|_{\hat{h}=\hat{h}_{\rm CE}}, \tag{A6a}$$

$$D^{(1)} = \varepsilon_{ijk}[(\mathsf{B})_{1i}(\mathsf{A})_{2j}(\mathsf{A})_{3k} + (\mathsf{A})_{1i}(\mathsf{B})_{2j}(\mathsf{A})_{3k} + (\mathsf{A})_{1i}(\mathsf{A})_{2j}(\mathsf{B})_{3k}], \tag{A6b}$$

and ε_{ijk} is the Eddington epsilon. With these expressions, the argument of the exponential function in $\hat{\mathcal{G}}$ [Eq. (19b)], evaluated with $\hat{h} = \hat{h}_{\rm tot}$, can be expressed as

$$-[\zeta_i - (\hat{v}_{\rm tot})_i]\left(\hat{\mathsf{T}}|^{-1}_{\hat{h}=\hat{h}_{\rm tot}}\right)_{ij}[\zeta_j - (\hat{v}_{\rm tot})_j] - \frac{\hat{\mathcal{E}}}{(\hat{T}_{\rm rel})_{\rm tot}} = \mathcal{P}^{(0)} + \mathcal{P}^{(1)}\epsilon + O(R_h S\epsilon^2), \tag{A7}$$

where

$$\mathcal{P}^{(0)} = -(\zeta_i - \hat{v}_i)(\mathsf{A}^{-1})_{ij}(\zeta_j - \hat{v}_j) - \frac{\hat{\mathcal{E}}}{\hat{T}_{\rm rel}}, \tag{A8a}$$

$$\begin{aligned}\mathcal{P}^{(1)} &= (\zeta_i - \hat{v}_i)(\mathsf{A}^{-1}\mathsf{B}\,\mathsf{A}^{-1})_{ij}(\zeta_j - \hat{v}_j)\\ &\quad + [(\zeta_i - \hat{v}_i)\hat{v}^{(1)}_{{\rm K}j} + \hat{v}^{(1)}_{{\rm K}i}(\zeta_j - \hat{v}_j)](\mathsf{A}^{-1})_{ij} + \frac{\hat{T}^{(1)}_{\rm relK}}{\hat{T}^2_{\rm rel}}\hat{\mathcal{E}},\end{aligned} \tag{A8b}$$

and $\hat{v}_i$ and $\hat{T}_{\rm rel}$ are the Chapman–Enskog macroscopic quantities. In the remainder in Eq. (A7), S indicates an appropriate function of $\boldsymbol{\zeta}$ and $\hat{\mathcal{E}}$ that decays fast enough when multiplied by a rapidly decaying function of $\boldsymbol{\zeta}$ and $\hat{\mathcal{E}}$. Therefore, the Gaussian $\hat{\mathcal{G}}$ [Eq. (19b)] evaluated with $\hat{h} = \hat{h}_{\rm tot} = \hat{h}_{\rm CE} + \hat{h}_{\rm K}$ can be expanded in the following form:

$$\hat{\mathcal{G}}|_{\hat{h}=\hat{h}_{\rm tot}} = \hat{\mathcal{G}}^{(0)} + \hat{\mathcal{G}}^{(1)}\epsilon + O(R_f\epsilon^2), \tag{A9}$$

where

$$\hat{\mathcal{G}}^{(0)} = \frac{\hat{\rho}}{\pi^{3/2}\sqrt{D^{(0)}}\hat{T}^{\delta/2}_{\rm rel}\Gamma(\delta/2)}\hat{\mathcal{E}}^{\delta/2-1}\exp\left(-(\zeta_i - \hat{v}_i)(\mathsf{A}^{-1})_{ij}(\zeta_j - \hat{v}_j) - \frac{\hat{\mathcal{E}}}{\hat{T}_{\rm rel}}\right), \tag{A10a}$$

$$\hat{\mathcal{G}}^{(1)} = \hat{\mathcal{G}}^{(0)}\left(\frac{\hat{\rho}^{(1)}_{\rm K}}{\hat{\rho}} - \frac{1}{2}\frac{D^{(1)}}{D^{(0)}} - \frac{\delta}{2}\frac{\hat{T}^{(1)}_{\rm relK}}{\hat{T}_{\rm rel}} + \mathcal{P}^{(1)}\right). \tag{A10b}$$

