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Slip/Jump Coefficients and Knudsen-Layer Corrections for the ES Model in the Generalized Slip-Flow Theory

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Abstract. The slip/jump coefficients and the Knudsen-layer functions for the time-dependent version of the generalized slip-flow theory have been obtained for the Ellipsoidal Statistical (ES) model up to the second order of the Knudsen number expansion. In particular, simple but exact conversion formulas between the ES and Bhatnagar–Gross–Krook (BGK) model have been established.

INTRODUCTION

Recently, in [1, 2, 3], the first two authors have extended the generalized slip-flow theory, established by Sone (see, e.g., [4]), for stationary flows of slightly rarefied gases to non-stationary ones, where the system of the fluid-dynamical equations, their slip/jump boundary conditions, and the Knudsen-layer corrections has been obtained explicitly up to the second order of the Knudsen number expansion. The extension was made in the linearized framework, and the numerical data for completing the system are available from the Kyoto University Research Information Repository (<http://hdl.handle.net/2433/199811>). The data have been prepared for the hard-sphere (HS) gas, as well as the Bhatnagar–Gross–Krook (BGK) model [5], under the diffuse reflection condition. In the present paper, we provide the corresponding data for the Ellipsoidal Statistical (ES) model [6].

The ES model, first proposed by Holway, is an extended relaxation model that includes the celebrated BGK model as a special case. The advantage of the ES model over the BGK model is that it can adjust the Prandtl number to realistic values while meeting the Boltzmann's H-theorem [7]. Since, in marked contrast to the classical fluid, the thermal and mechanical phenomena are mostly coupled in rarefied gases, this advantageous feature is appealing enough to induce further researches of model equations in the same spirit (see, e.g., [8] and the references therein). The present paper aims at newly providing the slip/jump coefficients and the Knudsen-layer functions for the ES model, thereby making it easier to access the generalized slip-flow theory in current trends.

In the ES model the velocity distribution function (VDF) is driven not to the local Maxwellian as in the BGK model but to the (three-dimensional) local Gaussian, which resembles the Maxwellian but is not necessarily isotropic. The flexibility of the Gaussian enables us to adjust the Prandtl number to realistic values, while its resemblance to the Maxwellian enables us to find simple conversion formulas between the two models, when the deviation from the local equilibrium state is small (see, e.g., [9, p. 319] and [10, 11, 12]). In the present work, we especially focus on this fact and discuss in details the conversion formulas occurring at the level of the VDF as well as the transport coefficients, the slip/jump coefficients, and the structure of the Knudsen layer.

GENERALIZED SLIP-FLOW THEORY: A BRIEF SUMMARY

According to the time-dependent version of the generalized slip-flow theory [1, 2, 3], the behavior of a slightly rarefied monatomic gas with a small Reynolds number can be described in the bulk of the domain by the Stokes-type set of equations with slip/jump boundary conditions; in the layer with the thickness of a few mean free paths, which is adjacent to the boundary and is called the Knudsen layer, this fluid-dynamical description (to be referred to as the

fluid-dynamical part) is necessary to be corrected (the Knudsen-layer correction). The slip/jump conditions and the Knudsen-layer correction are required at the level of the first and higher orders of the Knudsen number.

Let us denote by $t_0 t$ the time, by Lx_i the space coordinates, by $\rho_0(1 + \omega)$, $p_0(1 + P)$, and $T_0(1 + \tau)$ the density, pressure, and temperature of the gas, by $(2RT_0)^{1/2}u_i$ the flow velocity, and by $(2RT_0)^{1/2}u_{iw}$ and $T_0(1 + \tau_w)$ the velocity and temperature of the boundary. Here t_0 is the reference time scale, L is the characteristic length of the system, R is the specific gas constant, ρ_0 , p_0 , and T_0 are the density, pressure, and temperature in the reference equilibrium state at rest and are related to each other by $p_0 = \rho_0 RT_0$. We also denote by n_i the unit normal to the boundary, pointed to the gas, and by t_i an arbitrary unit vector tangential to the boundary. The Knudsen number Kn is defined by $\text{Kn} = \ell_0/L$ with ℓ_0 being the mean free path of a molecule at the reference equilibrium state. In the present paper, we use the notation ε defined by $\varepsilon = (\sqrt{\pi}/2)\text{Kn}$, instead of Kn , to emphasize its smallness. In the above mentioned works [1, 2, 3], it is assumed that there is no external force and that the boundary does not deform and thus $u_{iw}n_i = 0$. Furthermore, the time scale is taken as $t_0 = L/[\varepsilon(2RT_0)^{1/2}]$ because of the slow evolution in time.

We shall tell apart the fluid-dynamical part and the Knudsen-layer correction by putting subscript H and K to the notation of quantities respectively. Each quantity, say $h = h_H + h_K$ ($h = \omega, P, \tau, u_i$, etc.), is expanded in a power series of ε as $h_H = h_{H0} + h_{H1}\varepsilon + h_{H2}\varepsilon^2 \cdots$ and $h_K = h_{K1}\varepsilon + h_{K2}\varepsilon^2 \cdots$. Boundary data u_{iw} and τ_w are expanded as well, e.g., $u_{iw} = u_{iw0} + u_{iw1}\varepsilon + \cdots$. Note that the expansion of h_K starts from $O(\varepsilon)$. Then, the above mentioned Stokes-type set of equations and the slip/jump boundary conditions over a smooth solid body are written in a compact form as follows:

