

On the Second-order Slip and Jump Coefficients for the General Theory of Slip Flow

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Abstract. The general theory of slip flow established in the late 1960s is revisited. For a long time, the complete set of data of the slip and jump coefficients up to the second order of the small Knudsen number have been available only for the Bhatnagar–Gross–Krook model. The present paper provides the complete set of data of those coefficients for a hard-sphere gas on the diffuse reflection boundary. The data are obtained by using the general identities that have been deduced from recently developed symmetry arguments. A few simple application examples are also presented.

Keywords: slip flow, second-order slip, slightly rarefied gas, kinetic theory, Boltzmann equation, Poiseuille flow, thermal transpiration, drag, thermophoresis

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INTRODUCTION

Recent development of micro device technologies enhances the research activity of gas flows in the slip-flow regime, both numerically and experimentally. The general theory of slip flow itself has been established with a firm foundation in 1960s and 1970s on the basis of the Bhatnagar–Gross–Krook (BGK or Boltzmann–Krook–Welander [1, 2]) model [3] and later on the basis of the original Boltzmann equation [4]. The slip and jump conditions up to the second order of the small Knudsen number, which are recent concerns of many researchers (e.g., [5, 6, 7, 8]), have also been clarified at such an early stage. They are compiled and can be found in [9, 10].

For a long time, the specific values of the second-order slip and jump coefficients occurring in that theory have been available only partially, except for the BGK model with the diffuse reflection condition. In the present work, we will take a step forward to provide all the values of those coefficients for a hard-sphere gas with the diffuse reflection condition. The symmetry argument recently developed by the first author [11] makes this step rather easy, compared with a straightforward numerical approach.

GENERAL THEORY OF SLIP FLOW

Let us denote by Lx_i the space coordinates, by $p_0(1+P)$ and $T_0(1+\tau)$ the pressure and temperature of the gas, by $(2RT_0)^{1/2}u_i$ the flow velocity, and by $(2RT_0)^{1/2}u_{wi}$ and $T_0(1+\tau_w)$ the velocity and temperature of the boundary. Here L is the characteristic length of the system, R is the specific gas constant, p_0 and T_0 are the pressure and temperature in the reference equilibrium state at rest. 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. We assume that the boundary does not deform and thus $u_{wi}n_i = 0$. The slip-flow theory describes the asymptotic behavior of the gas for small Knudsen numbers. Here 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.¹ In the present paper, we use the notation ε defined by $\varepsilon = (\sqrt{\pi}/2)\text{Kn}$, instead of Kn , to emphasize its smallness.

According to the general theory of slip flow [9, 10], the behavior of a slightly rarefied gas with a small Reynolds number can be described in the bulk of the domain by the Stokes set of equations with slip and 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 fluid-dynamical part) is necessary to be corrected

¹ For the BGK model, $\ell_0 = (2/\sqrt{\pi})(2RT_0)^{1/2}/(A_c\rho_0)$, where $\rho_0 = p_0/RT_0$ (the reference density) and $A_c\rho_0$ is the collision frequency (A_c is a positive constant). For a hard-sphere gas, $\ell_0 = (\sqrt{2}\pi d^2(\rho_0/m))^{-1}$, where d and m are the diameter and mass of a molecule.

(the Knudsen-layer correction). The slip and jump conditions and the Knudsen-layer correction are required at the level of the first and higher orders of the Knudsen number. This is a classical result derived by a systematic asymptotic analysis of the linearized Boltzmann equation for small Knudsen number. The primary concern of the present paper is the fluid-dynamical part. The Knudsen-layer corrections will be rarely discussed or mentioned hereafter.

We shall tell apart the fluid-dynamical part and the Knudsen-layer correction by putting subscript G and K to the notation of quantities respectively. Each quantity, say $h = h_G + h_K$ ($h = P, \tau, u_i$, etc.), is expanded in a power series of ε as $h_G = h_G^{(0)} + h_G^{(1)}\varepsilon + h_G^{(2)}\varepsilon^2 \dots$ and $h_K = h_K^{(1)}\varepsilon + h_K^{(2)}\varepsilon^2 \dots$. Note that the expansion of h_K starts from $O(\varepsilon)$ (see the previous paragraph). Then, the above mentioned Stokes set of equations and the slip and jump boundary conditions over a smooth solid body are written as follows:

Stokes set of equations

$$\frac{\partial P_G^{(0)}}{\partial x_i} = 0, \quad \frac{\partial u_{Gi}^{(m)}}{\partial x_i} = 0, \quad \gamma_1 \frac{\partial^2 u_{Gi}^{(m)}}{\partial x_j^2} = \frac{\partial P_G^{(m+1)}}{\partial x_i}, \quad \frac{\partial^2 \tau_G^{(m)}}{\partial x_j^2} = 0, \quad (m = 0, 1, 2, \dots), \quad (1)$$