Since $\hat{T}_{\rm tot} = \hat{T} + \hat{T}^{(1)}_{\rm K}\epsilon + O(R_h\epsilon^2)$, we have $\hat{A}_c(\hat{T}_{\rm tot}) = \hat{A}_c(\hat{T}) + \hat{A}'_c(\hat{T})\hat{T}^{(1)}_{\rm K}\epsilon + O(R_h\epsilon^2)$. Using these expansions and $\hat{\rho}_{\rm tot} = \hat{\rho} + \hat{\rho}^{(1)}_{\rm K}\epsilon + O(R_h\epsilon^2)$, in $\hat{Q}(\hat{f}_{\rm tot}) = \hat{Q}(\hat{f}_{\rm CE} + \hat{f}_{\rm K})$ and taking account of the fact that $\hat{Q}(\hat{f}_{\rm CE}) = O(\epsilon\hat{f}^{(0)})$, we obtain the following expression of the term in the square brackets in Eq. (A1):

$$\hat{Q}(\hat{f}_{\rm CE} + \hat{f}_{\rm K}) - \hat{Q}(\hat{f}_{\rm CE}) = \hat{A}_{\rm c}(\hat{T})\,\hat{\rho}\,(\hat{\mathcal{G}}^{(1)} - \hat{f}^{(1)}_{\rm K})\epsilon + O(R_f\epsilon^2). \tag{A11}$$

Now we derive the expression of $\hat{\mathcal{G}}^{(1)}$ that is correct within the error of $O(R_f\epsilon^2)$. Since $\hat{f}_{\rm CE} = \hat{f}^{(0)} + O(\epsilon)$, we have the following:

$$(\mathsf{A})_{ij} = \hat{T}\delta_{ij} + O(\epsilon), \tag{A12a}$$

$$(\mathsf{A}^{-1})_{ij} = \hat{T}^{-1}\delta_{ij} + O(\epsilon), \tag{A12b}$$

$$(\mathsf{B})_{ij} = \hat{T}d_{{\rm K}ij} + O(R_h\epsilon), \tag{A12c}$$

$$(\mathsf{A}^{-1}\mathsf{B}\ \mathsf{A}^{-1})_{ij} = \hat{T}^{-2}(\mathsf{B})_{ij} + O(R_h\epsilon) = \hat{T}^{-1}d_{{\rm K}ij} + O(R_h\epsilon), \tag{A12d}$$

where

$$d_{{\rm K}ij} = \left[(1-\theta)\frac{\hat{T}^{(1)}_{\rm trK}}{\hat{T}} + \theta\frac{\hat{T}^{(1)}_{\rm K}}{\hat{T}}\right]\delta_{ij} + (1-\theta)\nu\left[\frac{\hat{p}^{(1)}_{{\rm K}ij}}{\hat{\rho}\hat{T}} - \left(\frac{\hat{\rho}^{(1)}_{\rm K}}{\hat{\rho}} + \frac{\hat{T}^{(1)}_{\rm trK}}{\hat{T}}\right)\delta_{ij}\right]. \tag{A13}$$

These relations give the following expressions of $D^{(0)}$, $D^{(1)}$, and $\mathcal{P}^{(1)}$:

$$D^{(0)} = \hat{T}^3 + O(\epsilon), \tag{A14a}$$

$$D^{(1)} = \hat{T}^3 d_{{\rm K}ii} + O(R_h\epsilon), \tag{A14b}$$

$$\mathcal{P}^{(1)} = \frac{(\zeta_i - \hat{v}_i)(\zeta_j - \hat{v}_j)}{\hat{T}}d_{{\rm K}ij} + 2\frac{\hat{v}^{(1)}_{{\rm K}k}(\zeta_k - \hat{v}_k)}{\hat{T}} + \frac{\hat{T}^{(1)}_{\rm relK}}{\hat{T}^2}\hat{\mathcal{E}} + O(R_hS\epsilon). \tag{A14c}$$

Using these expressions in Eq. (A10b) and noting that $\hat{\mathcal{G}}^{(0)} = \hat{f}^{(0)} + O(\epsilon\hat{f}_{\rm CE})$, we have the following expression of $\hat{\mathcal{G}}^{(1)}$:

$$\begin{aligned}\hat{\mathcal{G}}^{(1)} = \hat{f}^{(0)}\Bigg[&\frac{\hat{\rho}^{(1)}_{\rm K}}{\hat{\rho}} - \frac{1}{2}d_{{\rm K}ii} - \frac{\delta}{2}\frac{\hat{T}^{(1)}_{\rm relK}}{\hat{T}} + \frac{(\zeta_i - \hat{v}_i)(\zeta_j - \hat{v}_j)}{\hat{T}}d_{{\rm K}ij} \\ &+2\frac{\hat{v}^{(1)}_{{\rm K}k}(\zeta_k - \hat{v}_k)}{\hat{T}} + \frac{\hat{T}^{(1)}_{\rm relK}}{\hat{T}^2}\hat{\mathcal{E}}\Bigg] + O(R_f\epsilon) \\ = \hat{\mathcal{G}}^{(1)}_{\rm K} &+ O(R_f\epsilon),\end{aligned} \tag{A15}$$

where $\hat{\mathcal{G}}^{(1)}_{\rm K}$ is defined in Eq. (56a). Equations (A1), (A11), and (A15) lead to Eqs. (55) and (56).

Appendix B: Data and accuracy for numerical computation

As mentioned in Sec. V B 4, the computation of the problems for (ϕ_v^{II}, c_v^{II}) and (ϕ_T^{II}, c_T^{II}) were carried out on the basis of the coupled equations for reduced distribution functions (G_v^{II}, H_v^{II}) and those for (G_T^{II}, H_T^{II}), respectively. The scheme, the method how to determine the unknown constants c_v^{II} and c_T^{II}, and the grid points used here are essentially the same as those in Ref. [33]. However, since we do not need to compute the collision integral of the Boltzmann equation as Ref. [33], the scheme is much simpler, and the primary grid system for the molecular velocity used for capturing the collision integral in Ref. [33] is unnecessary here. To be more specific, the actual computation was performed in the variables (y, σ, ζ), where $\sigma = \zeta_{\rm n}/\zeta$, instead of the original variables $(y, \zeta_{\rm n}, \zeta)$. Note that (y, σ, ζ) in the present paper correspond to (η, μ, ζ) in Ref. [33], so that when the reader refers to Ref. [33], the symbols y and σ should be changed to η and μ, respectively. In the computation, the range of y and ζ were, respectively, restricted to $0 \le y \le d$ and $0 \le \zeta \le Z$ with suitably large constants d and Z, and these ranges, as well as the range of σ: $-1 \le \sigma \le 1$, were divided into small intervals by the grid points distributed nonuniformly. The distributions of the grid points and the values of d and Z are given in Appendix B in Ref. [33] [see Eqs. (B.1), (B.2), and (B.3) and Table B.3 there]. For nitrogen (N_2), methanol (CH_3OH), and water vapor (H_2O), we used the grid systems S1, S2, and S3 defined in Appendix B in Ref. [33] and S4, whose grid points are double of those of S1, for the space variable y. As for (σ, ζ), we used M1, M2, ..., and M7 in Ref. [33] for the same gases [note that we used the secondary grid system for the molecular velocity, i.e., grid points

$M^{(j)}$ ($j = -2N_M, ..., 2N_M$) and $\xi^{(k)}$ ($k = 0, ..., 2N_\xi$) in Ref. [33] for σ and ζ, respectively]. For pseudo-CO_2 gases $CO_2(n)$ ($n = 5$, 10, 20, and 50), we used the systems with wider range (i.e., larger d) and more grid points for y to handle the thicker Knudsen layer for these gases, especially for $CO_2(20)$ and $CO_2(50)$.

Our standard grid system is (S1, M1) for the gases except $CO_2(n)$ and (S5, M1) for these gases, where S5 is a system for y with the same grid intervals as S1 and a larger d. The numerical results shown in Tables III and IV and in Figs. 3–10 are based on these standard grid systems. The system S1 has $d = 44.46$ and 251 grid points with the minimum and maximum grid intervals being 7.3×10^{-7} (at $y = 0$) and 0.69 (at $y = d$), and the system S5 has $d = 64.16$ and 269 grid points with the minimum and maximum grid intervals being 7.3×10^{-7} (at $y = 0$) and 1.78 (at $y = d$). The system M1 has a complex structure for the purpose of an easy control of the distribution of the grid points near $\sigma = 0$ and $\zeta = 0$ [see Eqs. (B.2) and (B.3) in Ref. [33]]. It has $Z = 5$ and 449 grid points for σ and 161 grid points for ζ. The minimum and maximum grid intervals are 2.4×10^{-10} (at $\sigma = 0$) and 0.025 (at $\sigma = \pm 1$) for σ and 5.1×10^{-10} (at $\zeta = 0$) and 0.12 (at $\zeta = Z$) for ζ.

