

Slip-flow theory for thermo-osmosis based on a kinetic model with near-wall potential

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(Received 25 June 2025; revised 3 September 2025; accepted 16 October 2025; published 12 November 2025)

In this paper, thermal-slip coefficients in slip boundary conditions of the Stokes equation are derived using the generalized slip-flow theory, with special interest in the role of near-wall potential in micro- and nanoscale flows. As the model of fluids and fluid-solid interaction, we employ the model Boltzmann equation for dilute gases and the diffuse-reflection boundaries with near-wall potential, respectively. It is found that, when the mean free path of gas molecules and the effective range of potential are of the same order of magnitude, the thermal-slip boundary condition can be derived in the near-continuum limit. In the derived slip-flow theory, the thermal-slip coefficient and the boundary-layer corrections (i.e., Knudsen-layer corrections) are determined by solving the kinetic boundary-layer problems (i.e., Knudsen-layer problems) that include external-force terms and inhomogeneous terms both driven by the potential. As an application of the slip-flow theory, thermo-osmosis between two parallel plates with uniform temperature gradients is analyzed. The results of the slip-flow theory are validated by comparing them with those of the direct numerical analysis of the same problem. Furthermore, it is found that thermo-osmosis and thermal slip on the plates are significantly affected by the features of the near-wall potential; even the gas-flow direction can be reversed when the near-wall potential is repulsive. Such a flow reversal is qualitatively similar to thermo-osmosis in liquids reported in existing molecular dynamics simulation.

DOI: [10.1103/zpzj-ngrh](https://doi.org/10.1103/zpzj-ngrh)

I. INTRODUCTION

In conventional fluid mechanics based on the incompressible Navier-Stokes equations, the temperature field of a fluid is decoupled from the flow field. Therefore, the temperature variation of the fluid cannot induce fluid flows without the help of external forces such as temperature-dependent buoyancy forces. However, in micro- and nanoscale flows, the temperature variation of boundaries (i.e., channel walls) can induce fluid flows, which we call thermo-osmosis [1] or thermo-osmotic flows. Thermo-osmosis is induced mainly by surface effects and thus is practically significant in micro- and nanoscale confinements [2] where external body forces are negligible. [However, it should be remarked that, when being coupled with electric effects such as ionic motion, there may arise a thermally induced body force due to the variation of electric permittivity (see, e.g., Ref. [3]).] Thermo-osmosis is a conversion from heat to fluid motion

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and can be applied to various technologies. For instance, in the case of gases, where thermo-osmosis is often called thermal transpiration, thermally driven pumps without mechanically moving parts (the so-called Knudsen pump [4]) have been developed and prototypes have been put into practice using microfabrication techniques [5]. In the case of liquids, laser-heating-induced thermo-osmosis near a liquid-solid interface has been applied to the optothermal manipulation of nanomaterials [6].

From a macroscopic viewpoint, both for gases and liquids, thermo-osmosis can be regarded as a thermal-slip boundary condition of fluid-dynamic equations (e.g., the Stokes or Navier–Stokes equations), that is,

$$\mathbf{v} \cdot \mathbf{t} = -K_{\text{TS}} \mathbf{t} \cdot \nabla T \quad (\text{on boundaries}), \quad (1)$$

where $\mathbf{v}$ represents the flow velocity, $\mathbf{t}$ is a unit tangent on boundaries, K_{TS} is a thermal-slip coefficient, and ∇T is the temperature gradient of the fluid on the boundaries. The condition Eq. (1) is sometimes called thermo-osmotic slip [7–9]. The thermal-slip coefficient K_{TS} is usually negative in experiments, i.e., the flow is directed from cold to hot (see, e.g., Ref. [10] for gases and Refs. [2,9] for liquids). The concern in this paper is the derivation of Eq. (1) together with the determination of the thermal-slip coefficient K_{TS} , based on the molecular-scale description of fluids that includes interaction potential between fluid molecules and solid molecules.

Let us first take an overview of the current situation on the thermal-slip boundary condition [Eq. (1)] for gases. In the case of a gas, the ratio between the mean free path ℓ_0 of gas molecules and a reference length scale L_0 (e.g., the channel dimension) is defined as the Knudsen number ($\text{Kn} = \ell_0/L_0$), which represents the degree of gas rarefaction. When a gas is rarefied, i.e., Kn is not negligibly small, the gas is out of thermal equilibrium and a conventional fluid-mechanics framework becomes inapplicable; the Boltzmann equation based on the kinetic theory of gases must be employed [11,12]. However, in the regime of near-local thermal equilibrium where Kn is small, it is possible to use an asymptotic analysis of the Boltzmann equation (or its simplified models) to systematically derive fluid-dynamic equations and associated slip and jump boundary conditions that describe the gas behavior [12,13]. We refer to this framework as the generalized slip-flow theory in this paper. The thermal-slip boundary condition [Eq. (1)] can be obtained as one of the outcomes of the generalized slip-flow theory. A key significance of the generalized slip-flow theory is that, for a given set of intermolecular collision models and molecular scattering laws at boundaries, the thermal-slip coefficient K_{TS} can be determined by a systematic procedure. However, since the Boltzmann equation is formulated for dilute gases, the generalized slip-flow theory is not directly applicable to dense gases or liquids. Also note that thermally induced gas flows still occur for moderate or large Knudsen numbers. However, such flows lie outside the scope of fluid-dynamic equations and require an analysis based on the Boltzmann equation [11,12,14] (see also experimental results for straight channels [15,16]).

Regarding liquids, the derivation of the thermal-slip boundary condition [Eq. (1)] is more complicated due to the dense nature of the medium. A theoretical approach was proposed by Derjaguin *et al.* [1] using the linear-response theory, and, more recently, a microscopic theory of thermo-osmosis was presented [8,17,18]. However, to compute the thermal-slip coefficient K_{TS} , these theories require microscopic information such as excess enthalpy profiles near boundaries, which are difficult to measure in experiments. In this respect, the prediction of thermo-osmosis for liquids is more difficult than for gases, since the generalized slip-flow theory for gases uses the information that is experimentally accessible; for instance, the molecular scattering laws at solid surfaces can be measured using molecular-beam experiments [19]. Therefore, up to now, molecular dynamics (MD) simulation has been the primary practical tool for investigating thermo-osmosis in liquids, and MD simulations have been carried out for various systems such as Lennard-Jones (LJ) fluids [7,20–24], water [20,25], and aqueous electrolytes [26–28]. A remarkable trend observed in MD studies is that the direction of thermo-osmosis is reversible depending on hydrophilic properties at liquid-solid interfaces. To be more precise, the thermal-slip coefficient tends to be $K_{\text{TS}} < 0$ (or $K_{\text{TS}} > 0$) for hydrophilic (or hydrophobic) surfaces [20–24]. Since the hydrophilic

properties are strongly influenced by the interaction potential between fluid and solid molecules, the near-wall potential is considered to play a crucial role in thermo-osmosis. This paper therefore focuses on elucidating the impact of the near-wall interaction potential on the thermal-slip boundary condition [Eq. (1)]. (We also note that the sign reversal of thermo-osmosis was also discussed recently for a near-critical binary fluid mixture [29].) Now, the central question addressed here is how to obtain the thermal-slip coefficient K_{TS} under the effect of near-wall fluid-solid interactions.

The influence of the near-wall interaction potential on slip coefficients has been extensively investigated in the literature, with primary focus on the so-called shear slip. Here the shear slip is described by the boundary condition $\mathbf{v} \cdot \mathbf{t} \approx L_S \dot{\gamma}$, where L_S is the slip length and $\dot{\gamma}$ is the shear rate. For instance, using MD simulations (or in experiments), the effects on the slip length L_S caused by the shear-rate dependence [30] (or Ref. [31]), the wetting properties at liquid-solid interfaces [32] (or Refs. [33–36]), and the electrical charge distribution [37] (or Ref. [38]) have been reported. Various theoretical frameworks and models to predict L_S have also been elaborated: the results of equilibrium and/or nonequilibrium MD simulations were utilized to obtain L_S [39–42] and the modeling of molecular motion in a thin layer adjacent to solid surfaces was proposed [43–46] (see also the recent review article [47]). However, the effect of the near-wall potential on thermal slip has not yet been investigated using the existing theoretical frameworks mentioned above. In this paper, given that the generalized slip-flow theory has succeeded in obtaining slip coefficients for gases, we try to apply the generalized slip-flow theory to account for the effect of the near-wall potential on the thermal-slip coefficient. This serves as a primary step toward developing the model of thermal-slip boundary condition for both gases and liquids based on molecular-scale descriptions. (Note that the generalized slip-flow theory also provides shear-slip and temperature-jump coefficients as we will discuss later.) As a proof-of-concept study, we adopt a simplified physical setting using the Bhatnager-Gross-Krook (BGK) model [48,49] of the Boltzmann equation to describe the intermolecular interaction, along with diffuse reflection as the molecular scattering law at boundaries. The equation is supplemented by a force field representing a near-wall interaction potential. In particular, we focus on the case in which the bulk flow is not directly affected by the near-wall potential; only the thermal-slip boundary condition and the boundary-layer corrections are modified by the potential.

The paper is organized as follows. In Sec. II, we describe the physical setting and formulate the problem in detail. In Sec. III, we develop a slip-flow theory under near-wall interactions based on the generalized slip-flow theory. In Sec. IV, we apply the slip-flow theory to the problem of thermo-osmosis, which is a special case of the problem defined in Sec. II, and compare the results with the direct numerical analysis of the same problem. This allows us to validate the slip-flow theory and examine the effects of the near-wall potential on thermo-osmosis. In Sec. V, we provide a brief comparison with previous studies and highlight some key features of the present slip-flow theory. Finally, Sec. VI summarizes the main findings and provides future perspectives.

II. FORMULATION

A. Description of the problem

Let us consider an ideal monatomic gas contained between two parallel plates. Cartesian coordinates X_i ($i = 1, 2, 3$) are introduced such that the X_1 direction is perpendicular to the plates, as shown in Fig. 1(a). The plates are placed at $X_1 = \pm D/2$, where D is the distance between the plates. The volume average of the gas density is denoted by ρ_0 . Then, the mean free path of gas molecules at a reference equilibrium state with density ρ_0 and temperature T_0 is defined as ℓ_0 , where T_0 is the reference temperature of the plates. The Knudsen number Kn , which characterizes the degree of gas rarefaction, is defined by $\text{Kn} = \ell_0/D$.

The velocity and the temperature of the plates at $X_1 = \pm D/2$ are kept at $v_{wi}^\pm$ ($i = 1, 2, 3$) and $T_w^\pm$, respectively. The velocities of the plates are tangential to the surfaces, meaning that $v_{w1}^\pm = 0$, while

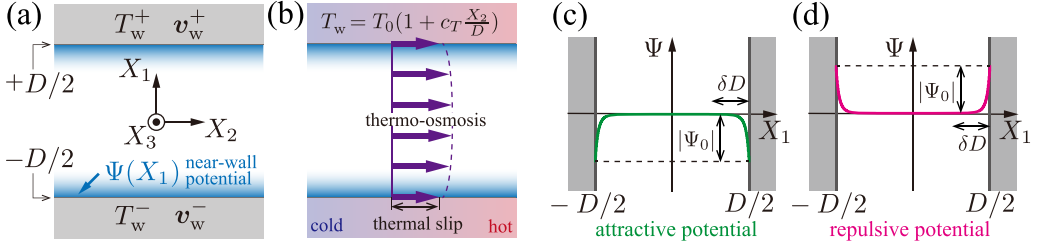


FIG. 1. Schematic of the problem. (a) General setting of the slip-flow theory (Sec. III). (b) Application of the slip-flow theory to the thermo-osmosis problem (Sec. IV). [(c) and (d)] Schematic examples of Ψ for (c) purely attractive and (d) purely repulsive potentials.