Stokes-type set of equations

$$\partial_i P_{H0} = 0, \quad (1a)$$

$$\partial_t \omega_{Hm-1} + \partial_i u_{iHm} = 0, \quad (1b)$$

$$\partial_t u_{iHm} + \frac{1}{2} \partial_i P_{Hm+1}^* - \frac{1}{2} \gamma_1 \Delta u_{iHm} + \frac{1}{4} (\gamma_1 \gamma_{10} - 2\gamma_6) \Delta^2 u_{iHm-2} = 0, \quad (1c)$$

$$\partial_t \tau_{Hm} - \frac{2}{5} \partial_t P_{Hm} - \frac{1}{2} \gamma_2 \Delta \tau_{Hm} + \frac{1}{10} (\gamma_2 \gamma_3 - \frac{13}{2} \gamma_{11}) \Delta^2 \tau_{Hm-2} = 0, \quad (1d)$$

where $\partial_i = \partial/\partial x_i$, $\partial_t = \partial/\partial t$, $\Delta = \partial_j^2$, and

$$P_{Hm+1}^* = P_{Hm+1} - \frac{1}{6} (\gamma_2 \gamma_1 - 4\gamma_3) \Delta \tau_{Hm-1} + \frac{1}{5} \gamma_1 \partial_t P_{Hm-1}, \quad (1e)$$

$$P_{Hm} = \omega_{Hm} + \tau_{Hm}. \quad (1f)$$

Slip/jump boundary conditions

$$u_{iHm} n_i = a_1^{(1)} \overline{\partial_i \partial_j u_{kHm-2} n_i n_j n_k} + a_2^{(1)} (2\bar{\kappa} \partial_i \tau_{Hm-2} n_i - \Delta \tau_{Hm-2} + \partial_i \partial_j \tau_{Hm-2} n_i n_j), \quad (2a)$$

$$u_{iHm} t_i = u_{iwm} t_i + b_1^{(1)} \overline{\partial_i u_{jHm-1} n_i t_j} + b_2^{(1)} \overline{\partial_i \tau_{Hm-1} t_i} + b_3^{(1)} \overline{\partial_i \partial_j \tau_{Hm-2} n_i t_j} + b_4^{(1)} \overline{\partial_i \partial_j u_{kHm-2} n_i n_j t_k} \\ + b_5^{(1)} \overline{\bar{\kappa} \partial_j u_{kHm-2} n_j t_k} + b_6^{(1)} \overline{\kappa_{ij} \partial_j u_{kHm-2} n_k t_i} + b_7^{(1)} \overline{\kappa_{ij} \partial_i \tau_{Hm-2} t_j} + b_8^{(1)} \overline{\bar{\kappa} \partial_i \tau_{Hm-2} t_i}, \quad (2b)$$

$$\tau_{Hm} = \tau_{wm} + c_1^{(0)} \overline{\partial_i \tau_{Hm-1} n_i} - c_2^{(0)} \overline{\partial_i \partial_j \tau_{Hm-2} n_i n_j} + c_3^{(0)} \overline{\partial_i \partial_j u_{kHm-2} n_i n_j n_k} + c_4^{(0)} \overline{\bar{\kappa} \partial_i \tau_{Hm-2} n_i} \\ + c_5^{(0)} \overline{\partial_i u_{iHm-1}} + (c_6^{(0)} + c_2^{(0)}) \Delta \tau_{Hm-2}. \quad (2c)$$

Here $m = 0, 1, 2$ and the quantities h_{H-1} and h_{H-2} should be read as zero. The same convention applies to (3) as well. In (1), γ 's are dimensionless transport coefficients at the reference state and are constants depending on the gas model. Among them, γ_1 and γ_2 are respectively the dimensionless viscosity and thermal conductivity and their ratio yields the Prandtl number, i.e., $\text{Pr} = \gamma_1/\gamma_2$.¹ In (2) b 's, a 's, c 's are the slip/jump coefficients, which depend both on the gas and the surface-scattering models, and $\bar{f}_{ij} = f_{ij} + f_{ji} - (2/3)f_{kk}\delta_{ij}$, where δ_{ij} is the Kronecker delta. κ_{ij}/L and $\bar{\kappa}/L$ are respectively the curvature matrix and mean curvature of the boundary.² The system (1)–(2) determines the

¹The viscosity $\mu(T)$ is a positive function of temperature T . At the reference state, it is given by $\mu(T_0) = (\sqrt{\pi}/2)\gamma_1 p_0 (2RT_0)^{-1/2} \ell_0$.

² κ_{ij}/L and $\bar{\kappa}/L$ are defined by $\kappa_{ij} = \kappa_1 m_i m_j + \kappa_2 \ell_i \ell_j$ and $\bar{\kappa} = (\kappa_1 + \kappa_2)/2$, where κ_1/L and κ_2/L are the principal curvatures of the boundary and m_i and ℓ_i are the direction cosines of the principal directions corresponding to κ_1/L and κ_2/L . Here κ_1 and κ_2 are taken negative when the corresponding center of curvature lies on the gas side.

behavior of the gas in the bulk region from the lowest order. Namely, (1a) yields the uniform pressure at the leading order. Equations (1b)–(1d) and boundary condition (2) for $m = 0$ determine the leading order of temperature and flow velocity, together with the first order of pressure; those for $m = 1$ determine the first order of temperature and flow velocity, together with the second order of pressure; and so on. Note that (2) for $m = 0$ is just the non-slip/non-jump condition.