Slip and jump boundary conditions [up to $O(\varepsilon^2)$]

the leading order (non-slip and non-jump)

$$u_{Gi}^{(0)} = u_{wi}^{(0)}, \quad \tau_G^{(0)} = \tau_w^{(0)}, \quad (2)$$

the first order

$$u_{Gi}^{(1)} n_i = 0, \quad u_{Gi}^{(1)} t_i = u_{wi}^{(1)} t_i - k_0 \left(\frac{\partial u_{Gi}^{(0)}}{\partial x_j} + \frac{\partial u_{Gj}^{(0)}}{\partial x_i} \right) n_i t_j - K_1 \frac{\partial \tau_G^{(0)}}{\partial x_i} t_i, \quad (3)$$

$$\tau_G^{(1)} = \tau_w^{(1)} + d_1 \frac{\partial \tau_G^{(0)}}{\partial x_i} n_i, \quad (4)$$

the second order

$$\begin{aligned} u_{Gi}^{(2)} t_i = & u_{wi}^{(2)} t_i - k_0 \left(\frac{\partial u_{Gi}^{(1)}}{\partial x_j} + \frac{\partial u_{Gj}^{(1)}}{\partial x_i} \right) n_i t_j - K_1 \frac{\partial \tau_G^{(1)}}{\partial x_i} t_i - a_1 \left[\frac{\partial}{\partial x_k} \left(\frac{\partial u_{Gi}^{(0)}}{\partial x_j} + \frac{\partial u_{Gj}^{(0)}}{\partial x_i} \right) \right] n_j n_k t_i \\ & - a_2 \bar{\kappa} \left(\frac{\partial u_{Gi}^{(0)}}{\partial x_j} + \frac{\partial u_{Gj}^{(0)}}{\partial x_i} \right) n_i t_j - a_3 \kappa_{ij} \left(\frac{\partial u_{Gk}^{(0)}}{\partial x_j} + \frac{\partial u_{Gj}^{(0)}}{\partial x_k} \right) n_k t_i \\ & - (a_4 - d_1 K_1) \frac{\partial^2 \tau_G^{(0)}}{\partial x_i \partial x_j} n_i t_j - a_5 \bar{\kappa} \frac{\partial \tau_G^{(0)}}{\partial x_i} t_i - (a_6 - d_1 K_1) \kappa_{ij} \frac{\partial \tau_G^{(0)}}{\partial x_j} t_i, \end{aligned} \quad (5)$$

$$u_{Gi}^{(2)} n_i = -2b_1 \frac{\partial^2 u_{Gi}^{(0)}}{\partial x_k \partial x_j} n_i n_j n_k - b_2 \left(\frac{\partial^2 \tau_G^{(0)}}{\partial x_i \partial x_j} n_i n_j + 2\bar{\kappa} \frac{\partial \tau_G^{(0)}}{\partial x_i} n_i \right), \quad (6)$$

$$\tau_G^{(2)} = \tau_w^{(2)} + d_1 \frac{\partial \tau_G^{(1)}}{\partial x_i} n_i + 2d_4 \frac{\partial^2 u_{Gi}^{(0)}}{\partial x_k \partial x_j} n_i n_j n_k + d_3 \frac{\partial^2 \tau_G^{(0)}}{\partial x_i \partial x_j} n_i n_j + d_5 \bar{\kappa} \frac{\partial \tau_G^{(0)}}{\partial x_i} n_i, \quad (7)$$

where γ_1 is the dimensionless viscosity², which is a constant depending on the molecular model (see Table 2 in the next section), while $k_0, K_1, a_1 \sim a_6, b_1, b_2, d_1$, and $d_3 \sim d_5$ are the slip and jump coefficients, which are a constant depending on both the molecular model and the kinetic boundary condition (i.e., the model of gas-surface interaction). κ_{ij}/L and $\bar{\kappa}/L$ are respectively the curvature matrix and mean curvature of the boundary.³ The system (1)–(7) determines the

² The viscosity μ at the reference state is given by $\mu = \gamma_1 p_0 (2RT_0)^{-1/2} L\varepsilon$.

³ 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.

TABLE 1. Slip and jump coefficients for the BGK model and the diffuse reflection condition (the data taken from [10, 9]).

first-order slip & jump		second-order slip				second-order jump			
k_0	-1.01619	a_1	0.76632	a_4	0.27922	d_3	0	b_1	0.11684
K_1	-0.38316	a_2	0.50000	a_5	0.26693	d_4	0.11169	b_2	0.26693
d_1	1.30272	a_3	-0.26632	a_6	-0.76644	d_5	1.82181		

behavior of the bulk gas from the lowest order. Namely, the first equation of (1) means the uniform pressure at the leading order. Equation (1) for $m = 0$ with (2) determines the leading order of temperature and flow velocity, together with the first order of pressure; Equation (1) for $m = 1$ with (3) and (4) determine the first order of temperature and flow velocity, together with the second order of pressure; and so on.