$v_{w2}^{\pm}$ and $v_{w3}^{\pm}$ are constants since the plates are rigid walls. The magnitude of the plate velocity $|v_{wi}^{\pm}|$ is small compared with the thermal speed $v_0 = \sqrt{2RT_0}$, where R is the specific gas constant, i.e.,

$$c_v^{\pm} = \frac{|v_{wi}^{\pm}|}{v_0} \ll 1. \quad (2)$$

The temperatures of the plates may vary with X_2 and X_3 , but the magnitude of the temperature gradient is assumed to be small, i.e.,

$$c_T^{\pm} = \frac{D}{T_0} \left| t_i \frac{\partial T_w^{\pm}}{\partial X_i} \right| \ll 1, \quad (3)$$

where t_i is a unit tangent on the plates. When the plates are stationary and have infinitesimal temperature gradients in the X_2 direction, that is,

$$|v_{wi}^{\pm}| = 0, \quad T_w^{\pm} = T_w(X_2) \equiv T_0 \left(1 + c_T \frac{X_2}{D} \right) \quad \left(c_T = \frac{D}{T_0} \frac{dT_w}{dX_2} \right), \quad (4)$$

($c_T \ll 1$), the problem is reduced to the fundamental setting of thermo-osmosis, as shown in Fig. 1(b). We will mainly analyze this thermo-osmosis setting later in Sec. IV, but Secs. II and III consider a more general case with $|v_{wi}^{\pm}| \neq 0$.

Gas molecules are subject to external forces per unit mass exerted by a potential field Ψ near the surfaces. The potential Ψ is assumed to depend only on X_1 , i.e., $\Psi = \Psi(X_1)$, and is symmetric with respect to $X_1 = 0$. The characteristic value of the potential (e.g., at the plates) is given by $\Psi_0 \equiv 2RT_0U$, where U is a dimensionless parameter of the order of unity. The potential decays to zero as the distance from the plate increases; the characteristic length of its effective range is denoted by δD with $\delta (\geq 0)$ a dimensionless parameter. For instance, two specific cases, the purely attractive and purely repulsive potentials, are shown in Figs. 1(c) and 1(d), respectively. These cases will be further discussed in Sec. IV.

We investigate the steady gas flow under the following assumptions. (i) The gas behavior is described by the BGK model of the Boltzmann equation [48,49]. (ii) Gas molecules undergo diffuse reflection [12] at the boundaries, i.e., at the surfaces of the plates. Specifically, molecules impinging on a boundary are reflected according to the half-range Maxwellian distribution with velocity $v_{wi}^{\pm}$ and temperature $T_w^{\pm}$ together with the condition that there is no net mass flux across the boundary. (iii) The magnitudes of the velocity and temperature gradient of the plates are small [see Eqs. (2) and (3)], allowing for linearization of the system around a local equilibrium state defined by setting $c_v^{\pm} = c_T^{\pm} = 0$. In the absence of interaction potential (that is, when $\delta = 0$ or $U = 0$), the problem is formally reduced to a classical two-surface problem of a rarefied gas. Therefore, without the potential, the slip-flow theory developed here becomes identical with the one described in the literature (e.g., Ref. [12]). In this study, we are interested in the effect of a finite interaction potential

characterized by $\delta(> 0)$, representing long-range fluid-solid interaction, in the fluid-dynamic limit ($\text{Kn} \ll 1$).

B. Basic equations

Let $f(X_i, \xi_i)$ denote the molecular velocity distribution function, where ξ_i is the molecular velocity vector; let $\rho(X_i)$, $v_i(X_i)$, and $T(X_i)$ denote the density, flow velocity, and temperature of the gas. Then the BGK model incorporating the effect of a potential is written as

$$\xi_i \frac{\partial f}{\partial X_i} - \frac{d\Psi}{dX_1} \frac{\partial f}{\partial \xi_1} = A_c \rho (f_e - f), \quad (5a)$$

$$f_e = \frac{\rho}{(2\pi RT)^{3/2}} \exp\left(-\frac{(\xi_i - v_i)^2}{2RT}\right), \quad (5b)$$

$$\begin{bmatrix} \rho \\ \rho v_i \\ 3\rho RT \end{bmatrix} = \int_{\text{all } \xi_i} \begin{bmatrix} 1 \\ \xi_i \\ (\xi_i - v_i)^2 \end{bmatrix} f \, d\xi, \quad (5c)$$

where A_c is a constant such that $A_c \rho$ represents the collision frequency and $d\xi$ is a short-hand notation of $d\xi_1 d\xi_2 d\xi_3$. Note that in this model, f is coupled with ρ , v_i , and T through Eqs. (5b) and (5c), while Ψ and A_c are prescribed. The relations between f and v_i and T are nonlinear. The reference density ρ_0 and the reference equilibrium distribution f_0 are expressed as $\rho_0 = (1/D) \int_{-D/2}^{D/2} \rho(X_1) dX_1$ and $f_0 = \rho_0 (2\pi RT_0)^{-3/2} \exp(-\xi_i^2/(2RT_0))$, respectively. The potential $\Psi(X_1)$ has a characteristic value of $\Psi_0 (= 2RT_0 U)$ near the plates and decays to zero as the distance from the plates increases. The full detail of Ψ will be specified [cf. Eq. (21)] in the analysis in Sec. IV.

The diffuse-reflection boundary condition [12] is given by

$$f = \frac{\sigma_{w\pm}}{(2\pi RT_w^\pm)^{3/2}} \exp\left(-\frac{(\xi_i - v_{wi}^\pm)^2}{2RT_w^\pm}\right) \quad \left(X_1 = \pm \frac{D}{2}, \xi_1 \leq 0\right), \quad (6a)$$

with

$$\sigma_{w\pm} = \pm \left(\frac{2\pi}{RT_w^\pm}\right)^{1/2} \int_{\xi_1 \geq 0} \xi_1 f \, d\xi. \quad (6b)$$

Here σ_{w+} and σ_{w-} are the quantities determined by f via Eq. (6b), which ensures that there are no net mass fluxes across the boundaries (the impermeability condition), i.e., $\int \xi_1 f d\xi = 0$ at $X_1 = \pm D/2$ [12]. It should be remarked that the kinetic boundary condition, Eq. (6), is defined for reflected molecules, i.e., $\xi_1 < 0$ at $X_1 = D/2$ or $\xi_1 > 0$ at $X_1 = -D/2$, and that no condition is imposed for the molecules arriving at the walls. Other macroscopic quantities, such as the pressure, stress tensor, and heat flux of the gas, are defined as

$$\begin{bmatrix} p \\ p_{ij} \\ q_i \end{bmatrix} = \int_{\text{all } \xi_i} \begin{bmatrix} \frac{1}{3}(\xi_i - v_i)^2 \\ (\xi_i - v_i)(\xi_j - v_j) \\ \frac{1}{2}(\xi_i - v_i)(\xi_j - v_j)^2 \end{bmatrix} f \, d\xi. \quad (7)$$

C. Linearized problem

The smallness assumption [Eqs. (2) and (3)] allows us to linearize the problem described by Eqs. (5) and (6). First, let us consider the case where $c_v^\pm = c_T^\pm = 0$ while the potential remains nonzero. In this case, the solution to Eqs. (5) and (6) is given by the local equilibrium $f = f_0^*$,

where

$$f_0^*(X_1, \xi_i) = \frac{\rho_0^*(X_1)}{(2\pi RT_0)^{3/2}} \exp\left(-\frac{\xi_i^2}{2RT_0}\right) \left(= \frac{\rho_0^*}{\rho_0} f_0\right), \quad (8a)$$

$$\rho_0^*(X_1) = \frac{\exp(-\Psi(X_1)/RT_0)}{\bar{\Psi}} \rho_0, \quad (8b)$$

$$\bar{\Psi} = \frac{1}{D} \int_{-D/2}^{D/2} \exp\left(-\frac{\Psi(X_1)}{RT_0}\right) dX_1. \quad (8c)$$

In the following, we consider the perturbation from the local Maxwellian distribution f_0^* . To this end, we first introduce dimensionless quantities as

$$\begin{aligned} x_i &= X_i/D, \quad \zeta_i = \xi_i/v_0, \quad \phi = f/f_0^* - 1, \quad \psi_\delta = \Psi/(2RT_0U), \\ \tau_w^\pm &= T_w^\pm/T_0 - 1, \quad u_{wi}^\pm = v_{wi}^\pm/v_0, \quad \omega = \rho/\rho_0^* - 1, \quad u_i = v_i/v_0, \\ \tau &= T/T_0 - 1, \quad P = p/p_0 - 1, \quad P_{ij} = p_{ij}/p_0 - \delta_{ij}, \quad Q_i = q_i/(p_0 v_0), \end{aligned} \quad (9)$$

where $p_0 = \rho_0 RT_0$ denotes the reference pressure, $v_0 = \sqrt{2RT_0}$ is taken as the reference speed, and the subscript δ of ψ_δ explicitly indicates that the (dimensionless) potential includes the parameter δ . Substituting Eq. (9) into Eqs. (5) and (6) and neglecting the higher-order terms of perturbation, i.e., $\phi, \omega, u_i, \tau, u_{wi}^\pm$, we obtain the following linearized BGK equation:

$$\zeta_i \frac{\partial \phi}{\partial x_i} - U \frac{d\psi_\delta}{dx_1} \frac{\partial \phi}{\partial \zeta_1} = \frac{\alpha}{k} (\phi_e - \phi), \quad (10a)$$

$$\phi_e = \omega + 2\zeta_i u_i + \left(\zeta^2 - \frac{3}{2}\right) \tau, \quad (10b)$$

$$\begin{bmatrix} \omega \\ u_i \\ \tau \end{bmatrix} = \int_{\mathbb{R}^3} \begin{bmatrix} 1 \\ \zeta_i \\ \frac{2}{3}(\zeta^2 - \frac{3}{2}) \end{bmatrix} \phi E \, d\boldsymbol{\zeta}, \quad (10c)$$

$$k = \frac{\sqrt{\pi}}{2} \text{Kn}, \quad \text{Kn} = \frac{\ell_0}{D}, \quad \ell_0 = \frac{2}{\sqrt{\pi}} \frac{v_0}{A_c \rho_0}, \quad (10d)$$

where $E = \pi^{-1/2} \exp(-\zeta^2)$, $\zeta = |\zeta_i| = (\zeta_j^2)^{1/2}$, and $d\boldsymbol{\zeta}$ is a short-hand notation of $d\zeta_1 d\zeta_2 d\zeta_3$. The auxiliary functions associated with the potential are given by

$$\alpha = \frac{\exp(-2U\psi_\delta)}{\bar{\psi}_\delta} \left(\bar{\psi}_\delta = \int_{-1/2}^{1/2} \exp(-2U\psi_\delta(x_1)) \, dx_1 \right). \quad (11)$$