Knudsen-layer correction Once the fluid-dynamic part has been obtained by the above process, the corrections to that part in the vicinity of the boundary, which we call the Knudsen-layer corrections, are given by the following formulas through the elemental functions Ω 's, Y 's, and Θ 's, which we call the Knudsen-layer functions:

$$u_{iKm}n_i = - \int_{\eta}^{\infty} Y_2^{(1)}(z) dz (2\bar{\kappa} \partial_i \tau_{Hm-2} n_i - \Delta \tau_{Hm-2} + \partial_i \partial_j \tau_{Hm-2} n_i n_j) - \frac{1}{2} \int_{\eta}^{\infty} Y_1^{(1)}(z) dz \partial_i \partial_j \overline{u_{kHm-2} n_i n_j n_k}, \quad (3a)$$

$$u_{iKm}t_i = Y_1^{(1)}(\eta) \overline{\partial_i u_{jHm-1} n_j t_j} + Y_2^{(1)}(\eta) \partial_i \tau_{Hm-1} t_i + Y_3^{(1)}(\eta) \partial_i \partial_j \tau_{Hm-2} n_i t_j + Y_4^{(1)}(\eta) \overline{\partial_i \partial_j u_{kHm-2} n_i n_j t_k} \\ + Y_5^{(1)}(\eta) \overline{\bar{\kappa} \partial_i u_{kHm-2} n_j t_k} + Y_6^{(1)}(\eta) \kappa_{ij} \overline{\partial_j u_{kHm-2} n_k t_i} + Y_7^{(1)}(\eta) \kappa_{ij} \partial_i \tau_{Hm-2} t_j + Y_8^{(1)}(\eta) \bar{\kappa} \partial_i \tau_{Hm-2} t_i, \quad (3b)$$

$$\begin{bmatrix} \omega_{Km} \\ \tau_{Km} \end{bmatrix} = \begin{bmatrix} \Omega_1^{(0)}(\eta) \\ \Theta_1^{(0)}(\eta) \end{bmatrix} \partial_i \tau_{Hm-1} n_i - \begin{bmatrix} \Omega_2^{(0)}(\eta) \\ \Theta_2^{(0)}(\eta) \end{bmatrix} \partial_i \partial_j \tau_{Hm-2} n_i n_j + \begin{bmatrix} \Omega_3^{(0)}(\eta) \\ \Theta_3^{(0)}(\eta) \end{bmatrix} \overline{\partial_i \partial_j u_{kHm-2} n_i n_j n_k} \\ + \begin{bmatrix} \Omega_4^{(0)}(\eta) \\ \Theta_4^{(0)}(\eta) \end{bmatrix} \bar{\kappa} \partial_i \tau_{Hm-2} n_i + \begin{bmatrix} \Omega_6^{(0)}(\eta) + \Omega_2^{(0)}(\eta) \\ \Theta_6^{(0)}(\eta) + \Theta_2^{(0)}(\eta) \end{bmatrix} \Delta \tau_{Hm-2} + \begin{bmatrix} \Omega_5^{(0)}(\eta) \\ \Theta_5^{(0)}(\eta) \end{bmatrix} \partial_i u_{iHm-1}. \quad (3c)$$

Here η is the stretched coordinate normal to the boundary defined by $x_i = x_{wi} + \varepsilon \eta n_i$, where Lx_{wi} is a boundary position, and all the quantities with subscript H represent their values at $x_i = x_{wi}$ (or $\eta = 0$). Taking into account the no net flow through the solid boundary, $0 = u_i n_i = u_{iH} n_i + u_{iK} n_i$ on the boundary, so that a 's in (2a) are related to Y 's as $a_1^{(1)} = (1/2) \int_0^{\infty} Y_1^{(1)}(z) dz$ and $a_2^{(1)} = \int_0^{\infty} Y_2^{(1)}(z) dz$. Further detailed information is available from [1, 2, 3].

Elemental half-space problems In deriving (2) and (3), a locally isotropic property [4, 1] is assumed for the kinetic boundary condition. The Knudsen-layer functions Ω 's and Θ 's (or Y 's) are, then, expressed as moments of elemental solutions of the form $\phi_j^{(0)}(\eta, \zeta_n, \zeta)$ ($j = 1, 2, \dots, 6$) [or $\phi_j^{(1)}(\eta, \zeta_n, \zeta)$ ($j = 1, 2, \dots, 8$)] for the half-space problems (4) [or (5)] below, where $\zeta = |\zeta| = (\zeta_i^2)^{1/2}$ and $\zeta_n = \zeta_i n_i$ with $(2RT_0)^{1/2} \zeta$ being the molecular velocity. The jump coefficients $c_j^{(0)}$ [or the slip coefficients $b_j^{(1)}$] are determined together with those solutions.

Elemental problem for $\phi_j^{(0)}(\eta, \zeta_n, \zeta)$ ($j = 1, 2, \dots, 6$):

$$\zeta_n \partial_{\eta} \phi_j^{(0)} = \mathcal{L}(\phi_j^{(0)}) - I_j^{(0)}, \quad (4a)$$

$$\phi_j^{(0)} = -\tilde{\mathcal{K}}(\zeta^2) c_j^{(0)} + \mathcal{K}(\phi_j^{(0)}) + \tilde{\mathcal{K}}(g_j^{(0)}), \quad \zeta_n > 0, \eta = 0, \quad (4b)$$

$$\phi_j^{(0)} \rightarrow 0 \quad \text{as} \quad \eta \rightarrow \infty, \quad (4c)$$

where $\mathcal{L}$ is the linearized collision operator, $\mathcal{K}$ is the linear scattering operator, which admits the above functional form of ϕ 's in the molecular velocity variables, $\tilde{\mathcal{K}}(f) = f - \mathcal{K}(f)$, and