If we sum up the terms in the above system, the behavior of the bulk gas is seen to be described correctly up to $O(\varepsilon^2)$ as follows:

$$\frac{\partial u_{Gi}}{\partial x_i} = 0, \quad \varepsilon \gamma_1 \frac{\partial^2 u_{Gi}}{\partial x_j^2} = \frac{\partial P_G}{\partial x_i}, \quad \frac{\partial^2 \tau_G}{\partial x_j^2} = 0, \quad (8)$$

with the slip and jump conditions

$$\begin{aligned} u_{Gi} t_i &= u_w t_i - \varepsilon k_0 \left(\frac{\partial u_{Gi}}{\partial x_j} + \frac{\partial u_{Gj}}{\partial x_i} \right) n_i t_j - \varepsilon K_1 \frac{\partial \tau_G}{\partial x_i} t_i - \varepsilon^2 a_1 \left[\frac{\partial}{\partial x_k} \left(\frac{\partial u_{Gi}}{\partial x_j} + \frac{\partial u_{Gj}}{\partial x_i} \right) \right] n_j n_k t_i \\ &\quad - \varepsilon^2 a_2 \bar{\kappa} \left(\frac{\partial u_{Gi}}{\partial x_j} + \frac{\partial u_{Gj}}{\partial x_i} \right) n_i t_j - \varepsilon^2 a_3 \kappa_{ij} \left(\frac{\partial u_{Gk}}{\partial x_j} + \frac{\partial u_{Gj}}{\partial x_k} \right) n_k t_i \\ &\quad - \varepsilon^2 (a_4 - d_1 K_1) \frac{\partial^2 \tau_G}{\partial x_i \partial x_j} n_i t_j - \varepsilon^2 a_5 \bar{\kappa} \frac{\partial \tau_G}{\partial x_i} t_i - \varepsilon^2 (a_6 - d_1 K_1) \kappa_{ij} \frac{\partial \tau_G}{\partial x_j} t_i, \end{aligned} \quad (9)$$

$$u_{Gi} n_i = -2\varepsilon^2 b_1 \frac{\partial^2 u_{Gi}}{\partial x_j \partial x_k} n_i n_j n_k - \varepsilon^2 b_2 \left(\frac{\partial^2 \tau_G}{\partial x_i \partial x_j} n_i n_j + 2\bar{\kappa} \frac{\partial \tau_G}{\partial x_i} n_i \right), \quad (10)$$

$$\tau_G = \tau_w + \varepsilon d_1 \frac{\partial \tau_G}{\partial x_i} n_i + 2\varepsilon^2 d_4 \frac{\partial^2 u_{Gi}}{\partial x_j \partial x_k} n_i n_j n_k + \varepsilon^2 d_3 \frac{\partial^2 \tau_G}{\partial x_i \partial x_j} n_i n_j + \varepsilon^2 d_5 \bar{\kappa} \frac{\partial \tau_G}{\partial x_i} n_i. \quad (11)$$

The system (8)–(11) might be preferred as a concise form of (1)–(7), especially for numerical computations.

In order to apply the theory to specific problems, a complete set of data of k_0 , K_1 , $a_1 \sim a_6$, b_1 , b_2 , d_1 , and $d_3 \sim d_5$ is desired. However, it is available only for the BGK model with the diffuse reflection condition ([3, 9]; see Table 1). Even for a hard-sphere gas with the diffuse reflection condition, only a partial set of data (i.e., k_0 , K_1 , a_4 , b_1 , b_2 , d_1 , and d_4) has been available [12, 13, 14, 15], thus having restricted the application of the theory to the level of $O(\varepsilon)$.

In the next section, we provide a complete set of numerical data of the slip and jump coefficients for a hard-sphere gas on the diffuse reflection boundary, which was obtained by using the symmetric relation developed in [11].

IDENTITIES AMONG THE SLIP AND JUMP COEFFICIENTS

Each slip and jump coefficient is related to a specific thermal or fluid-dynamical state (shear stress, temperature gradient, thermal stress, etc.) of the bulk gas at the boundary and is determined (together with the solution, namely the velocity distribution function) through the analysis of the corresponding half-space problem of the linearized Boltzmann equation with/without a source term. This half-space problem is generically written as

$$\zeta_n \frac{\partial \phi^\alpha}{\partial \eta} = \mathcal{L}[\phi^\alpha] + I^\alpha(\eta, \boldsymbol{\zeta}), \quad (12a)$$

$$\phi^\alpha = \widetilde{\mathcal{K}}[-2\zeta_j(\delta_{ij} - n_i n_j) b_i^\alpha - |\boldsymbol{\zeta}|^2 c^\alpha + g^\alpha(\boldsymbol{\zeta})] + \mathcal{K}[\phi^\alpha], \quad \zeta_n > 0, \quad \eta = 0, \quad (12b)$$