Here α represents the dimensionless reference density corresponding to Eq. (8b). Once the functional form of the potential ψ_δ is specified, Eq. (10) forms a system of equations for unknown functions ϕ, ω, u_i , and τ , while U, α , and k are external parameters. In the following, we use k in place of Kn [see Eq. (10d)] for notational simplicity. The usual BGK model is formally recovered by setting $U = 0$ and $\alpha = 1$. The boundary condition is linearized in the same manner as

$$\phi = \phi_w^\pm \left(x_1 = \pm \frac{1}{2}, \quad \zeta_1 \leq 0 \right), \quad (12a)$$

with

$$\phi_w^\pm = 2\zeta_i u_{wi}^\pm + (\zeta^2 - 2)\tau_w^\pm \pm 2\sqrt{\pi} \int_{\zeta_1 \geq 0} \zeta_1 \phi E \, d\boldsymbol{\zeta}. \quad (12b)$$

The $\phi_w^\pm$ are functions of ζ_i , in which $u_{wi}^\pm$ and $\tau_w^\pm$ are prescribed. Note that $\phi_w^\pm$ depends on ϕ through the integral on the right-hand side (i.e., the last term). The other (dimensionless) macroscopic

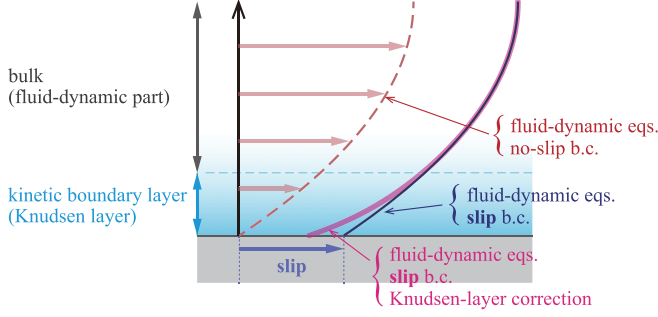


FIG. 2. Schematics of the slip-flow theory. As an illustrative example, a parallel flow near a stationary boundary is considered. The entire region is described by the fluid-dynamic equations with no-slip boundary conditions (red). Near the boundary, the Knudsen layer plays two roles: (i) the slip boundary condition modifies the fluid-dynamic part (blue) and (ii) the Knudsen-layer correction modifies the macroscopic quantities near the boundary. The Knudsen-layer correction rapidly decays as the distance from the boundary increases.

quantities are defined as

$$P = \omega + \tau, \quad P_{ij} = 2 \int_{\mathbb{R}^3} \zeta_i \zeta_j \phi E \, d\zeta, \quad Q_i = \int_{\mathbb{R}^3} \zeta_i \zeta^2 \phi E \, d\zeta - \frac{5}{2} u_i. \quad (13)$$

In the following, we analyze Eqs. (10)–(12) based on the generalized slip-flow theory, presented in Sec. III, to obtain the slip and jump coefficients in the presence of the near-wall potential Ψ (or ψ_δ) of the plates. Then, in Sec. IV, we compare the slip-flow theory with the direct numerical analysis of Eqs. (10)–(12) for the thermo-osmosis problem.

III. SLIP-FLOW THEORY WITH NEAR-WALL POTENTIAL

A. Assumptions

Hereafter, we assume $k \ll 1$ and apply the generalized slip-flow theory to investigate the gas behavior. In this framework, the whole gas domain is decomposed into the bulk region and the kinetic boundary layer adjacent to the boundary (i.e., the Knudsen layer). The schematics of the bulk and the Knudsen layer are shown in Fig. 2. In short, using the generalized slip-flow theory, the fluid-dynamic part in the entire region, i.e., the bulk and the Knudsen layer, will be described by the fluid-dynamic equations of the macroscopic quantities (e.g., the Stokes equation); the boundary-layer analysis (i.e., the Knudsen-layer analysis) provides appropriate slip and jump boundary conditions for the fluid-dynamic equations, along with corrections that are significant only in the boundary layer.

We further assume that the range of interaction, δ , is as small as the Knudsen number k , meaning we consider the scaling

$$\chi \equiv \delta/k = O(1), \quad k \ll 1. \quad (14)$$

The validity of this scaling assumption Eq. (14) will be examined later in Sec. IV E 4. Under the scaling Eq. (14), we perform an asymptotic analysis based on a power-series expansion in k , with particular attention to the differences between the cases with and without the near-wall potential ψ_δ . In Eq. (10a), these differences appear in the terms $U(d\psi_\delta/dx_1)(\partial\phi/\partial\zeta_1)$ and $\alpha(\neq 1)$. However, under the assumption Eq. (14), these differences are only significant within the boundary layer, which has a length scale of k . Consequently, we neglect these terms in the analysis of fluid-dynamic part, while retaining them as inhomogeneous terms in the Knudsen-layer analysis. In this way, the fluid-dynamic part remains unchanged from the generalized slip-flow theory without the near-wall potential. However, the scaling Eq. (14) suggests that the range of the potential (e.g., the molecular

size) is of the same order as the mean free path, implying that the effect of finite volume fraction should become relevant. In this study, we neglect finite-volume effects to focus on the influence of the near-wall potential.

When χ is small, say, $\chi = O(k)$ [or equivalently $\delta = O(k^2)$], a different situation arises: The range of the potential is localized within an inner layer that is thinner than the Knudsen layer. In this case, the kinetic boundary condition can be derived [50] by analyzing the inner layer problem, where gas molecules interact with solid molecules through attractive-repulsive potential. The inner layer problem was further mathematically justified [51].

B. Main results

We describe only the main results here, leaving the details and the derivation in Supplemental Material S1 [52].

The macroscopic quantities h ($h = \omega, u_i, \tau$, etc.) are decomposed as

$$h = h_G + h_K. \quad (15)$$

Here h_G , referred to as the Hilbert part hereafter, describes the overall gas behavior throughout the gas region, while h_K , referred to as the Knudsen-layer correction, corresponds to the corrections to the Hilbert part required near the plate surfaces. The Hilbert part h_G is moderately varying, i.e., $\partial h_G / \partial x_i = O(h_G)$. On the other hand, h_K varies in the scale of the Knudsen number (or the mean free path) in the direction normal to the boundary and decays fast as the distance from the plates increases.

The results of the slip-flow theory are summarized as follows. First, neglecting the terms of $O(k^2)$, the Hilbert part is governed by the following fluid-dynamic equations:

$$\frac{\partial u_{iG}}{\partial x_i} = 0 \quad (\text{the equation of continuity}), \quad (16a)$$

$$\frac{\partial P_G}{\partial x_i} = k \frac{\partial^2 u_{iG}}{\partial x_j^2} \quad (\text{the Stokes equation}), \quad (16b)$$

$$\frac{\partial^2 \tau_G}{\partial x_j^2} = 0 \quad (\text{the heat equation}), \quad (16c)$$

$$\omega_G = P_G - \tau_G \quad (\text{the equation of state}), \quad (16d)$$

where the dimensionless viscosity in Eq. (16b) is reduced to k in the case of the BGK model. The system is supplemented by the slip and jump boundary conditions

$$(u_{iG} - u_{wi}^\pm) t_i = \mp k b_1^{(1)} t_i \frac{\partial u_{iG}}{\partial x_1} + k b_2^{(1)} t_i \frac{\partial \tau_G}{\partial x_i} \quad \left(x_1 = \pm \frac{1}{2} \right) \quad (\text{slip boundary condition}), \quad (17a)$$

$$\tau_G - \tau_w^\pm = \mp k c_1^{(0)} \frac{\partial \tau_G}{\partial x_1} \quad \left(x_1 = \pm \frac{1}{2} \right) \quad (\text{jump boundary condition}), \quad (17b)$$

and the impermeability condition

$$u_{1G} = 0 \quad (x_1 = \pm \frac{1}{2}). \quad (17c)$$

Here t_i denotes the unit tangent vector on the boundaries and $b_1^{(1)}$, $b_2^{(1)}$, and $c_1^{(0)}$ represent the shear-slip, thermal-slip, and temperature-jump coefficients, respectively. Notations for these constants follow those of Ref. [13]. The slip and jump coefficients are predefined constants that depend on the intermolecular collision model, the molecular scattering law at the boundaries, and the near-wall potential, and can be obtained by solving the Knudsen-layer problems summarized in Appendix [Eqs. (A1), (A2), and (A3)]. These problems are formulated as boundary-value problems for linearized BGK-type equations with external forces, and the derivation of the problems is fully described in Supplemental Material S1 B [52]. Because the potential considered here is symmetric

about the channel center ($x_1 = 0$), the coefficients $b_1^{(1)}$, $b_2^{(1)}$, and $c_1^{(0)}$ take identical values at both boundaries $x_1 = \pm 1/2$. The expressions for the stress tensor and the heat flux are given in Supplemental Material S1 A [52].

Next, we describe the Knudsen-layer corrections h_K . We introduce a stretched coordinate in the Knudsen layer near the plate at $x_1 = 1/2$ as

$$\eta = \frac{1/2 - x_1}{k}. \quad (18)$$

Then, the potential near the plate in the stretched coordinate is denoted by $\tilde{\psi}_\chi(\eta)$, where the subscript χ indicates explicitly that the potential includes the parameter χ [Eq. (14)]. The overall potential ψ_δ is divided as $\psi_\delta = \psi_\delta^+ + \psi_\delta^-$, where $\psi_\delta^\pm(x_1)$ represents the potential by the plate at $x_1 = \pm 1/2$. We define $\tilde{\psi}_\chi(\eta) = \psi_\delta^+(x_1)$, that is, the contribution from ψ_δ^- is discarded in $\tilde{\psi}_\chi(\eta)$ since the potentials are assumed to be localized near the plates at $x_1 = \pm 1/2$. The description of the region $x_1 \geq 0$ is sufficient due to the symmetry with respect to $x_1 = 0$, and the effect of the potential ψ_δ^- is negligible in this region. Then, the Knudsen-layer corrections near the plate $x_1 = 1/2$ are given as

$$u_{iK}t_i = -kY_1^{(1)}(\eta)t_i \frac{\partial u_{iG}}{\partial x_1} \Big|_{x_1=1/2} + kY_2^{(1)}(\eta)t_i \frac{\partial \tau_G}{\partial x_i} \Big|_{x_1=1/2}, \quad (19a)$$

$$u_{1K} = 0, \quad (19b)$$

$$\tau_K = -k\Theta_1^{(0)}(\eta) \frac{\partial \tau_G}{\partial x_1} \Big|_{x_1=1/2}, \quad (19c)$$

$$\omega_K = 2U\tilde{\psi}_\chi(\eta)\tau_G|_{x_1=1/2} - k\Omega_1^{(0)}(\eta) \frac{\partial \tau_G}{\partial x_1} \Big|_{x_1=1/2}, \quad (19d)$$

$$P_K = \omega_K + \tau_K, \quad (19e)$$

where $h_K = h_K(\eta, x_2, x_3)$ with $h_K = u_{iK}, \tau_K, \omega_K$, and P_K . The functions $Y_1^{(1)}(\eta)$, $Y_2^{(1)}(\eta)$, $\Omega_1^{(0)}(\eta)$, and $\Theta_1^{(0)}(\eta)$ represent the so-called Knudsen-layer functions. These Knudsen-layer functions are predefined functions determined alongside the slip and jump coefficients $b_1^{(1)}$, $b_2^{(1)}$, and $c_1^{(0)}$ by solving the Knudsen-layer problems. Note that $Y_1^{(1)}(\eta)$, $Y_2^{(1)}(\eta)$, $\Omega_1^{(0)}(\eta)$, and $\Theta_1^{(0)}(\eta)$ all decays as $\eta \rightarrow \infty$, as we will see later in Sec. IV E 3 for $Y_2^{(1)}(\eta)$.