$$\begin{aligned} I_1^{(0)} &= 0, \quad g_1^{(0)} = \zeta_n A, \quad I_2^{(0)} = \frac{1}{2}(\zeta^2 - \zeta_n^2) \phi_2^{(1)}, \quad g_2^{(0)} = 2a_2^{(1)} \zeta_n + \frac{1}{2}(\zeta^2 - 3\zeta_n^2)(b_2^{(1)} B + F), \\ I_3^{(0)} &= -\frac{1}{4}(\zeta^2 - \zeta_n^2) \phi_1^{(1)}, \quad g_3^{(0)} = -2a_1^{(1)} \zeta_n - \frac{1}{4}b_1^{(1)}(\zeta^2 - 3\zeta_n^2)B - \frac{1}{2}\zeta_n(D_1 - (\zeta^2 - 2\zeta_n^2)D_2), \\ I_4^{(0)} &= (\zeta^2 - \zeta_n^2)(\partial_{\zeta_n} \phi_1^{(0)} - \phi_2^{(1)}), \quad g_4^{(0)} = -4a_2^{(1)} \zeta_n - b_2^{(1)}(\zeta^2 - 3\zeta_n^2)B, \\ I_5^{(0)} &= 0, \quad g_5^{(0)} = -\frac{1}{3}(\zeta^2 - 3\zeta_n^2)B, \quad I_6^{(0)} = 0, \quad g_6^{(0)} = -\frac{1}{3}(\zeta^2 - 3\zeta_n^2)F + F_d. \end{aligned}$$

Elemental problem for $\phi_j^{(1)}(\eta, \zeta_n, \zeta)$ ($j = 1, 2, \dots, 8$):

$$\zeta_n \partial_{\eta} \zeta_t \phi_j^{(1)} = \mathcal{L}(\zeta_t \phi_j^{(1)}) - \zeta_t I_j^{(1)}, \quad (5a)$$

$$\zeta_t \phi_j^{(1)} = -2\tilde{\mathcal{K}}(\zeta_t) b_j^{(1)} + \mathcal{K}(\zeta_t \phi_j^{(1)}) + \tilde{\mathcal{K}}(\zeta_t g_j^{(1)}), \quad \zeta_n > 0, \eta = 0, \quad (5b)$$

$$\zeta_t \phi_j^{(1)} \rightarrow 0 \quad \text{as} \quad \eta \rightarrow \infty, \quad (5c)$$

where $\zeta_t = \zeta_i t_i$ and

$$\begin{aligned} I_1^{(1)} &= 0, \quad g_1^{(1)} = \zeta_n B, \quad I_2^{(1)} = 0, \quad g_2^{(1)} = A, \quad I_3^{(1)} = \phi_1^{(0)}, \quad g_3^{(1)} = 2\zeta_n F, \quad I_4^{(1)} = 0, \quad g_4^{(1)} = -(D_1 + \zeta_n^2 D_2), \\ I_5^{(1)} &= \frac{1}{2}(\zeta^2 - \zeta_n^2)\partial_{\zeta_n}\phi_1^{(1)}, \quad g_5^{(1)} = -2D_1 - \frac{1}{2}(\zeta^2 - \zeta_n^2)D_2, \quad I_6^{(1)} = \frac{1}{2}\partial_{\zeta_n}((\zeta^2 - \zeta_n^2)\phi_1^{(1)}), \quad g_6^{(1)} = g_5^{(1)} - g_4^{(1)}, \\ I_7^{(1)} &= \frac{1}{2}\partial_{\zeta_n}((\zeta^2 - \zeta_n^2)\phi_2^{(1)}) + \phi_1^{(0)}, \quad g_7^{(1)} = 0, \quad I_8^{(1)} = \frac{1}{2}(\zeta^2 - \zeta_n^2)\partial_{\zeta_n}\phi_2^{(1)}, \quad g_8^{(1)} = 0. \end{aligned}$$

It should be noted that I 's and g 's in the above are given sources in the equation and boundary condition. The functions A, B, D_1, D_2, F , and F_d occurring in g 's are functions of ζ which solve the following integral equations:

$$\begin{aligned} \mathcal{L}(\zeta_i A) &= -\zeta_i(\zeta^2 - \frac{5}{2}) \quad \text{with } \langle \zeta^2 A \rangle = 0, \quad \mathcal{L}(\zeta_{ij} B) = -2\zeta_{ij}, \quad \mathcal{L}(\zeta_{ij} F) = \zeta_{ij} A, \\ \mathcal{L}[(\zeta_i \delta_{jk} + \zeta_j \delta_{ik} + \zeta_k \delta_{ij})D_1 + \zeta_i \zeta_j \zeta_k D_2] &= \gamma_1(\zeta_i \delta_{jk} + \zeta_j \delta_{ik} + \zeta_k \delta_{ij}) - \zeta_i \zeta_j \zeta_k B \quad \text{with } \langle \zeta^2(5D_1 + \zeta^2 D_2) \rangle = 0, \\ \mathcal{L}(F_d) &= -\frac{5}{6}\gamma_2(\zeta^2 - \frac{3}{2}) + \frac{1}{3}\zeta^2 A \quad \text{with } \langle F_d \rangle = \langle \zeta^2 F_d \rangle = 0, \end{aligned}$$

where $\zeta_{ij} = \zeta_i \zeta_j - (1/3)\zeta^2 \delta_{ij}$, $\langle f \rangle \equiv \int f E(\zeta) d\zeta$, and $E(z) = \pi^{-3/2} \exp(-z^2)$. The γ 's occurring in (1) are expressed through these functions as

$$\begin{aligned} \gamma_1 &= \frac{2}{15} \langle \zeta^4 B \rangle, \quad \gamma_2 = \frac{4}{15} \langle \zeta^4 A \rangle, \quad \gamma_3 = \frac{2}{15} \langle \zeta^4 AB \rangle, \quad \gamma_6 = \frac{1}{15} \langle \zeta^4 BD_1 \rangle + \frac{1}{35} \langle \zeta^6 BD_2 \rangle, \\ \gamma_{10} &= \frac{1}{15} \langle \zeta^4 B^2 \rangle, \quad \gamma_{11} = -\frac{2}{39} (\gamma_2(2\langle \zeta^2 A^2 \rangle) + \gamma_3) + \frac{16}{15} \langle \zeta^4 AF \rangle + 4\langle \zeta^2 AF_d \rangle. \end{aligned}$$