$$\phi^\alpha \rightarrow 0 \quad \text{as } \eta \rightarrow \infty, \quad (12c)$$

where $\zeta_n = \zeta_i n_i$, η is the (stretched dimensionless) coordinate in the direction of n_i , \mathcal{L} is the linearized collision operator, \mathcal{K} is the locally isotropic reflection operator on the boundary, $\widetilde{\mathcal{K}}[f] = f - \mathcal{K}[f]$, I^α and g^α are a given

function, δ_{ij} is the Kronecker delta, superscript α is the label for telling apart the elemental problems, and b_i^α and c^α correspond to the slip coefficient of tangential velocity and the jump coefficient of temperature, respectively. For instance, \mathcal{L} is given for the BGK model by

$$\mathcal{L}[\phi^\alpha] = \langle \phi^\alpha \rangle + 2\zeta_i \langle \zeta_i \phi^\alpha \rangle + \frac{2}{3} (|\boldsymbol{\zeta}|^2 - \frac{3}{2}) \langle (|\boldsymbol{\zeta}|^2 - \frac{3}{2}) \phi^\alpha \rangle,$$

and for a hard-sphere gas by

$$\begin{aligned} \mathcal{L}[\phi^\alpha] &= -v(|\boldsymbol{\zeta}|) \phi^\alpha(\boldsymbol{\zeta}) + \int k(\boldsymbol{\zeta}, \boldsymbol{\xi}) \phi^\alpha(\boldsymbol{\xi}) d\boldsymbol{\xi}, \\ v(z) &= \frac{1}{2\sqrt{2}} \left[\exp(-z^2) + \left(2z + \frac{1}{z}\right) \int_0^z \exp(-y^2) dy \right], \\ k(\boldsymbol{\zeta}, \boldsymbol{\xi}) &= \frac{1}{\sqrt{2\pi} |\boldsymbol{\zeta} - \boldsymbol{\xi}|} \exp\left(-|\boldsymbol{\xi}|^2 + \frac{|\boldsymbol{\xi} \times \boldsymbol{\zeta}|^2}{|\boldsymbol{\xi} - \boldsymbol{\zeta}|^2}\right) - \frac{|\boldsymbol{\zeta} - \boldsymbol{\xi}|}{2\sqrt{2\pi}} \exp(-|\boldsymbol{\xi}|^2), \end{aligned}$$

where

$$\langle \Phi \rangle(\eta) = \pi^{-3/2} \int \Phi(\boldsymbol{\eta}, \boldsymbol{\zeta}) \exp(-|\boldsymbol{\zeta}|^2) d\boldsymbol{\zeta}.$$

For the diffuse reflection condition, \mathcal{K} is given by

$$\mathcal{K}[\phi^\alpha] = 2\pi^{-1} \int_{\zeta_n^* < 0} |\zeta_n^*| \phi^\alpha(\boldsymbol{\zeta}^*) \exp(-|\boldsymbol{\zeta}^*|^2) d\boldsymbol{\zeta}^*, \quad \zeta_n > 0.$$

By applying the symmetric relation developed in [11], we obtain the following identity between the half-space problem for ϕ^α [(12) with $\alpha = \alpha$] and that for ϕ^β [(12) with $\alpha = \beta$]:

$$\begin{aligned} &\langle \zeta_n (2\zeta_j (\delta_{ij} - n_i n_j) b_i^\beta - |\boldsymbol{\zeta}|^2 c^\beta) (\phi^\alpha - g^\alpha) \rangle|_{\eta=0} + \langle \zeta_n g^{\beta-} (\phi^\alpha - \frac{1}{2} g^\alpha) \rangle|_{\eta=0} - \int_0^\infty \langle I^{\beta-} \phi^\alpha \rangle d\eta \\ &= \langle \zeta_n (2\zeta_j (\delta_{ij} - n_i n_j) b_i^\alpha - |\boldsymbol{\zeta}|^2 c^\alpha) (\phi^\beta - g^\beta) \rangle|_{\eta=0} + \langle \zeta_n g^{\alpha-} (\phi^\beta - \frac{1}{2} g^\beta) \rangle|_{\eta=0} - \int_0^\infty \langle I^{\alpha-} \phi^\beta \rangle d\eta, \end{aligned} \quad (13)$$

where superscript “ $-$ ” means that $\Phi^-(\cdot, \boldsymbol{\zeta}) = \Phi(\cdot, -\boldsymbol{\zeta})$. The specific form of I^α and g^α for various elemental half-space problems can be found in [16]. Here we simply summarize the identities between different slip and jump coefficients that have been obtained from (13) for various pairs of those half-space problems:

$$K_1 = \frac{1}{2\gamma_1} \left(-\gamma_3 + \int_0^\infty \langle (|\boldsymbol{\zeta}|^2 - \zeta_n^2) (|\boldsymbol{\zeta}|^2 - \frac{5}{2}) \phi^S \rangle d\eta \right), \quad (14)$$