The strategy of the flow-behavior analysis is as follows. (i) First, we solve the Knudsen-layer problems [Eqs. (A1), (A2), and (A3)]. This process is done numerically in principle, but the recipe has been presented in the literature [53]. Note that the Knudsen-layer problems does not include k as the physical parameter. (ii) Second, under the specific setting of boundary values $u_{wi}^\pm$ and $\tau_w^\pm$, we solve the fluid-dynamic equations Eq. (16) with the slip and jump boundary conditions Eq. (17) to obtain the Hilbert part. This process can be done either analytically or numerically, depending on the situations. In any case, the cost for solving the fluid-dynamics equations is expected to be much smaller than that for solving the original system Eqs. (10)–(12). (iii) Finally, we add the Knudsen-layer corrections Eq. (19) to the Hilbert part. If the flow behavior in the bulk is only interested, then the process (iii) may be omitted. In this paper, we will discuss the flow field near the boundary and include the Knudsen-layer corrections as we will see in Sec. IV.

We leave a couple of remarks as follows. (i) We consider the expansion up to the first-order in k and neglect the contributions of $O(k^2)$ in this paper. However, it is possible to extend the generalized slip-flow theory to incorporate higher-order effects, including the effects of curved surfaces [12]. (ii) The analysis presented so far is also applicable to the Boltzmann equation [12]. In this study, we have adopted the BGK model for simplicity, as it enables us to understand the framework of the generalized slip-flow theory more easily. A known limitation of the BGK model, however, is that it fixes the Prandtl number of the gas to unity. This drawback can be amended by

employing more sophisticated (but complex) models, such as the ellipsoidal-statistical model [54] or the Shakhov model [55]. The framework developed in the present paper is expected to be extendable to these models in a straightforward manner.

IV. ANALYSIS OF THERMO-OSMOSIS PROBLEM

In this section, we investigate the thermo-osmosis problem as defined by Eq. (4) and illustrated in Fig. 1(b). To analyze this problem, we employ two approaches: (i) the slip-flow theory developed in Sec. III and (ii) direct numerical analysis. We then compare both results for small Kn (or k) to validate the slip-flow theory. Note that the approach (i) provides an explicit analytical solution, although the numerical value of the thermal-slip coefficient [i.e., $b_2^{(1)}$], which is problem-independent, must be determined numerically.

A. Detailed setting

First, we set the boundary parameters as

$$v_{wi}^\pm = 0, \quad \tau_w^\pm = \tau_w \equiv c_T x_2 \quad (20)$$

[see Eq. (4)]. To obtain the flow field, the potential $\Psi(X_1)$ must be specified. We use the following pseudo-Sutherland-type potential [see Figs. 1(c) and 1(d)]:

$$\Psi = \Psi^+ + \Psi^-,$$

$$\Psi^\pm(X_1) = -\Psi_0 \left(\frac{\delta D}{\pm(1/2 + \delta)D - X_1} \right)^6, \quad (21)$$

where Ψ^+ and Ψ^- represent the potentials near the plates located at $X_1 = D/2$ and $-D/2$, respectively, and $\Psi_0 = 2RT_0U$. When U is positive (or negative), the potential is purely attractive (or repulsive). Physically, an attractive potential with the power r_0^{-6} , where r_0 is the distance from the wall, corresponds to the van der Waals interaction potential [56]. The interaction parameter δ determines the effective range of the potential and is assumed to be small. The corresponding dimensionless potential shape, $\psi_\delta(x_1)$, and its corresponding form in the Knudsen-layer analysis, $\tilde{\psi}_\chi(\eta)$, are given by

$$\psi_\delta = \psi_\delta^+ + \psi_\delta^-, \quad \psi_\delta^\pm(x_1) = -\left(\frac{\delta}{\pm(1/2 + \delta) - x_1} \right)^6,$$

$$\frac{d\psi_\delta}{dx_1} = \frac{6}{1/2 + \delta - x_1} \psi_\delta^+ + \frac{6}{-(1/2 + \delta) - x_1} \psi_\delta^-, \quad (22a)$$

$$\tilde{\psi}_\chi(\eta) = -\left(\frac{\chi}{\chi + \eta} \right)^6, \quad \frac{d\tilde{\psi}_\chi}{d\eta} = -\frac{6}{\chi + \eta} \tilde{\psi}_\chi. \quad (22b)$$

Note that $\tilde{\psi}_\chi$ depends on χ rather than δ [see Eq. (22b)].

The profiles of $U\psi_\delta(x_1)$ for $\delta = 0.01$ and $U = \pm 1$ are presented in Fig. 3(a). As shown in the figure, the effective range of the potential is restricted in the region $x_1 \in [1/2 - \delta, 1/2]$. The reference density α [Eq. (11)] for these cases are shown in Fig. 3(b). For the attractive (or repulsive) potential, the reference density increases (or decreases) near the plate at $x_1 = 1/2$. The bulk density is obtained as $\alpha \approx \bar{\psi}_\delta^{-1}$, with $\bar{\psi}_\delta \approx 1.014$ and 0.995 for $U = 1$ and $U = -1$, respectively.

B. Similarity solution

Since the unknown function ϕ depends on $(x_1, x_2, \zeta_1, \zeta_2, \zeta_3)$, the analysis of the problem requires substantial computational resources due to the high dimensionality. A useful approach to simplifying the problem is to introduce a similarity solution [12]. Based on the similarity solution for the

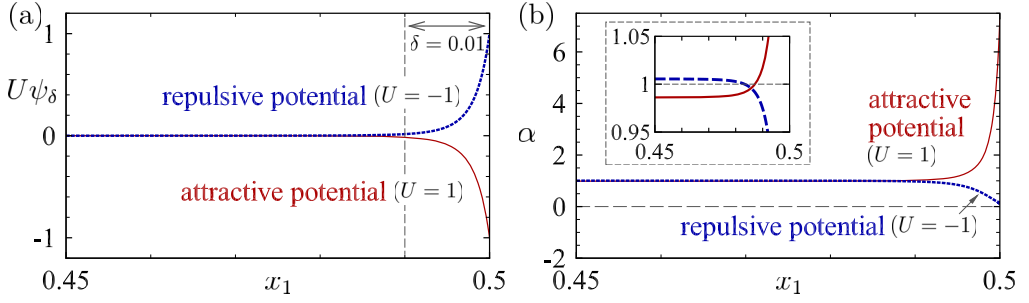


FIG. 3. (a) Dimensionless potential $U\psi_\delta(x_1)$ [Eq. (22a)] for $\delta = 0.01$ near the plate at $x_1 = 1/2$. The cases of $U = 1$ and $U = -1$ are shown by red solid and blue dashed curves, respectively. (b) Corresponding reference density profile α [Eq. (11)], where the inset shows the magnification near $\alpha = 1$.

thermal transpiration [53], the following form of the similarity solution can be applied:

$$\phi = c_T \left[\left(\zeta^2 - \frac{5}{2} \right) x_2 + 2U\psi_\delta(x_1)x_2 + \zeta_2\phi_T(x_1, \zeta_1, \zeta_\rho) \right], \quad \zeta_\rho = (\zeta_2^2 + \zeta_3^2)^{1/2}. \quad (23)$$

Without any approximation, this form is compatible with Eqs. (10)–(12) in the presence of the potential, where ϕ_T is an alternative unknown function that depends only on $(x_1, \zeta_1, \zeta_\rho)$. The macroscopic quantities are then expressed as

$$\frac{u_2}{c_T} = u_T(x_1), \quad u_1 = u_3 = 0, \quad (24a)$$

$$\frac{\omega}{c_T} = -[1 - 2U\psi_\delta(x_1)]x_2, \quad \frac{\tau}{c_T} = x_2, \quad \frac{P}{c_T} = 2U\psi_\delta(x_1)x_2. \quad (24b)$$

The functions $\phi_T(x_1, \zeta_1, \zeta_\rho)$ and $u_T(x_1)$ remain unknowns. Therefore, we are mainly interested in obtaining the flow field u_T in the following. Here, it should be noted that temperature perturbation, τ , is uniform in x_1 and linearly depends on x_2 , being identical to the temperature variation of the wall ($\tau = \tau_w$). Physically, this means that the effect of flow on the temperature profile is negligible and pure thermal conduction is dominant.

C. Approach (i): The slip-flow theory

Under the condition (20), the heat equation with Eq. (17b) yields $\tau_G = c_T x_2$. Then the thermal-slip boundary condition turns out to be

$$u_{2G} = b_2^{(1)} \frac{\partial \tau_G}{\partial x_2} = c_T b_2^{(1)}, \quad u_{1G} = u_{3G} = 0, \quad \left(x_1 = \pm \frac{1}{2} \right). \quad (25)$$

The Stokes equation with the thermal-slip boundary condition [Eq. (17a)] then gives the solution $u_{2G} = c_T b_2^{(1)}$, $u_{1G} = u_{3G} = 0$, $P_G = \text{const}$, indicating that thermo-osmosis is a plug flow. The additive constant in P_G should be zero because of Eq. (24b). The equation of states leads to $\omega_G = -c_T x_2$. All of these are for the Hilbert part. Because of the symmetry at $x_1 = 0$, we consider only the region $0 \leq x_1 \leq 1/2$ hereafter. Then, using the results of Hilbert part, we can immediately compute the Knudsen-layer corrections Eq. (19) for $0 \leq x_1 \leq 1/2$: $\tau_K = 0$, $\omega_K = P_K = 2U\psi_\chi(\eta)c_T x_2$, $u_{1K} = u_{3K} = 0$, $u_{2K} = kY_2^{(1)}(\eta)$ with $\eta = (1/2 - x_1)/k$.

Summarizing these results, the nontrivial flow fields are given by

$$\frac{u_2}{c_T} = u_T = k \left[b_2^{(1)} + Y_2^{(1)} \left(\frac{1}{k} \left(\frac{1}{2} - x_1 \right) \right) \right] + O(k^2). \quad (26)$$

Since $b_2^{(1)}$ and $Y_2^{(1)}$ have been numerically obtained by solving Eq. (A1) (see Supplemental Material S3 A [52] for the detail of numerical analysis), Eq. (26) provides an explicit form of the approximate solution to the thermo-osmosis problem [Eqs. (10)–(12), (20), and (22a)] for small k . Note that Eq. (26) is uniform (i.e., pluglike) if the Knudsen-layer correction $Y_2^{(1)}$, describing spatial variations near the walls, is neglected.

It should be remarked that the forms of u_1 , u_3 , ω , τ , and P described above are consistent with those in Eq. (24), up to the first order in k .