Once ϕ 's are known, the Knudsen-layer functions Ω 's, Θ 's, and Y 's are obtained as the following moments:

$$\Omega_j^{(0)} = \langle \phi_j^{(0)} \rangle, \quad \Theta_j^{(0)} = \frac{2}{3} \langle (\zeta^2 - \frac{3}{2}) \phi_j^{(0)} \rangle, \quad Y_j^{(1)} = \frac{1}{2} \langle (\zeta^2 - \zeta_n^2) \phi_j^{(1)} \rangle.$$

Finally the momentum conservation of (5a) in the tangential direction yields the following identities that are to be used later in the reduction to the BGK model:

$$\langle \zeta_n(\zeta^2 - \zeta_n^2) \phi_j^{(1)} \rangle = \frac{3}{2} \int_{\eta}^{\infty} [\Omega_1^{(0)}(z) + \Theta_1^{(0)}(z)] dz \quad (j = 3, 7), \quad \langle \zeta_n(\zeta^2 - \zeta_n^2) \phi_j^{(1)} \rangle = 0, \quad (j = 1, 2, 4, 5, 6, 8). \quad (6)$$

ES MODEL AND ITS RELATION TO BGK MODEL

Preparation

Denoting by $\tilde{t}$ the time, by X_i the spatial coordinates, by ξ_i the molecular velocity, and by f the velocity distribution function, the original Boltzmann equation without external force is symbolically written as

$$\frac{\partial f}{\partial \tilde{t}} + \xi_i \frac{\partial f}{\partial X_i} = Q(f).$$

The ES model is defined by setting the collision integral $Q(f)$ as

$$Q(f) = Q_{\text{ES}}(f) \equiv A_c(T; \text{Pr}) \rho [\mathcal{G}(f) - f], \quad A_c(T; \text{Pr}) = \frac{\text{Pr} RT}{\mu(T)}, \quad (7)$$

$$\mathcal{G}(f) = \frac{\rho}{\sqrt{\det(2\pi\mathcal{T})}} \exp\left(-\frac{1}{2}\mathcal{T}_{ij}^{-1}(\xi_i - v_i)(\xi_j - v_j)\right), \quad \mathcal{T}_{ij} = [RT\delta_{ij} + (\text{Pr} - 1)(p_{ij}/\rho)]/\text{Pr}, \quad (8)$$

where ρ, v_i, T, p_{ij} , and $\mu(T)$ are respectively the density, the flow velocity, the temperature, the stress tensor, and the viscosity. The ES model equation is proved in [7] to satisfy the H theorem for $2/3 \leq \text{Pr} (< \infty)$. When $\text{Pr} = 1$,

$\mathcal{T}_{ij} = RT\delta_{ij}$ and $\mathcal{T}_{ij}^{-1} = (RT)^{-1}\delta_{ij}$, so that Q_{ES} is reduced to the collision integral Q_{BGK} for the BGK model:³

$$Q_{\text{ES}}(f)|_{\text{Pr}=1} = Q_{\text{BGK}}(f) \equiv A_c(T; 1)\rho[\mathcal{M}(f) - f], \quad \mathcal{M}(f) = \frac{\rho}{(2\pi RT)^{3/2}} \exp\left(-\frac{(\xi_i - v_i)^2}{2RT}\right). \quad (9)$$

Hereinafter, subscripts ES, BGK, and HS are used for other quantities as well, to indicate the model, if necessary.

By setting $\ell_0 = \sqrt{8RT_0/\pi}/[A_c(T_0; \text{Pr})\rho_0]$, we have $\mathcal{L}$ in (4) and (5) for the ES model, say $\mathcal{L}_{\text{ES}}$, in the form

$$\mathcal{L}(\phi) = \mathcal{L}_{\text{ES}}(\phi) \equiv \mathcal{L}_{\text{BGK}}(\phi) + 2\left(1 - \frac{1}{\text{Pr}}\right)\langle \zeta_{ij}\phi \rangle \zeta_i \zeta_j, \quad (10)$$

$$\mathcal{L}_{\text{BGK}}(\phi) \equiv \langle \phi \rangle + 2\langle \zeta_i \phi \rangle \zeta_i + \frac{2}{3}\langle (\zeta^2 - \frac{3}{2})\phi \rangle (\zeta^2 - \frac{3}{2}) - \phi. \quad (11)$$

Here $\mathcal{L}_{\text{BGK}}$ is the linearized collision operator for the BGK model. As is seen from (10), even when $\text{Pr} \neq 1$, the difference between $\mathcal{L}_{\text{ES}}$ and $\mathcal{L}_{\text{BGK}}$ occurs only when $\langle \zeta_{ij}\phi \rangle \neq 0$, i.e., only when the traceless part of the (linearized) stress tensor does not vanish. In case it vanishes or is a given function of specific form, the solution for the ES model can be recovered from that for the BGK model (e.g., [9, 10, 11, 12]), which will be the clue in the discussions in the next subsection.

Before going into details, we here summarize the explicit form of the functions $A, B, \dots, F_d$ and the dimensionless transport coefficients γ 's for the ES model:

$$\gamma_1 = \text{Pr}, \quad \gamma_2 = 1, \quad \gamma_3 = \text{Pr}, \quad \gamma_6 = \text{Pr}^2, \quad \gamma_{10} = \text{Pr}^2, \quad \gamma_{11} = 1 + \frac{2}{13}(\text{Pr} - 1), \quad (12a)$$

$$A = \zeta^2 - \frac{5}{2}, \quad B = 2\text{Pr}, \quad D_1 = -\text{Pr}, \quad D_2 = 2\text{Pr}, \quad F = -\zeta^2 + \frac{5}{2} - (\text{Pr} - 1), \quad F_d = -\frac{1}{3}(\zeta^4 - 5\zeta^2 + \frac{15}{4}). \quad (12b)$$

They are obtained straightforwardly, thanks to the simple form of $\mathcal{L}_{\text{ES}}$. Note that the case of the BGK model is recovered by setting $\text{Pr} = 1$ in (12).