$$\begin{aligned} a_4 &= d_1 K_1 - \frac{1}{\gamma_1} k_0 \left(\gamma_3 + \int_0^\infty \langle |\boldsymbol{\zeta}|^2 \phi^T \rangle d\eta \right) + \frac{1}{\gamma_1} \int_0^\infty \eta \left(\langle |\boldsymbol{\zeta}|^2 \phi^T \rangle + \langle (|\boldsymbol{\zeta}|^2 - \zeta_n^2) (|\boldsymbol{\zeta}|^2 - \frac{5}{2}) \phi^S \rangle \right) d\eta \\ &\quad + \frac{1}{2\gamma_1} \int_0^\infty \langle (|\boldsymbol{\zeta}|^2 - \zeta_n^2) (\zeta_n B + \phi^{S-}) \phi^T \rangle d\eta, \end{aligned} \quad (15)$$

$$a_1 = \frac{\gamma_6}{\gamma_1} + \frac{1}{2} \int_0^\infty \langle (|\boldsymbol{\zeta}|^2 - \zeta_n^2) \phi^S \rangle d\eta, \quad (16)$$

$$\begin{aligned} a_3 &= -\frac{1}{4\gamma_1} \left(\int_0^\infty \langle |\boldsymbol{\zeta}|^2 (|\boldsymbol{\zeta}|^2 - \zeta_n^2) B \phi^S \rangle d\eta - \frac{4}{15} \langle |\boldsymbol{\zeta}|^4 (D_1 - \frac{1}{7} |\boldsymbol{\zeta}|^2 D_2) B \rangle \right. \\ &\quad \left. + 2 \langle \zeta_n (|\boldsymbol{\zeta}|^2 - \zeta_n^2) (D_1 + \frac{1}{2} (|\boldsymbol{\zeta}|^2 - 3\zeta_n^2) D_2) \phi^S \rangle|_{\eta=0} - \int_0^\infty \langle (|\boldsymbol{\zeta}|^2 - \zeta_n^2)^2 \phi^{S-} \frac{\partial \phi^S}{\partial \zeta_n} \rangle d\eta \right), \end{aligned} \quad (17)$$

$$a_2 = a_1 + a_3, \quad (18)$$

$$d_4 = \frac{2}{5} \frac{\gamma_1}{\gamma_2} a_4, \quad (19)$$

$$\begin{aligned} d_3 &= \frac{4}{5\gamma_2} \left(-\gamma_3 K_1 - K_1 \int_0^\infty \langle |\boldsymbol{\zeta}|^2 \phi^T \rangle d\eta + \frac{1}{2} \int_0^\infty (2\eta + d_1) \langle (|\boldsymbol{\zeta}|^2 - \zeta_n^2) (|\boldsymbol{\zeta}|^2 - \frac{5}{2}) \phi^C \rangle d\eta + \frac{2}{15} \langle |\boldsymbol{\zeta}|^4 A F \rangle \right. \\ &\quad \left. + \frac{1}{2} \int_0^\infty \langle (|\boldsymbol{\zeta}|^2 - \zeta_n^2) \phi^C - |\boldsymbol{\zeta}|^2 A \phi^{T-} \rangle d\eta \right), \end{aligned} \quad (20)$$

TABLE 2. Dimensionless transport coefficients $\gamma_1 \sim \gamma_3$ and γ_6 (the data taken from [10]).

	definition	BGK	hard sphere		definition	BGK	hard sphere
γ_1	$\frac{2}{15} \langle \boldsymbol{\zeta} ^4 B \rangle$	1	1.270042427	γ_3	$\frac{2}{15} \langle \boldsymbol{\zeta} ^4 AB \rangle$	1	1.947906335
γ_2	$\frac{4}{15} \langle \boldsymbol{\zeta} ^4 A \rangle$	1	1.922284066	γ_6	$\frac{1}{15} \langle \boldsymbol{\zeta} ^4 (D_1 + \frac{3}{7} \boldsymbol{\zeta} ^2 D_2) B \rangle$	1	1.419423836

$$d_5 = 2d_3 + \frac{8}{5\gamma_2} \left(\int_0^\infty \langle |\boldsymbol{\zeta}|^2 A \phi^T \rangle d\eta - \frac{2}{15} \langle |\boldsymbol{\zeta}|^4 AF \rangle - \frac{1}{2} \int_0^\infty \langle (|\boldsymbol{\zeta}|^2 - \zeta_n^2) \phi^T - \frac{\partial \phi^T}{\partial \zeta_n} \rangle d\eta \right), \quad (21)$$