Our accuracy check consists of the following:

(i) We have checked the accuracy of the results using different combinations of the grid systems for the accommodation coefficient $\alpha = 0.2$, 0.5, and 1 in the case of N_2, CH_3OH, and H_2O and for $\alpha = 1$ in the case of $CO_2(n)$. For instance, we have confirmed that the numerical values shown for these values of α in Tables III and IV are accurate up to the last digit.

(ii) We have checked if the values of $|G_v^{II}|$, $|H_v^{II}|$, $|G_T^{II}|$, and $|H_T^{II}|$ are small enough at the outer edges of the computational domain, i.e., $y = d$ and $\zeta = Z$ for $\alpha = 0.2$, 0.5, and 1. We have confirmed that $\max_{y=d}|G_\kappa^{II}|/\max|G_\kappa^{II}|$, $\max_{\zeta=Z}|G_\kappa^{II}|/\max|G_\kappa^{II}|$, $\max_{y=d}|H_\kappa^{II}|/\max|H_\kappa^{II}|$, and $\max_{\zeta=Z}|H_\kappa^{II}|/\max|H_\kappa^{II}|$ ($\kappa = v$, T) are less than 1.6×10^{-9} for N_2, CH_3OH, and H_2O, where max without a subscript means the maximum in the computational domain. We have also confirmed that $\max_{\zeta=Z}|G_\kappa^{II}|/\max|G_\kappa^{II}|$ and $\max_{\zeta=Z}|H_\kappa^{II}|/\max|H_\kappa^{II}|$ ($\kappa = v$, T) are less than 1.5×10^{-9} for $CO_2(n)$ ($n = 5$, 10, 20, and 50). However, $\max_{y=d}|G_\kappa^{II}|/\max|G_\kappa^{II}|$ and $\max_{y=d}|H_\kappa^{II}|/\max|H_\kappa^{II}|$ ($\kappa = v$, T) become worse for $CO_2(n)$ as n increases. To be more precise, $\max_{y=d}|G_\kappa^{II}|/\max|G_\kappa^{II}|$ and $\max_{y=d}|H_\kappa^{II}|/\max|H_\kappa^{II}|$ are less than 3.8×10^{-10} for $CO_2(5)$, less than 8.8×10^{-8} for $CO_2(10)$, less than 8.4×10^{-6} for $CO_2(20)$, and less than 7.0×10^{-4} for $CO_2(50)$. That is, the decay of $|G_\kappa^{II}|$ and $|H_\kappa^{II}|$ for large y becomes slow for $CO_2(n)$ as n increases. This is the reason why we were not able to solve the problem for (ϕ_κ^{II}, c_κ^{II}) for $CO_2(n)$ with n greater than 50.

(iii) The scheme used in the present computation is not conservative in the sense that the conservation of mass, momentum, and energy is not imposed artificially on the scheme. Therefore, whether the conservation laws are satisfied accurately or not provides a good measure of accuracy. The conservation of mass, momentum, and energy in the following form holds:

$$I[F] = I_-[F] + I_+[F] = 0, \tag{B1}$$

where

$$I[F] = \int \zeta_n F d\boldsymbol{\zeta}, \qquad I_-[F] = \int_{\zeta_n<0} \zeta_n F d\boldsymbol{\zeta}, \qquad I_+[F] = \int_{\zeta_n>0} \zeta_n F d\boldsymbol{\zeta}, \tag{B2}$$

and $F = G_\kappa^{II}$ for the mass conservation, $F = \zeta_n G_\kappa^{II}$ for the momentum conservation, and $F = \zeta^2 G_\kappa^{II} + (\delta/2) H_k^{II}$ for the energy conservation ($\kappa = v$, T). We have checked how accurately the conservation laws are fulfilled for $\alpha = 0.2$, 0.5, and 1. The numerical solutions show that $\max_y |I[F]|/\max_y |I_-[F]|$ with the three Fs listed above is less than 2.7×10^{-5} for N_2, CH_3OH, and H_2O; $\max_y |I[F]|/\max_y |I_-[F]|$ with the same Fs is less than 3.4×10^{-5} for $CO_2(5)$ and $CO_2(10)$; $\max_y |I[F]|/\max_y |I_-[F]|$ with $F = G_\kappa^{II}$ and $F = \zeta^2 G_\kappa^{II} + (\delta/2) H_k^{II}$ is less than 2.6×10^{-5}, but $\max_y |I[F]|/\max_y |I_-[F]|$ with $F = \zeta_n G_\kappa^{II}$ is only less than 2.5×10^{-4} for $CO_2(20)$ and $CO_2(50)$.