In the case of the hard-sphere gas, $\ell_0 = 1/(\sqrt{2}\pi d_m^2 \rho_0/m)$ with m and d_m being the mass and diameter of a molecule. The functions $A, B, \dots, F_d$ take different forms from those in (12b), and consequently γ 's take the following values:

$$\begin{aligned} \gamma_1 &= 1.270042427, & \gamma_2 &= 1.922284066, & (\text{Pr} = \gamma_1/\gamma_2 = 0.6606944569), & \gamma_3 &= 1.947906335, \\ \gamma_6 &= 1.419423836, & \gamma_{10} &= 1.63607346, & \gamma_{11} &= 2.7931173. \end{aligned}$$

In comparing the data based on different collision models, it is common in the literature to take the viscosity or thermal conductivity as a reference quantity, i.e., to make $\gamma_1 \ell_0$ or $\gamma_2 \ell_0$ being common. This leads to the conversion rule of the mean free path ℓ_0 between the ES and HS models such that $\text{Pr}_{\text{ES}} \ell_{0\text{ES}} = 1.270042427 \ell_{0\text{HS}}$ or $\ell_{0\text{ES}} = 1.922284066 \ell_{0\text{HS}}$, i.e., $\text{Pr}_{\text{ES}} \varepsilon_{\text{ES}} = 1.270042427 \varepsilon_{\text{HS}}$ or $\varepsilon_{\text{ES}} = 1.922284066 \varepsilon_{\text{HS}}$. Since $\text{Pr}_{\text{HS}} = 0.6606944569$ is close to $2/3$, the viscosity based conversion is practically identical to the thermal-conductivity based one between ES with $\text{Pr}_{\text{ES}} = 2/3$ and HS, which is an advantage of the ES model over the BGK model.

Reduction to the BGK Model

In the present subsection, we discuss the feasibility of the reduction of the problems (4) and (5) for the ES model to those for the BGK model. Let us first consider the elemental problems (4). The parity of $\phi_j^{(0)}$ makes the non-diagonal parts of the stress tensor vanished, but the diagonal parts remain. Consequently, we do not find a simple conversion between $\mathcal{L}_{\text{ES}}(\phi_j^{(0)})$ and $\mathcal{L}_{\text{BGK}}(\phi_j^{(0)})$. The reduction of the problems is not expected. As to the problems (5), however, the desired reduction can be made for most of them, which we explain below.

Thanks to the parity of $\phi_j^{(1)}$, the diagonal parts of the stress tensor vanish. As to the non-diagonal parts, thanks to the property (6) (see [1, Appendix G.2] as well), they vanish as well, except for $\phi_3^{(1)}$ and $\phi_7^{(1)}$. Consequently, in the

³In the original BGK model, A_c is a positive constant because it is a simplified model for the pseudo-Maxwell molecular gas. Here, A_c is extended to be a function of the temperature as in [7]. The extension does not make a difference from the original under the linearized situation.

TABLE 1. Slip/jump coefficients for the ES model ($\text{Pr} = 2/3$), the BGK model, and the hard-sphere gas. I.

	ES	BGK [4]	HS [1]		ES	BGK [4]	HS [1]
$c_1^{(0)}$	1.30160	1.30272	2.4001	$c_2^{(0)}$	-0.02537	0	-0.4992
$c_3^{(0)}$	0.00041	0.11169	0.0087	$c_4^{(0)}$	1.69117	1.82181	4.6181
$c_5^{(0)}$	0.28954	0.44045	0.4596	$c_6^{(0)}$	-1.35138	-1.4276	-3.1800
$b_3^{(1)}$	-0.50025	-0.77837	-1.5846				

TABLE 2. Slip/jump coefficients for the ES model ($\text{Pr} = 2/3$), the BGK model, and the hard-sphere gas. II.

	ES (present results)			BGK [4]	HS [1]
	direct computation	formula (13)	symmetry relation [1]		
$b_1^{(1)}$	0.67746	0.67746	0.67746	1.01619	1.2540
$b_2^{(1)}$	0.38316	0.38316	0.38316	0.38316	0.6465
$b_4^{(1)}$	-0.51088	-0.51088	-0.51088	-0.76632	-0.9039
$b_5^{(1)}$	-0.33334	-0.33333	-0.33333	-0.50000	-0.6601
$b_6^{(1)}$	0.17753	0.17755	0.17756	0.26632	0.2438
$b_7^{(1)}$	0.20667	0.20668	0.20667	0.26729	0.4472
$b_8^{(1)}$	-0.26693	-0.26693	-0.26693	-0.26693	-0.2336
$2a_1^{(1)}$	-0.15578	-0.15579	-0.15578	-0.23368	-0.2137
$a_2^{(1)}$	-0.26693	-0.26693	-0.26693	-0.26693	-0.4782

elemental problems for $\phi_j^{(1)}$ ($j = 1, 2, 4, 5, 6, 8$), $\mathcal{L}_{\text{ES}}$ is reduced to $\mathcal{L}_{\text{BGK}}$. Taking into account the similarity of $I_j^{(1)}$ and $g_j^{(1)}$ between the two models originated from (12), we obtain the following simple conversions:

$$\phi_j^{(1)}_{\text{ES}} = \text{Pr } \phi_j^{(1)}_{\text{BGK}} \quad (j = 1, 4, 5, 6), \quad \phi_j^{(1)}_{\text{ES}} = \phi_j^{(1)}_{\text{BGK}} \quad (j = 2, 8). \quad (13a)$$

The corresponding slip coefficients and Knudsen-layer functions obey the same conversion.