$$a_6 = a_4 + k_0 \frac{\gamma_3}{\gamma_1} - \frac{1}{\gamma_1} \int_0^\infty \eta \langle (|\boldsymbol{\zeta}|^2 - \zeta_n^2) (|\boldsymbol{\zeta}|^2 - \frac{5}{2}) \phi^S \rangle d\eta - \frac{1}{4\gamma_1} \int_0^\infty \langle |\boldsymbol{\zeta}|^2 (|\boldsymbol{\zeta}|^2 - \zeta_n^2) B \phi^C \rangle d\eta \\ + \frac{1}{4\gamma_1} \int_0^\infty \langle (|\boldsymbol{\zeta}|^2 - \zeta_n^2)^2 \phi^S - \frac{\partial \phi^C}{\partial \zeta_n} \rangle d\eta, \quad (22)$$

$$a_5 = -a_4 + a_6 - \frac{\gamma_3}{\gamma_1} k_0 + \frac{1}{\gamma_1} \int_0^\infty \eta \langle (|\boldsymbol{\zeta}|^2 - \zeta_n^2) (|\boldsymbol{\zeta}|^2 - \frac{5}{2}) \phi^S \rangle d\eta. \quad (23)$$

Here $\phi^T(\eta, \zeta_n, |\boldsymbol{\zeta}|)$, $\zeta_i \phi^S(\eta, \zeta_n, |\boldsymbol{\zeta}|)$, and $\zeta_i \phi^C(\eta, \zeta_n, |\boldsymbol{\zeta}|)$ ($\zeta_i = \zeta_i t_i$) are the solution of the classical temperature-jump, shear-slip, and thermal creep problems occurring at the first order of the Knudsen number, namely the solution of (12) for $\alpha = T, S,$ and C with

$$I^T = 0, \quad b_i^T = 0, \quad c^T = d_1, \quad g^T = \zeta_n A(|\boldsymbol{\zeta}|), \\ I^S = 0, \quad b_i^S = -k_0 t_i, \quad c^S = 0, \quad g^S = \zeta_n \zeta_i B(|\boldsymbol{\zeta}|), \\ I^C = 0, \quad b_i^C = -K_1 t_i, \quad c^C = 0, \quad g^C = \zeta_i A(|\boldsymbol{\zeta}|).$$

It should be mentioned that the coefficients b_1 and b_2 are given by definition [10] as

$$b_1 = -\frac{1}{4} \int_0^\infty \langle (|\boldsymbol{\zeta}|^2 - \zeta_n^2) \phi^S \rangle d\eta, \quad b_2 = -\frac{1}{2} \int_0^\infty \langle (|\boldsymbol{\zeta}|^2 - \zeta_n^2) \phi^C \rangle d\eta.$$

As explicitly indicated in the above equation, A, B, D_1, D_2 and F are isotropic functions of $\boldsymbol{\zeta}$, which are defined as the solution of the following linear integral equations:

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

and $\gamma_1 \sim \gamma_3$ and γ_6 are dimensionless transport coefficients, which are constants defined as their integral. The specific values of γ 's depend on the molecular model and are listed in Table 2.

We stress that the identities (14)–(23) are general and hold for various intermolecular potential models (the inverse-power law, Lennard-Jones, VHS [17], VSS [18], etc.) and boundary conditions.⁴ Moreover, they show that the complete data set of the slip and jump coefficients can be obtained, once we have the solutions of the three classical half-space problems ϕ^T , ϕ^S , and ϕ^C . Since the accurate numerical method to solve these problems [12, 13] has been established in the late 1980s, we have recomputed the problems using the same method. Then, from the identities (14)–(23), we obtain the complete data set of the slip and jump coefficients for a hard-sphere gas with diffuse reflection condition. The results are listed in Table 3. Accuracy of the data of K_1 and b_2 has been improved from those given in [9, 10] at the last decimal because of the recomputation with a refined grid. Incidentally, we have also confirmed that the data for the BGK model in Table 1 were recovered by the same procedure from the identities (14)–(23).

⁴ See [11, 16] for the class of the boundary conditions to which the symmetric relation can be applied. In addition, it should be noted that the scattering kernel is locally isotropic and that the accommodation coefficient is $O(1)$. These are basic assumptions that are made in Sone's theory of the present concern [9, 10]. For the boundary with accommodation coefficient of $O(\varepsilon)$, e.g., the (nearly) specular reflection boundary, the slip/jump condition is known to be qualitatively different. See, e.g., Y. Sone and K. Aoki, Phys. Fluids **20**, 571 (1977) and K. Aoki, T. Inamuro, and Y. Onishi, J. Phys. Soc. Jpn **47**, 663 (1979).