Appendix C: Outline of the derivation of Eq. (131)

Equation (130a) can be written in terms of ψ_κ^I [Eq. (106b)] as

$$Y_\kappa(y) = \frac{1}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \psi_\kappa^I e^{-\zeta_{\rm n}^2} d\zeta_{\rm n}, \tag{C1}$$

with $\kappa = v$, T. Therefore, the first equations of Eqs. (131a) and (131b) follow immediately from Eqs. (121) and (122).

In order to derive the second equations of Eqs. (131a) and (131b), we introduce the additional reduced velocity distribution functions σ_κ^I and λ_κ^I:

$$\sigma_\kappa^I(y,\zeta_{\rm n}) = \frac{1}{\pi}\frac{2}{\delta} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_0^{\infty} \hat{\mathcal{E}}(\zeta_{\rm s}^2+\zeta_{\rm t}^2)\phi_\kappa^I(y,\zeta_{\rm n},\zeta,\hat{\mathcal{E}}) e^{-\zeta_{\rm s}^2-\zeta_{\rm t}^2} \frac{\hat{\mathcal{E}}^{\delta/2-1}}{\Gamma(\delta/2)} e^{-\hat{\mathcal{E}}} d\hat{\mathcal{E}} d\zeta_{\rm t} d\zeta_{\rm s}, \tag{C2}$$

$$\lambda_\kappa^I(y,\zeta_{\rm n}) = \frac{1}{2\pi} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_0^{\infty} (\zeta_{\rm s}^2+\zeta_{\rm t}^2)^2\phi_\kappa^I(y,\zeta_{\rm n},\zeta,\hat{\mathcal{E}}) e^{-\zeta_{\rm s}^2-\zeta_{\rm t}^2} \frac{\hat{\mathcal{E}}^{\delta/2-1}}{\Gamma(\delta/2)} e^{-\hat{\mathcal{E}}} d\hat{\mathcal{E}} d\zeta_{\rm t} d\zeta_{\rm s}. \tag{C3}$$

If we derive the equations and boundary conditions for σ_κ^I and λ_κ^I by taking the appropriate moments of Eqs. (99) and (100) and compare the results with the problems for ψ_v^I [Eq. (109) with Eq. (111) and Eq. (112)] and for ψ_T^I [Eq. (115)], we find the following relations:

$$\sigma_v^I = \lambda_v^I = \psi_v^I, \tag{C4a}$$

$$\sigma_T^I = \lambda_T^I = \psi_T^I + r_T, \tag{C4b}$$

where

$$r_T = \begin{cases} \alpha e^{-y/\zeta_{\rm n}} & (\zeta_{\rm n} > 0), \\ 0 & (\zeta_{\rm n} < 0). \end{cases} \tag{C5}$$

The function $H_\kappa(y)$ defined by Eq. (130g) can be written in terms of ψ_κ^I, σ_κ^I, and λ_κ^I in the following form:

$$\begin{aligned} H_\kappa(y) =& \frac{1}{2}\left\langle \left(\zeta_{\rm s}^2+\zeta_{\rm t}^2\right)\left[\zeta_{\rm n}^2 + \left(\zeta_{\rm s}^2+\zeta_{\rm t}^2\right) + \hat{\mathcal{E}} - \frac{5+\delta}{2}\right]\phi_\kappa^I \right\rangle \\ =& \frac{1}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \left[\left(\zeta_{\rm n}^2 - \frac{5+\delta}{2}\right)\psi_\kappa^I + \frac{\delta}{2}\sigma_\kappa^I + 2\lambda_\kappa^I\right] e^{-\zeta_{\rm n}^2} d\zeta_{\rm n}. \end{aligned} \tag{C6}$$

On the other hand, we can derive the following relation for the BGK model:

$$H_{\kappa\rm BGK}(y) = \frac{1}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \left[\left(\zeta_{\rm n}^2 - \frac{5}{2}\right)\psi_{\kappa\rm BGK}^I + 2\lambda_{\kappa\rm BGK}^I\right] e^{-\zeta_{\rm n}^2} d\zeta_{\rm n}, \tag{C7}$$

and can find that

$$\lambda_{v\rm BGK}^I = \psi_{v\rm BGK}^I, \tag{C8a}$$

$$\lambda_{T\rm BGK}^I = \psi_{T\rm BGK}^I + r_T. \tag{C8b}$$

By comparing Eq. (C6) [with Eq. (C4)] and Eq. (C7) [with Eq. (C8)] and by making use of Eqs. (121) and (122), we obtain the second equations of Eqs. (131a) and (131b).

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