D. Approach (ii): The numerical analysis

We solve the thermo-osmosis problem [Eqs. (10)–(12), (20), and (22a)] numerically by applying the similarity solution ϕ_T [Eq. (23)]. By substituting Eq. (23) into the BGK equations [Eqs. (10)–(12)], it turns out that the similarity solution ϕ_T solves the following boundary-value problem:

$$\zeta_1 \frac{\partial \phi_T}{\partial x_1} - U \frac{d\psi_\delta}{dx_1} \frac{\partial \phi_T}{\partial \zeta_1} = \frac{\alpha}{k} (2u_T - \phi_T) - \left(\zeta_1^2 + \zeta_\rho^2 - \frac{5}{2} \right) - 2U \psi_\delta, \quad (27a)$$

$$u_T = \frac{1}{2} \int_{\mathbb{R}^3} \zeta_\rho^2 \phi_T E \, d\zeta, \quad (27b)$$

$$\phi_T = 0 \quad \left(x_1 = \pm \frac{1}{2}, \zeta_1 \leq 0 \right), \quad (27c)$$

where Eq. (27) includes the Knudsen number k as a physical parameter. The detail of the numerical analysis is given in Supplemental Material S3 B [52].

Let us denote by $b_{2,\text{num}}^{(1)}$ the thermal-slip coefficient $b_2^{(1)}$ estimated from the result of numerical analysis. Recalling Eq. (26), we can set $b_{2,\text{num}}^{(1)}$ as

$$b_{2,\text{num}}^{(1)} = \frac{u_2|_{x_1=0}}{k c_T} + O(k) \quad \text{as } k \rightarrow 0. \quad (28)$$

Note that u_2 in Eq. (28) is evaluated at $x_1 = 0$ (i.e., the channel center) at which the Knudsen-layer function $Y_2^{(1)}$ vanishes. By comparing $b_2^{(1)}$ obtained from the Knudsen-layer problem [Eq. (A1)] and $b_{2,\text{num}}^{(1)}$ obtained from Eq. (28), we can assess the validity of the slip-flow theory developed in Sec. III.

E. Results of thermo-osmosis problem

Numerical method used in the subsequent results is summarized in Supplemental Material S3 [52]. In particular, numerical parameters, including the number of lattice points, are presented in Supplemental Material S3 C [52]. Although the velocity distribution functions in the present problem are known to exhibit discontinuities in the (x_1, ζ_1) space (see, e.g., the similar case for convex boundaries [57]), the present scheme naively neglects the discontinuity. To compensate, we use a relatively large number of lattice points and assess the accuracy in Supplemental Material S3 D [52]. For highly accurate numerical analysis, however, the discontinuities should be treated properly, e.g., using a hybrid scheme [58] or the method of characteristics [59].

1. Comparison of the thermal-slip coefficients between the slip-flow theory and the numerical analysis

In this section, we compare the thermal-slip coefficient $b_2^{(1)}$ and $b_{2,\text{num}}^{(1)}$ for representative cases of attractive ($U = 1$) and repulsive ($U = -1$) potentials with various values of $\chi (= \delta/k)$ that characterizes the effective range of the potential. Recall that we are interested in developing a slip-flow theory for small k and thus we choose $k \leq 0.05$ below. Recall also that the value of χ is assumed to be $O(1)$ quantity by the assumption Eq. (14).

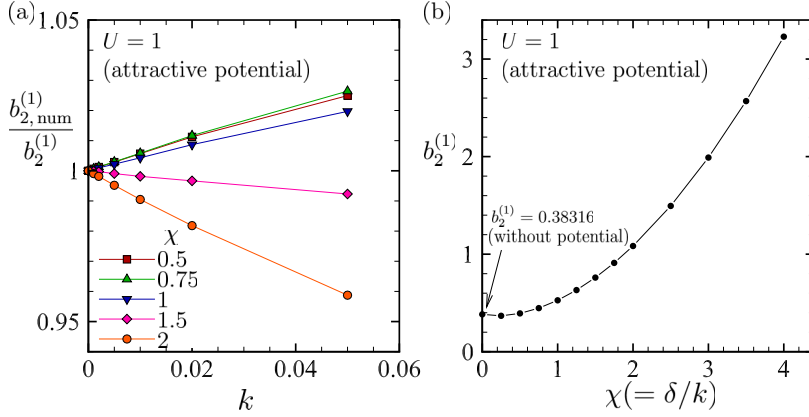


FIG. 4. Thermal-slip coefficients for attractive potential $U = 1$. (a) The ratio $b_{2,\text{num}}^{(1)}/b_2^{(1)}$ between the thermal-slip coefficient obtained by the numerical analysis $b_{2,\text{num}}^{(1)}$ and that by the slip-flow theory $b_2^{(1)}$. (b) The thermal-slip coefficient $b_2^{(1)}$ as a function of the range of the potential χ .

First, let us consider the case of $U = 1$ (attractive potential). For a fixed $\chi > 0$, Fig. 4(a) shows that the ratio $b_{2,\text{num}}^{(1)}/b_2^{(1)}$ varies linearly with k , that is, $b_{2,\text{num}}^{(1)}/b_2^{(1)} \approx 1 + \lambda_\chi k$, where λ_χ is a slope depending on χ . These trends are consistent with Eqs. (26) and (28), although it is seen that the higher-order analysis is necessary to obtain the information of slope λ_χ . To further check the trends of Fig. 4(a), the numerical values of $b_{2,\text{num}}^{(1)}$ and $b_2^{(1)}$ for some k and χ are provided in Table I. Without the potentials (i.e., $U = 0$), the present thermo-osmosis problem is reduced to a classical thermal transpiration problem (see, e.g., Refs. [14,60]). The thermal-slip coefficient $b_2^{(1)}$ in Table I for this case, $b_2^{(1)} = 0.38316$, is the same as that reported in Ref. [12] up to five decimal points, ensuring the accuracy of the present numerical analysis. As the range of the potential χ increases, Fig. 4(b) shows that $b_2^{(1)}$ also increases except for $\chi = 0.25$ at which a slight decrease is observed.

Next, we consider the case with $U = -1$ (repulsive potential). Figure 5(a), corresponding to Fig. 4(a), shows that $b_{2,\text{num}}^{(1)} \rightarrow b_2^{(1)}$ as $k \rightarrow 0$ for various values of χ (see also Table I). As the range of the potential χ increases, Fig. 5(b) shows that $b_2^{(1)}$ decreases for $\chi > 0$ (the case of $\chi \rightarrow 0$ will be discussed below) and eventually changes the sign at $\chi \approx 0.6$. Thus, the effect of the potential on the thermal-slip coefficient is more pronounced in the repulsive case than in the attractive one, as increasing χ ultimately reverses the flow direction. Moreover, the rate of increase

TABLE I. Thermal-slip coefficients $b_{2,\text{num}}^{(1)}$ and $b_2^{(1)}$ for $U = 0$ (no potential), $U = 1$ (attractive potential), and $U = -1$ (repulsive potential) for various sets of k and χ . See also Figs. 4(a) and 5(a) for corresponding plots. More complete dataset, including the values for other parameter values, is found in Supplemental Material S4 [52].

U	χ	$b_{2,\text{num}}^{(1)}$				$b_2^{(1)}$
		$k = 0.05$	$k = 0.01$	$k = 0.005$	$k = 0.001$	
$U = 0$	—	0.38213	0.38316	0.38316	0.38317	0.38316
$U = 1$	$\chi = 0.5$	0.40254	0.39498	0.39388	0.39301	0.39275
$U = 1$	$\chi = 1$	0.53745	0.52933	0.52822	0.52733	0.52706
$U = 1$	$\chi = 2$	1.0389	1.0733	1.0784	1.0826	1.0836
$U = -1$	$\chi = 0.5$	0.18523	0.20032	0.20197	0.20343	0.20388
$U = -1$	$\chi = 1$	-0.90738	-0.87713	-0.87369	-0.87074	-0.86994
$U = -1$	$\chi = 2$	-3.1643	-3.0984	-3.0907	-3.0842	-3.0825

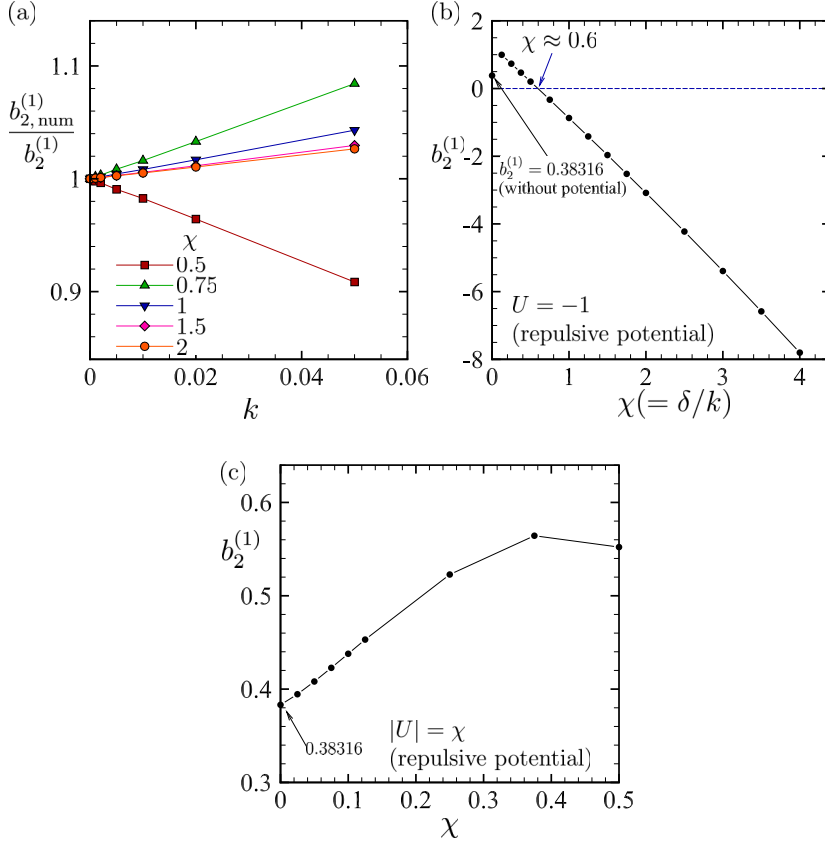


FIG. 5. Thermal-slip coefficients for repulsive potential. (a) The ratio $b_{2,\text{num}}^{(1)}/b_2^{(1)}$ between the thermal-slip coefficient obtained by the numerical analysis $b_{2,\text{num}}^{(1)}$ and that by the slip-flow theory $b_2^{(1)}$ for $U = -1$. [(b) and (c)] The thermal-slip coefficient $b_2^{(1)}$ as a function of the range of the potential χ for (b) $U = -1$ and (c) $U < 0$ with $|U| = \chi$.

in the magnitude $|b_2^{(1)}|$ with respect to χ is steeper than that observed for $U = 1$ (attractive potential). A more quantitative discussion of this behavior will be provided later in Sec. IV E 3.