TABLE 3. Slip and jump coefficients for a hard-sphere gas on the diffuse reflection boundary.

first-order slip & jump		second-order slip			second-order jump				
k_0	-1.2540	a_1	0.9039	a_4	0.0330	d_3	0.4992	b_1	0.1068
K_1	-0.6465	a_2	0.6601	a_5	0.2336	d_4	0.0087	b_2	0.4782
d_1	2.4001	a_3	-0.2438	a_6	-1.9987	d_5	4.6181		

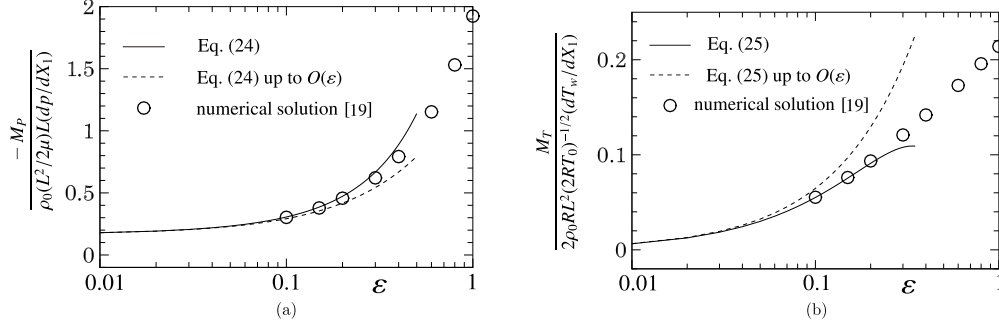


FIGURE 1. Mass flow rate per unit width in a straight channel. (a) Poiseuille flow, (b) thermal transpiration.

SIMPLE EXAMPLES

We show a few examples (see, e.g., [10]) for which the analytical solution is easily obtained by the slip flow theory.

Mass flow rate of the Poiseuille flow and thermal transpiration

Consider a slightly rarefied gas in a channel or tube. The flow that is induced by imposing a (small) uniform gradient of pressure along the channel or tube is called the Poiseuille or Hagen–Poiseuille flow, while the flow when a (small) uniform gradient of temperature is imposed along the channel or tube wall is called the thermal transpiration. The Poiseuille and Hagen–Poiseuille flows are commonly observed, while the thermal transpiration is specific to a rarefied gas. The X_1 -direction of the space coordinates X_i will be taken along the channel or tube. The quantity with subscript P and T denotes that for Poiseuille (or Hagen–Poiseuille) flow and thermal transpiration, respectively. The pressure and the wall temperature will be denoted by p and T_w , respectively.

First consider the case of a straight channel. Let L be the separation distance between the channel walls. Mass flow $(M, 0, 0)$ per unit time for unit spanwise width can be computed to yield [10, 19]

$$\frac{M_P}{\rho_0(L^2/2\mu)L(dp/dX_1)} = -\frac{1}{6} + k_0\epsilon - 2(a_1 - 2b_1)\epsilon^2, \quad (24)$$

$$\frac{M_T}{2\rho_0RL^2(2RT_0)^{-1/2}(dT_w/dX_1)} = -(K_1 + 2b_2\epsilon)\epsilon. \quad (25)$$

It should be noted that the expansion has been completed in the above expression (the third and higher order terms do not appear). However, the above should be recognized as the asymptotic solution and can be applied only for small ϵ . The results for a hard-sphere gas are plotted and compared with the direct numerical solution [19] in Fig. 1.

Next, consider the case of a straight tube with a circular cross-section. Let L be the radius of the tube. Mass flow $(M, 0, 0)$ per unit time can be computed [20] to yield

$$\frac{M_P}{\rho_0(\pi L^3/2\mu)L(dp/dX_1)} = -\frac{1}{4} + k_0\epsilon + (4b_1 - a_1 - \frac{a_2}{2})\epsilon^2 + \dots, \quad (26)$$

$$\frac{M_T}{2\rho_0R(\pi L^3)(2RT_0)^{-1/2}(dT_w/dX_1)} = -K_1\epsilon - (2b_2 - \frac{a_5}{2})\epsilon^2 + \dots. \quad (27)$$

The results for a hard-sphere gas are plotted and compared with the numerical solution [21] in Fig. 2.

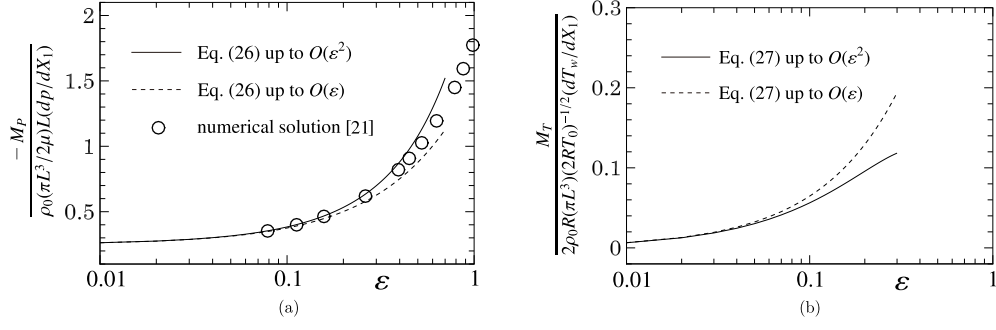


FIGURE 2. Mass flow rate in a straight tube with a circular cross-section. (a) Hagen–Poiseuille flow, (b) thermal transpiration.