Although similar conversions are not found for $\phi_3^{(1)}$ and $\phi_7^{(1)}$ separately, their difference $\phi_{73}^{(1)} \equiv \phi_7^{(1)} - \phi_3^{(1)}$ allows the reduction of $\mathcal{L}_{\text{ES}}(\phi_{73}^{(1)})$ to $\mathcal{L}_{\text{BGK}}(\phi_{73}^{(1)})$. Then, with the aid of (12b) and (13a) with $j = 2$, we obtain the conversion

$$\phi_{73}^{(1)}_{\text{ES}} = \phi_{73}^{(1)}_{\text{BGK}} + (\text{Pr} - 1) \phi_1^{(1)}_{\text{BGK}}. \quad (13b)$$

Here, in the last equality, we use (13a) with $j = 1$. Again, the corresponding slip coefficients and Knudsen-layer functions obey the same conversion.

To summarize, the jump coefficients and related Knudsen-layer functions require the direct numerical solutions of the problems (4) for the ES model. Among the remaining problems (5), only the problem for $\phi_3^{(1)}$ is required to be solved. The others are obtained by the simple conversion rules in (13) from the data for the BGK model, if they are available. The conversion rules in (13) hold for arbitrary values of the Prandtl number, provided that $\text{Pr} \geq 2/3$. Furthermore, they hold for any locally isotropic boundary conditions supposed in [1], which includes the diffuse reflection as a special case. In the next section, we show the results for $\text{Pr} = 2/3$ and the diffuse reflection condition.

Incidentally, once $\phi_1^{(0)}$, $\phi_1^{(1)}$, and $\phi_2^{(1)}$ are known, all the slip/jump coefficients can be obtained with the aid of the symmetry relation [13, 14, 15], as is done in [1]. Therefore, as far as the slip/jump coefficients are concerned, the newly required computation for the ES model is only for $\phi_1^{(0)}$.

NUMERICAL RESULTS

The problems (4) and (5) for the ES model can be converted to the integral equations for macroscopic variables as in the case of the BGK model (see, e.g., [16], [4, Appendix A.4]). In the meantime, the first and second authors have already established a direct accurate numerical method [2, 3] for the original formalism (4) and (5), which can

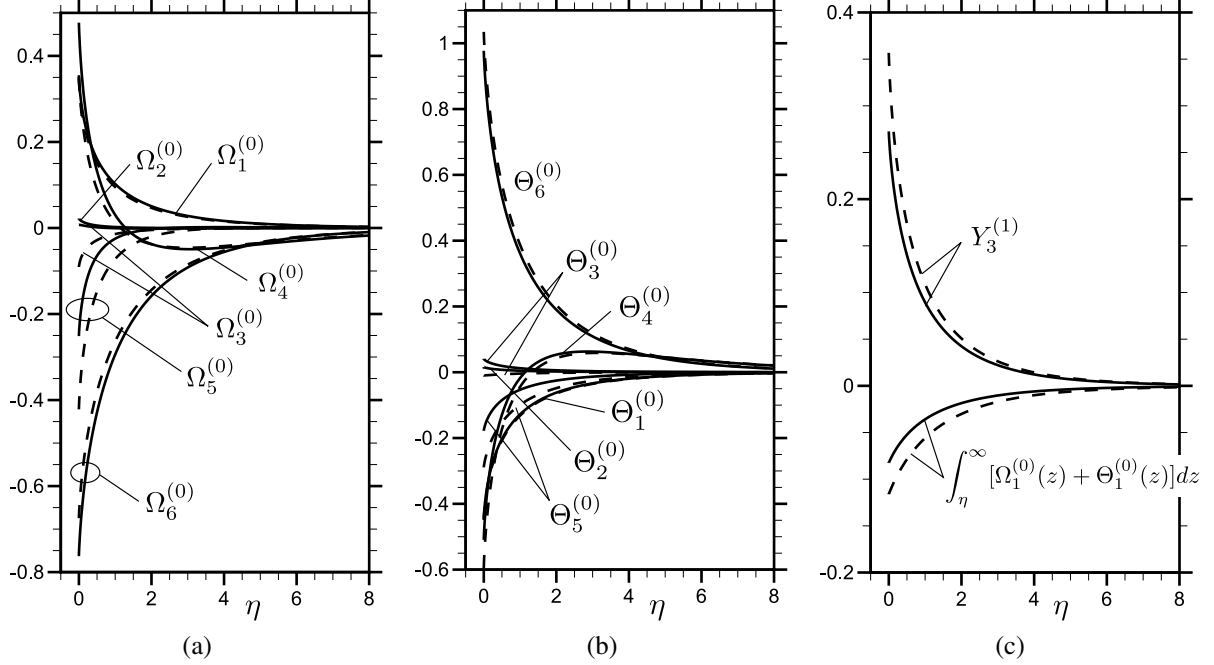


FIGURE 1. Knudsen-layer functions. (a) Density corrections $\Omega_1^{(0)}, \dots, \Omega_6^{(0)}$, (b) temperature corrections $\Theta_1^{(0)}, \dots, \Theta_6^{(0)}$, and (c) tangential velocity correction $Y_3^{(1)}$ and $\int_{\eta}^{\infty} (\Omega_1^{(0)} + \Theta_1^{(0)}) d\eta$ in (6). Solid lines: the ES model. Dashed lines: the BGK model. $\Omega_2^{(0)}$ and $\Theta_2^{(0)}$ for the BGK model are omitted in (a) and (b), because they are identically zero.

safely handle the emergence of a localized divergent singularity at the level of the VDF (see [3] for details). Here, we present the results obtained by the latter method. Owing to the limitations of space, we limit ourselves to show the slip/jump coefficients and a part of the Knudsen-layer functions for $\text{Pr} = 2/3$ and the diffuse reflection condition. Further detailed information, such as the VDFs and the compact tables and raw data of the Knudsen-layer functions, is available from Kyoto University Research Information Repository (<http://hdl.handle.net/2433/199811>).