It is worth noting that, for $U = -1$ [Fig. 5(b)], the thermal-slip coefficient $b_2^{(1)}$ does not converge to the value corresponding to the case without potential ($\chi = 0$) as $\chi \rightarrow 0$. This singular behavior is not observed in the attractive case ($U = 1$) [Fig. 4(b)]. To clarify this singular behavior, we show in Fig. 5(c) the values of $b_2^{(1)}$ versus χ for $|U|/\chi = 1$ ($U < 0$) instead of $U = -1$. Then $b_2^{(1)}$ for $\chi \rightarrow 0$ smoothly approaches that for the case without potential. The singularity comes from the fact that, in the Knudsen-layer problem [Eq. (A1)], we can estimate $U(d\tilde{\psi}_\chi/d\eta)|_{\eta=0} \approx U/\chi$. Hence, the limit $\chi \rightarrow 0$ leads to the blow up of the term $U(d\tilde{\psi}_\chi/d\eta)$ when U is finite, although its support vanishes. In the case of $U = -1$, it is expected that the blow up of $U(d\tilde{\psi}_\chi/d\eta)$ with the vanishing support results in a nonvanishing effect on $b_2^{(1)}$. The behavior of $b_2^{(1)}$ observed in Fig. 5(c) supports the above discussion.

2. Comparison of the thermo-osmotic flow profiles between the slip-flow theory and the numerical analysis

In this section, we discuss the spatial profiles of the thermo-osmosis flow, i.e., u_2 [see Fig. 1(b)]. As in the previous section, we compare the results obtained from the slip-flow theory [Eq. (26)] with those from the numerical analysis [Eqs. (24a) and (27)].

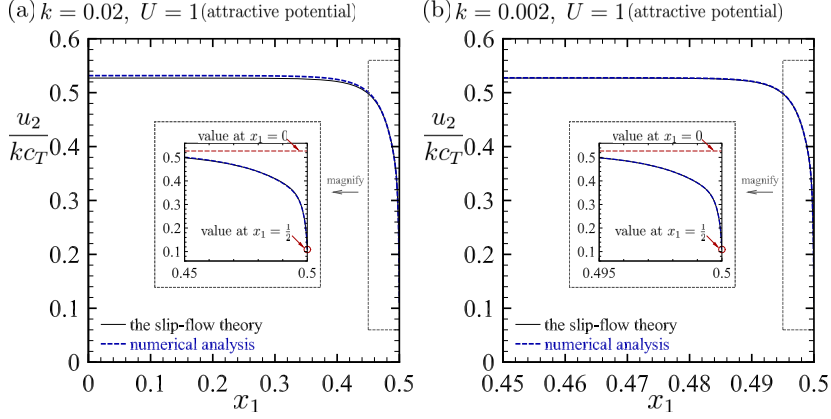


FIG. 6. Profiles of thermo-osmosis under the near-wall attractive potential: $u_2 = u_2(x_1)$ obtained from the slip-flow theory [black solid curve; Eq. (26)] and from the numerical analysis [blue dashed curve; Eq. (24a)]. The profiles are normalized by kc_T , where $k \approx$ Knudsen number and c_T is the magnitude of (dimensionless) temperature gradient. (a) $k = 0.02$ and (b) $k = 0.002$ with $\chi = 1$ and $U = 1$. The insets show the magnification near the plate $x_1 = 1/2$.

For $U = 1$ (attractive potential) and $\chi = 1$, we show the profiles of $u_2(x_1)$ in Fig. 6 for (a) $k = 0.02$ and (b) $k = 0.002$. In Fig. 6(b), the x_1 range is restricted to $x_1 \in [0.45, 0.5]$, since u_2 remains nearly constant for $x_1 \in [0, 0.45]$. Recall that c_T denotes the magnitude of the dimensionless temperature gradient of the plates [see Eq. (3)], and the velocity profiles are normalized by kc_T . Note that $u_2 \rightarrow 0$ as $k \rightarrow 0$. For both values of k presented in the figure, the slip-flow theory accurately reproduces the results of the numerical analysis, including regions near the plate surface (see the insets). The discrepancy between the two approaches is smaller for smaller k , which is consistent with the fact that the slip-flow theory is an asymptotic approximation valid in the limit $k \rightarrow 0$.

For $U = -1$ (repulsive potential) and $\chi = 1$, the corresponding velocity profiles are shown in Fig. 7 for (a) $k = 0.02$ and (b) $k = 0.002$. The main differences from the attractive case ($U = 1$; see Fig. 6) are found in the sign of u_2 , which is now negative when $U = -1$ (see Fig. 7), and in the behavior of u_2 near $x_1 = 1/2$. As discussed in Sec. IVE 1, thermo-osmosis can be directed from hot to cold, i.e., $u_2 < 0$, in the presence of a repulsive potential. The profiles of u_2 near the plate $x_1 = 1/2$ exhibit singular behavior, where $|\partial u_2 / \partial x_1|$ appears to diverge at the boundary $x_1 = 1/2$. This singularity is not observed in the attractive case ($U = 1$; see Fig. 6). Such singular (or regular) behavior of macroscopic quantities under a repulsive (or attractive) near-wall potential can be attributed to the fact that the velocity distribution function on the plate is discontinuous (or continuous) in the velocity variables. This observation is reminiscent of the singular or regular behavior of the macroscopic quantities near convex or concave boundaries [57,61], although we do not explore this connection in detail here.

3. Effect of near-wall potential on thermo-osmosis, thermal slip, and Knudsen-layer correction

So far we have fixed $|U| = 1$. In this section, we investigate the effect of U . Figure 8(a) shows the profiles of thermo-osmosis $u_2(x_1)$ for various values of $U = -0.8, -0.6, 0, 0.6$, and 0.8 in the case of $\chi = 1$ and $k = 0.02$. For attractive potential ($U = 0.6, 0.8$), u_2 is larger than that of the case without potential ($U = 0$), indicating that the flow is enhanced due to the potential. In contrast, for repulsive potential ($U = -0.6, -0.8$), the overall flow in the bulk is reduced ($U = -0.6$) and eventually reversed ($U = -0.8$). Near the plate, a more complex behavior is observed for $U = -0.6$, as shown in the inset. That is, u_2 is positive away from the plate but is negative near the plate. These observations suggest a general trend: Attractive potentials tend to enhance

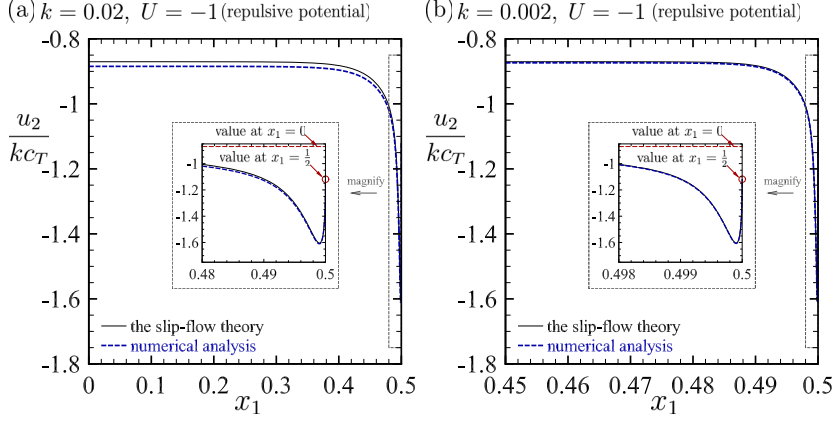


FIG. 7. Profiles of thermo-osmosis under the near-wall repulsive potential: $u_2 = u_2(x_1)$ obtained from the slip-flow theory [black solid curve; Eq. (26)] and from the numerical analysis [blue dashed curve; Eq. (24a)]. The profiles are normalized by kc_T , where $k \approx$ Knudsen number and c_T is the magnitude of (dimensionless) temperature gradient. (a) $k = 0.02$ and (b) $k = 0.002$ with $\chi = 1$ and $U = -1$. The insets show the magnification near the plate $x_1 = 1/2$.

thermo-osmosis from the cold to the hot region, whereas repulsive potentials tend to suppress or even reverse it.

However, the situation is more complex. Figure 8(b) shows the thermal-slip coefficient $b_2^{(1)}$, which determines the overall characteristics of the flow, as a function of U for $\chi = 0.5, 1, 2$. For large χ ($\chi = 2$), the previously discussed trend appears to hold, that is, attractive (or repulsive) potential increases (or diminishes) thermo-osmosis. However, for smaller χ ($\chi = 0.5$) and for small values of $|U|$, the inset shows a slight but opposite tendency. The case of $\chi = 1$ appears to be a rough threshold between these two behaviors. For all values of χ shown in the figure, the rate of change of the thermal-slip coefficient with respect to U (i.e., $|\partial b_2^{(1)}/\partial U|$) is larger for repulsive

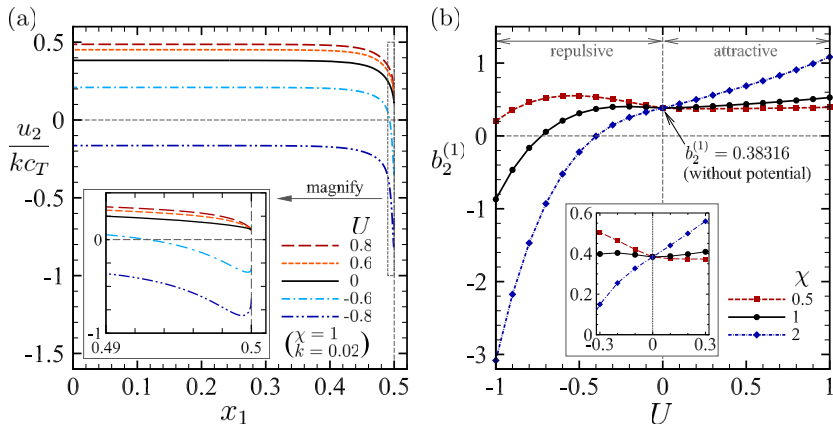


FIG. 8. (a) Profiles of thermo-osmosis u_2 and (b) the thermal-slip coefficient $b_2^{(1)}$ for various magnitude of the potential U obtained by the slip-flow theory. (a) $u_2(x_1)$ for $U = 0.8$ (red dashed), $U = 0.6$ (orange dotted), $U = 0$ (black solid), $U = -0.6$ (cyan dash-dotted), and $U = -0.8$ (blue dash-dot-dotted), where $\chi = 1$ and $k = 0.02$. The inset shows the magnification near $x_1 = 1/2$. (b) $b_2^{(1)}$ as a function of U for $\chi = 0.5$ (red squares), $\chi = 1$ (black circles), and $\chi = 2$ (blue diamonds). The inset shows the magnification near $U = 0$.

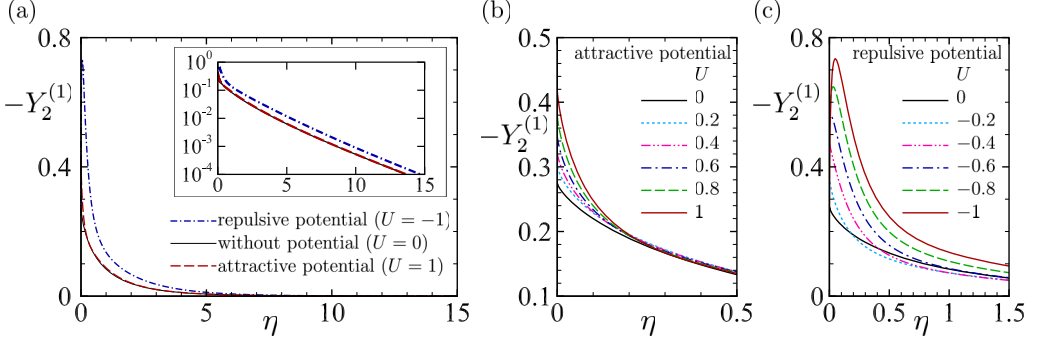


FIG. 9. Profiles of the Knudsen-layer function $Y_2^{(1)}(\eta)$ for $\chi = 1$. (a) The cases of repulsive potential ($U = -1$; blue dash-dotted), without potential ($U = 0$; black solid), and attractive potential ($U = 1$; red dashed), where the inset shows the semilogarithmic plot. Panels (b) and (c) show $Y_2^{(1)}(\eta)$ for the cases of attractive potential and repulsive potential, respectively, near $\eta = 0$ with various U .

potentials than for attractive potentials. Phenomenologically, the parameter U models the “affinity” of the interaction between fluid molecules and solid surface. The present model indicates that the thermal-slip coefficient $b_2^{(1)}$ is sensitive to the fluid-solid interaction, especially under repulsive conditions.