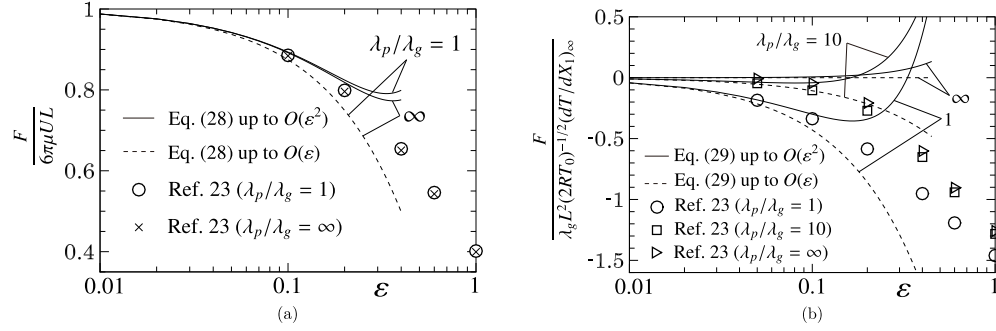


FIGURE 3. Forces acting on a spherical particle. (a) Drag force, (b) thermal force.

Drag and thermal forces acting on a spherical particle

Consider a spherical particle of radius L suspended in a slightly rarefied gas. The thermal conductivities of the particle and the gas will be denoted by λ_p and λ_g , respectively. The origin of the space coordinates X_i is the center of the sphere.

The drag force $(F, 0, 0)$ acting on the sphere in a slow uniform gas flow $(U, 0, 0)$ can be computed [10, 22] to yield

$$\frac{F}{6\pi\mu UL} = 1 + k_0\epsilon + \left(3k_0^2 - 3a_1 + 2a_3 + 2b_1 + \frac{8}{5} \frac{\text{Pr}K_1^2}{\lambda_p/\lambda_g + 2}\right)\epsilon^2 + \dots, \quad (28)$$

where μ is the viscosity, $\text{Pr}(= \gamma_1/\gamma_2)$ is the Prandtl number. This formula is taken from [10], but is simplified by using (14) and (18). The results for a hard-sphere gas are plotted and compared with the direct numerical solution [23] in Fig. 3(a).

When there is a small temperature gradient in the background gas, namely when the temperature of the gas in the absence of the sphere is given by $T_0 + (dT/dX_1)_\infty X_1$, the sphere is subjected to a force from the gas (the thermal force). The thermal force $(F, 0, 0)$ is computed [10, 22] to yield

$$\frac{F}{\lambda_g L^2 (2RT_0)^{-1/2} (dT/dX_1)_\infty} = \frac{48\pi}{5} \text{Pr} \left(\frac{K_1}{2 + \lambda_p/\lambda_g} \epsilon + \left(a_4 - \frac{C}{2 + \lambda_p/\lambda_g} \right) \epsilon^2 \right) + \dots, \quad (29a)$$

$$C = -b_2 - 3K_1 k_0 + 3a_4 - a_5 - a_6 + \frac{2K_1}{2 + \lambda_p/\lambda_g} \left(d_1 \frac{\lambda_p}{\lambda_g} - \frac{4}{5\gamma_2} \int_0^\infty H_B d\eta \right), \quad (29b)$$

$$\int_0^\infty H_B d\eta = 1.2765 \text{ (hard sphere)}, \quad 0.41556 \text{ (BGK)}. \quad (29c)$$

The results for a hard-sphere gas are plotted and compared with the direct numerical solution [23] in Fig. 3(b). When λ_p/λ_g is finite, the first term is dominant, and the thermal force is acting in the direction opposite to the imposed

gradient of temperature (the usual thermophoresis) because $K_1 < 0$. When λ_p/λ_g is very large or ideally infinite, only the $a_4\varepsilon^2$ remains in the parenthesis, and the thermal force is acting in the same direction as the temperature gradient (the negative thermophoresis [24, 14]) because $a_4 > 0$. Therefore, the direction of the thermophoresis may change depending on the material of the particle, though the negative thermophoresis has not been verified experimentally.

The reversal of the thermal force is due to the change of its physical mechanism. In the usual thermophoresis, the surface temperature of the sphere is nonuniform because of the finite thermal conductivity of the particle. The nonuniform surface temperature, then, induces the thermal creep flow and is subjected to the reaction from the gas. The first term of (29a) represents this effect. On the other hand, in the negative thermophoresis, the surface temperature is uniform because of the infinite thermal conductivity of the particle, thus the thermal creep effect is absent. Then, the higher-order effect of the thermal-stress slip is dominant, inducing a flow (thermal-stress slip flow) in the opposite to the thermal creep. Thus, the reaction from the gas is in the opposite direction to the case of the thermal creep effect.

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