Table 1 shows the slip/jump coefficients $c_1^{(0)}, \dots, c_6^{(0)}$ and $b_3^{(1)}$ for which new computations for the ES model are required. The table includes those for the BGK model and the hard-sphere gas as well for reference.

Table 2 shows the remaining slip coefficients for the ES model, BGK model, and hard-sphere gas. There are three columns for the ES model: the first column shows the data obtained by new direct computations, the second those obtained by the conversion (13) from the existing data for the BGK model, and the third those obtained by the identities in [1, Sec. 7], which are the consequence of the theory of symmetric relation. Fairly good agreements of the data among the three columns confirm the validity of the conversion formulas in (13) and, at the same time, the achievement of highly accurate computations in the present work.

Figure 1 shows the profiles of the Knudsen-layer functions $\Omega_1^{(0)}, \dots, \Omega_6^{(0)}$, $\Theta_1^{(0)}, \dots, \Theta_6^{(0)}$, $Y_3^{(1)}$, and $\int_{\eta}^{\infty} (\Omega_1^{(0)} + \Theta_1^{(0)}) d\eta$, which are computed from the numerical data of $\phi_1^{(0)}, \dots, \phi_6^{(0)}$ and $\phi_3^{(1)}$. Remember that η is the stretched normal coordinate to the boundary and that Ω 's, Θ 's, and Y 's are the density, temperature, and tangential flow velocity corrections to the fluid-dynamical description inside the Knudsen layer [see (3)]. The quantities in the figure cannot be recovered from those for the BGK model. Nevertheless, $\Omega_1^{(0)}, \Omega_4^{(0)}, \Omega_6^{(0)}, \Theta_1^{(0)}, \Theta_4^{(0)}, \Theta_6^{(0)}, Y_3^{(1)}$, and $\int_{\eta}^{\infty} (\Omega_1^{(0)} + \Theta_1^{(0)}) d\eta$ are rather close to those for the BGK model. The others, i.e., $\Omega_2^{(0)}, \Omega_3^{(0)}, \Omega_5^{(0)}, \Theta_2^{(0)}, \Theta_3^{(0)}$, and $\Theta_5^{(0)}$, are more dependent on the model. Their magnitude is, however, relatively small. The same observation applies to the slip/jump coefficients in Table 1.

Finally we would like to call the attention of the reader to two remarkable things. The first is that the ES model does not inherit the special property of the BGK model that $c_2^{(0)}, \Omega_2^{(0)}$, and $\Theta_2^{(0)}$ all vanish even if $\phi_2^{(0)}$ does not. They are, however, smaller than those for the hard-sphere gas in their magnitude by one order. The second is that $c_3^{(0)}$ is positive, irrespective of the choice of the model (see Table 1). Its positivity leads to the theoretical prediction of the negative

thermophoresis of a spherical particle with uniform temperature (or with extremely high thermal conductivity). This is the topic in the next section.

APPLICATION EXAMPLE: NEGATIVE THERMOPHORESIS

Consider a spherical particle of radius L suspended in a slightly rarefied gas. When there is a temperature gradient in the background gas, the sphere is subjected to a force from the gas (the thermal force).

Let the origin of the space coordinates X_i be the center of the sphere and the temperature of the gas in the absence of the sphere be $T_0 + (dT/dX_1)_\infty X_1$, where T_0 is the reference temperature. When the thermal conductivity of the particle is by far larger than that of the gas, the thermal force $(F_T, 0, 0)$ acting on the particle is given by

$$\frac{F_T}{\lambda_g L^2 (2RT_0)^{-1/2} (dT/dX_1)_\infty} = 24\pi c_3^{(0)} \varepsilon^2 + o(\varepsilon^2), \quad (14)$$

where λ_g is the thermal conductivity of the gas; see, e.g., [4, p. 252].⁴ Here are two remarks. If the thermal conductivity of the particle is comparable to that of the gas, the thermal force is larger by one order in ε and is in the direction opposite to the temperature gradient. The force (14) is, however, in the same direction as the temperature gradient, because $c_3^{(0)}$ is positive, irrespective of the gas model (see Table 1). The former case is simply referred to as the thermophoresis, while the latter case, i.e., (14), is referred to as the *negative* thermophoresis. The reversal of the force direction, as well as the change of magnitude by one order in ε , is due to the change of the dominant physical mechanism. The reader is referred to [4] for the comprehensive explanation on this issue.

Comparisons of the data of $c_3^{(0)}$ in Table 1 show that the ES model predicts by far smaller negative thermophoresis than the BGK model and the hard-sphere gas. However, in order to make fair comparisons, the mean free path of different molecular models should be converted, as is noted at the end of **Preparation**. In view of (14), the conversion that makes the thermal conductivity λ_g common is suitable, namely $\varepsilon_{\text{ES}} = \varepsilon_{\text{BGK}} = 1.922284066\varepsilon_{\text{HS}}$. Even if this conversion is taken into account, the thermal force F_T in (14) for the ES model is only about 17% of that for the hard-sphere gas.

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⁴The coefficient $c_3^{(0)}$ is related to a_4 in [4, p. 252] as $a_4 = -c_1^{(0)}b_2^{(1)} - b_3^{(1)} = (5/2)c_3^{(0)}/\text{Pr}$. See (57) in [1, Sec. 7] for the last equality.