Finally, Fig. 9 shows the Knudsen-layer correction $Y_2^{(1)}(\eta)$ for $\chi = 1$, which represents the behavior of the macroscopic quantity inside the Knudsen layer [see Eq. (A1)]. The overall behavior of $Y_2^{(1)}(\eta)$ is shown in Fig. 9(a) for the cases of repulsive potential ($U = -1$), no potential ($U = 0$), and attractive potential ($U = 1$). The inset, shown on a logarithmic scale, confirms that $Y_2^{(1)}$ decays exponentially as η increases. Figures 9(b) and 9(c) show close-up views near the boundary ($\eta \approx 0$) for the attractive and repulsive potential cases, respectively, for various U . For the attractive potential, the influence of the potential is rather localized near the plate. In contrast, for the repulsive potential, the decay of $Y_2^{(1)}$ appears to be slower, though it remains exponentially fast. It is worth noting that while exponential decay is well established in the absence of potential, its persistence in the present case is nontrivial, as the potential considered in this study follows a power-law function.

4. Adequateness of the scaling assumption

In this section, we demonstrate the adequacy of the scaling relation (14) in the slip-flow theory. Figure 10 shows the thermo-osmosis velocity at the channel center $u_2|_{x_1=0}$ for various values of k and δ , obtained by direct numerical analysis. For the case without a potential ($U = 0$; black solid curve), the flow magnitude is proportional to k , being consistent with the prediction of the generalized slip-flow theory. Note that the slope of the curve corresponds to the slip coefficient [Eq. (28)]. However, this linear relation breaks down when k is varied while δ is fixed (red circles), indicating that an asymptotic analysis based on an expansion with respect to k is inadequate to describe the gas behavior for $k \ll 1$. In contrast, when $\chi = \delta/k$ is kept constant (blue squares), a clear linear relationship $u_2 \propto k$ is observed. This result validates the appropriateness of the scaling in Eq. (14) and illustrates the reasoning behind its adoption in the present theory.

V. DISCUSSION

In the dimensional form, the thermal-slip boundary condition [Eq. (17a) or (25)] is written as, up to the first order of k ,

$$\mathbf{v} \cdot \mathbf{t} = -K_{\text{TS}} \mathbf{t} \cdot \nabla T, \quad K_{\text{TS}} = -\frac{\sqrt{\pi}}{2} \frac{v_0 \ell_0}{T_0} b_2^{(1)} \quad (\text{on boundaries}), \quad (29)$$

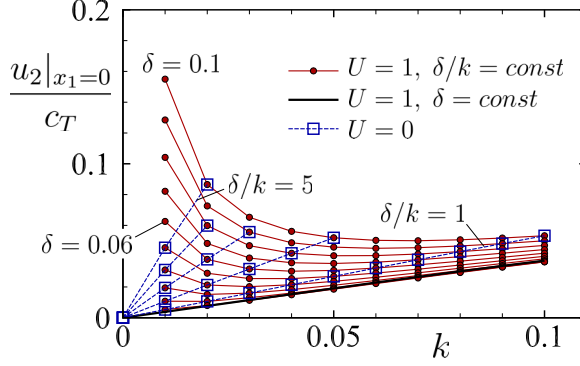


FIG. 10. Thermo-osmosis at the channel center, $u_2|_{x_1=0}/c_T$, as a function of k for various $\delta = 0.01, 0.02, \dots, 0.09, 0.1$, obtained by the direct numerical analysis. The case without the potential ($U = 0$) is shown by the black solid curve. The cases with $U = 1$ are shown in two different manners: red circles (or blue squares) connect the data point under the condition $\delta = 0.01, 0.02, \dots, 0.09, 0.1$ (or $\delta/k = \chi = 1, \dots, 5$).

where K_{TS} [the unit $\text{m}^2/(\text{s K})$] is the thermal-slip coefficient and $b_2^{(1)}$ is the corresponding dimensionless thermal-slip coefficient of order unity, as obtained in Secs. III and IV. Here $v_0 = \sqrt{2RT_0}$ is the thermal speed at the reference state, ℓ_0 is the mean free path at the reference state, and T_0 is the reference temperature. Note that $b_2^{(1)}$ can be either positive or negative signs, although positive values $b_2^{(1)} > 0$ (corresponding to flow from cold to hot) have been more commonly observed. In the following, we discuss the validity of Eq. (29) for gas and liquid phases separately.

A. Gases

In the case of gases, which we have considered throughout this study based on the BGK model [Eq. (5)], the viscosity μ is related to the mean free path ℓ_0 as [12]

$$\mu = \frac{\sqrt{\pi}}{2} \frac{p_0 \ell_0}{v_0}, \quad (30)$$

where p_0 is the reference pressure. Consequently, the dimensionless viscosity is given by $\mu/(p_0 D/v_0) = (\sqrt{\pi}/2)(\ell_0/D) = k$, as shown in the Stokes equation Eq. (16b). Using this relation of μ and $p_0 = \rho_0 R T_0$, the thermal-slip coefficient K_{TS} can be rewritten as

$$K_{TS} = -\frac{\mu}{\rho_0 T_0} \sigma_T \quad (\sigma_T = 2b_2^{(1)}). \quad (31)$$

In the experiment by Yamaguchi *et al.* [16], σ_T was measured to be approximately $\sigma_T \approx 0.9 - 1$ for several monatomic gases, which is of the same order of magnitude as the present results [i.e., $b_2^{(1)} = O(1)$; see Table I]. This agreement is reasonable, since the experimental estimation of σ_T in Ref. [16] is also based on fitting the thermal-slip boundary condition to measured mass flow rates to obtain the thermal-slip coefficient. It is worth noting that the Stokes equations for incompressible viscous fluid, i.e., $\partial p/\partial X_i = \mu(\partial^2 v_i/\partial X_j^2)$ can be recovered for the Hilbert part when $k \ll 1$ [12].

Purely attractive ($U > 0$) and purely repulsive ($U < 0$) potentials considered here represent two limiting cases of typical favorable and unfavorable solid-gas molecular interactions, respectively. Therefore, if we consider more realistic LJ-type potentials, which may lie between these two limiting cases, then the values of $b_2^{(1)}$ is expected to fall well within the range of $b_2^{(1)}$ presented here in Table I. In Ref. [62], molecular dynamics simulations for an LJ gaseous system were carried out to investigate thermo-osmosis in a nanochannel. The estimated values of K_{TS} are in qualitative agreement between the molecular simulation and Eq. (29). That is, using $b_2^{(1)} = 0.52706$

for $U = 1$ and $\chi = 1$ in Eq. (29), we obtain $K_{TS} \approx -4.9 \times 10^{-10} \text{ m}^2/(\text{s K})$ (Ref. [62]) and $K_{TS} \approx -1.6 \times 10^{-10} \text{ m}^2/(\text{s K})$ [Eq. (29)] for $\text{Kn} \approx 0.1$ and $K_{TS} \approx -7.2 \times 10^{-10} \text{ m}^2/(\text{s K})$ (Ref. [62]) and $K_{TS} \approx -4.9 \times 10^{-10} \text{ m}^2/(\text{s K})$ [Eq. (29)] for $\text{Kn} \approx 0.3$ (see Supplemental Material S5 [52] for the detail of the estimation). However, it should be remarked that a potential including both attractive and repulsive parts (such as a LJ-type potential) complicates the numerical analysis of Knudsen-layer problems, since the external-force term $(\partial\Psi/\partial X_1)(\partial f/\partial \xi_1)$ [see Eq. (5)] is locally positive or negative for such cases, making it difficult to apply an implicit upwind finite-difference method widely used in the literature as well as in the present paper.

We also make some comparisons with a recent study [18], which applied the framework of linear response theory to thermo-osmosis of gases and liquids in a closed channel consisting of two parallel confinements in both X_1 and X_2 directions. The major difference between the present study and Ref. [18] is that here we consider an open channel, i.e., the longitudinal pressure gradient in the bulk is zero [Eq. (24b)], whereas in Ref. [18] the effect of the backflow caused by a pressure gradient in the closed channel is present (no net mass flux condition is imposed in the longitudinal direction). The details of fluid-solid molecular interactions and the range of parameters (Kn and volume fraction) are also different. Despite these differences, there are some qualitative agreements as follows. (i) The velocity reversal between attractive-type and repulsive-type fluid-solid intermolecular interaction potentials is observed in both studies. In particular, gas flow is driven from the cold to hot sides (or the hot to cold sides) for attractive (or repulsive) potentials near the wall. (In Ref. [18], the backflow in the opposite direction occurs away from the wall.) (ii) The velocity profile is flat (i.e., pluglike) away from the wall in both studies. (iii) For a hard wall, i.e., the specular reflection boundary condition with no potential, the flow vanishes (no thermo-osmosis occurs). The point (iii) can be seen in our problem by replacing Eq. (12) with a specular reflection condition and by neglecting the external-force term. For this case,

$$\phi = c_T \left(\zeta^2 - \frac{5}{2} \right) x_2 - c_T k \zeta_2 \left(\zeta^2 - \frac{5}{2} \right), \quad (32)$$

is a solution that indeed realizes the thermo-osmosis setting $\tau = c_T x_2$ (linear temperature increase) and $P = 0$ (uniform pressure) but results in $u_i = 0$ (no flow), regardless of the value of Kn . To further comparisons, we will need to find a solution that induces backflows due to a pressure gradient, for which the shear-slip coefficient $b_1^{(1)}$ will be necessary.

B. Liquids

The slip-flow theory can be basically applied to gases, since it is based on the Boltzmann equation (or its model equations), which describes the evolution of the one-particle velocity distribution functions. The Boltzmann equation is valid for the entire range of $0 < \text{Kn} < \infty$, provided that the volume fraction $\mathcal{V} (\propto n d^3)$ is negligibly small, where n is the number density of fluid molecules and d the molecular diameter. Due to the smallness of volume fraction $\mathcal{V}$, long-range intermolecular potentials, which are important in liquids [i.e., $\mathcal{V} = O(1)$], and finite-size effects of molecules are not incorporated into the Boltzmann equation, and macroscopic quantities such as pressure are defined differently from those of liquids. Nevertheless, the present BGK model of the Boltzmann equation can be interpreted as describing a simplified “fluid” (say, a BGK fluid), in which fluid molecules interact locally in space to drive the system toward local thermal equilibrium. From this perspective, the BGK fluid can be viewed as a toy model for studying certain phenomena in liquids.

In the context of liquids, the quantity $K_{TS} T_0$, also denoted by M_{21} or β_{21} , is often used [7,20] as a measure of thermal-slip coefficients. Accordingly, we consider the quantity $M_{21} = K_{TS} T_0 = -(\sqrt{\pi}/2) v_0 \ell_0 b_2^{(1)}$ for comparison and provide rough estimates of its magnitude. In Eq. (29), we may estimate each parameter as follows:

- (i) the average molecular speed $v_0 \approx 10^2\text{--}10^3 \text{ m/s}$,
- (ii) the “mean free path” $\ell_0 \approx$ effective range of the potential $\delta D \approx 0.1\text{--}1 \text{ nm}$,
- (iii) the (dimensionless) thermal-slip coefficient $|b_2^{(1)}| \approx 0.1\text{--}1$.

In the second estimate, we have used the assumption $\chi = \delta/k = \delta/(\ell_0/D) = O(1)$, implying that ℓ_0 is on the order of δD . Note that the mean free path is not well defined for liquids, and ℓ_0 here is interpreted as a characteristic length scale associated with the interaction potential. With the above estimates, the (dimensional) thermal-slip coefficient M_{21} can be evaluated as $|M_{21}| = |K_{TS}T_0| \approx 10^{-9}-10^{-6} \text{ m}^2/\text{s}$. In the literature, using the MD simulations, Ref. [20] reported $|M_{21}| \approx 1-400 \times 10^{-8} \text{ m}^2/\text{s}$ for LJ-potential-based liquid-solid interfaces and $|M_{21}| \approx 250 \times 10^{-8} \text{ m}^2/\text{s}$ for water-graphene surfaces, Ref. [7] reported $|M_{21}| \approx 0.85-3.8 \times 10^{-8} \text{ m}^2/\text{s}$ for less-attractive LJ potential interaction and $|M_{21}| \approx 4.2-5.6 \times 10^{-6} \text{ m}^2/\text{s}$ for purely repulsive potential interaction at liquid-solid interfaces, and Ref. [24] reported $|M_{12}| \approx 1-5 \times 10^{-7} \text{ m}^2/\text{s}$ for LJ-potential-based liquid-solid interfaces, while experimental studies [2,9] reported $|M_{21}| \approx 10^{-10}-10^{-9} \text{ m}^2/\text{s}$. It should be also noted that MD simulations have shown that the sign of M_{21} (i.e., the direction of thermo-osmosis) can reverse depending on the degree of hydrophilicity [20–24]. Our present results qualitatively reproduce this sign-reversal trend, as shown in Fig. 8(b), where the thermal-slip coefficient $b_2^{(1)}$ changes sign with the variation of the potential strength U . It should also be noted that the “viscosity” in our BGK fluid is given by Eq. (30), which is different from the standard microscopic definition of liquid viscosity based on the time correlation of the stress tensor [63]. This is the why we regard the BGK fluid as a toy model when applied to liquids.

Despite the oversimplified treatment from a molecular-physics perspective (e.g., long-range interaction, finite-volume effects, layering near interfaces, and electric forces), the present approach based on a kinetic model exhibits some qualitative consistency with MD studies for liquids. Specifically, it captures (i) the correct order of magnitude and (ii) the trend with respect to the surface hydrophilic properties (i.e., attractive or repulsive potential). A notable strength of the present approach lies in its ability to systematically compute slip coefficients within the framework of the generalized slip-flow theory. In this framework, the slip coefficients are obtained by solving the Knudsen-layer problems [Eq. (A1)], which are spatially one-dimensional boundary-value problems for integro-differential kinetic equations. These problems are numerically tractable, and the well-established solution procedure exist (e.g., Ref. [53]). In particular, the computational cost for the BGK model is relatively low. For example, a standard single CPU is sufficient to compute the thermal-slip coefficient with decent accuracy within a few minutes, using approximately $O(10^4)$ lattice points in the two-dimensional phase space. The main limitation of the present model is its omission of intermolecular potential effects and finite-molecular-volume effects. Nevertheless, it may be possible to extend the model to include such effects by using kinetic models for nonideal gases, such as those developed for the van der Waals fluids [64].

VI. CONCLUSION

In this paper, we have developed a slip-flow theory to predict slip coefficients in the slip-boundary condition of the Stokes equation, which describes micro- and nanoscale gas flows between two parallel plates in the presence of a near-wall potential. The approach is based on the generalized slip-flow theory in kinetic theory of gases, whereby the determination of slip coefficients is reduced to solving the Knudsen-layer problems (i.e., kinetic boundary-layer problems), namely, Eq. (A1). This framework offers a pathway to explore systematically the influence of near-wall potentials on slip coefficients, while avoiding computationally costly molecular simulations.

Using the developed slip-flow theory, we investigated thermo-osmosis between two parallel plates with a uniform temperature gradient, assuming the presence of a pseudo-Sutherland-type near-wall potential. A comparison between the predictions of the slip-flow theory and the results of numerical analysis showed good agreement, validating the proposed theoretical framework. We also systematically examined the influence of the near-wall potential on thermo-osmosis, thermal-slip coefficients, and Knudsen-layer corrections for various parameter sets corresponding to purely attractive and purely repulsive potentials. The results showed that a reversal in the flow direction of thermo-osmosis can occur when the near-wall potential becomes sufficiently repulsive. To be more

specific, under a purely repulsive potential of decent strength, the thermo-osmosis flow is directed from hot to cold, which is opposite to the direction typically observed in conventional cases.

There are several directions for extending the present slip-flow theory.

(1) The influence of the specific shape of a potential function (i.e., ψ_δ) has not been investigated in this study. Physically realistic potential profiles, such as the LJ type that includes both attractive and repulsive parts, should be investigated. It is worth noting that the potential considered in this study [Eq. (21)] is a power-law type. When the potential decays more slowly, say $\Psi^\pm \propto |x_1 \mp 1/2|^{-1}$, a straightforward application of the slip-flow theory may fail (or may be limited) because of the slow decay of the Knudsen-layer solutions. In such cases, an asymptotic matching procedure may be required, as in the case of a two-dimensional Knudsen layer (or Knudsen zone) [65]. Therefore, the applicability of the present slip-flow theory to more general classes of potentials remains an open question.

(2) The influence of kinetic boundary conditions, which is diffuse reflection here, is considered important. It is reported that, in the case of dense fluids, the temperature gradient can induce thermo-osmosis even with a smooth hard wall [18]. This contrasts with a rarefied-gas case, where the specular reflection (without near-wall potential) does not allow thermo-osmosis [see Eq. (32) and description below it], and therefore, is worth further investigation.

(3) The analysis of other slip and jump coefficients under near-wall potentials [Eqs. (A2) and (A3)] is also important. In particular, the shear-slip coefficient has been the subject of long-standing interest and deserves a detailed examination in the context of near-wall interactions.

(4) The present analysis is limited to planar geometries and any effects from curved surfaces were not included. As the Knudsen-layer correction begins at the zeroth order in the Knudsen number, the curvature effect is expected to manifest in the first-order Knudsen-layer corrections when a curved surface is considered. Thus, to investigate thermo-osmosis around curved surfaces, including a spherical particle, an extension of the slip-flow theory to curved geometries is required. This is particularly relevant for understanding the mechanism of thermophoresis, the motion of suspended particles driven by temperature gradients in fluids (see, e.g., Ref. [66] for gases and Ref. [67] for liquids).

(5) The inclusion of long-range intermolecular interactions and finite-molecular-volume effects is important. Assessing the potential and limitations of the framework of the slip-flow theory in describing not only rarefied gases but also more complex fluids will be addressed in future work.

ACKNOWLEDGMENTS

This work was supported by the Japan Society for the Promotion of Science KAKENHI Grants No. 22K18770, No. 22K03924, No. 24K00803, and No. 25K01156 and also by the Japan Science and Technology Agency PRESTO Grant No. JPMJPR2207.

DATA AVAILABILITY

The data that support the findings of this article are openly available [68].

APPENDIX: KNUDSEN-LAYER PROBLEMS

In this Appendix, we explain the details of the Knudsen-layer problems that determine the slip and jump coefficients $b_1^{(1)}$, $b_2^{(1)}$, and $c_1^{(0)}$ and the Knudsen-layer corrections $Y_1^{(1)}$, $Y_2^{(1)}$, $\Omega_1^{(0)}$, and $\Theta_1^{(0)}$. We note that the potentials are localized near the plates, and thus the boundary layer of the one side is not affected by the potential of the other side. Therefore, only the boundary layer near the plate at $x_1 = 1/2$ is described here.

To obtain $b_2^{(1)}$ and $Y_2^{(1)}$, which are necessary in the thermo-osmosis problem (Sec. IV), we consider the following boundary-value problem:

$$\zeta_n \frac{\partial \varphi_2^{(1)}}{\partial \eta} - U \frac{d\tilde{\psi}_\chi}{d\eta} \frac{\partial \varphi_2^{(1)}}{\partial \zeta_n} = \exp(-2U\tilde{\psi}_\chi)(2Y_2^{(1)} - \varphi_2^{(1)}) + \mathcal{I}_{TS}, \quad (\text{A1a})$$

$$Y_2^{(1)}(\eta) = \frac{1}{2} \int_{\mathbb{R}^3} \zeta_\rho^2 \varphi_2^{(1)} E \, d\boldsymbol{\zeta}, \quad (\text{A1b})$$

$$\mathcal{I}_{TS} = - \left(2U\tilde{\psi}_\chi + 2\zeta_n U \frac{d\tilde{\psi}_\chi}{d\eta} \right) + [\exp(-2U\tilde{\psi}_\chi) - 1] \left(\zeta_n^2 + \zeta_\rho^2 - \frac{5}{2} \right), \quad (\text{A1c})$$

$$\varphi_2^{(1)} = -2b_2^{(1)} + \zeta_n^2 + \zeta_\rho^2 - \frac{5}{2} \quad (\eta = 0, \zeta_n > 0), \quad (\text{A1d})$$

$$\varphi_2^{(1)} \rightarrow 0 \quad (\eta \rightarrow \infty), \quad (\text{A1e})$$

where the notations follow those in Ref. [13] and explained below one by one. First, the molecular velocity ζ_i is decomposed into $\zeta_n = \zeta_i n_i$ with n_i the unit normal on the boundary at $x_1 = 1/2$ pointing to the gas (i.e., $\zeta_n = -\zeta_1$) and $\zeta_\rho = \sqrt{\zeta_2^2 + \zeta_3^2}$. The unknown function $\varphi_2^{(1)} = \varphi_2^{(1)}(\eta, \zeta_n, \zeta_\rho)$ is the portion of the molecular velocity distribution function for the Knudsen-layer correction and is related with the temperature gradient of the Hilbert part (see Supplemental Material S1 B [52] for details). In short, the terms related with $\tilde{\psi}_\chi$ are the contributions found in this paper. Substituting $\tilde{\psi}_\chi = 0$ into Eq. (A1) formally reproduces the known result. This problem corresponds to the *thermal slip* under the presence of a near-wall potential field.

The Knudsen-layer problem that determines $c_1^{(0)}$, $\Omega_1^{(0)}$, and $\Theta_1^{(0)}$ is summarized as

$$\zeta_n \frac{\partial \varphi_1^{(0)}}{\partial \eta} - U \frac{d\tilde{\psi}_\chi}{d\eta} \frac{\partial \varphi_1^{(0)}}{\partial \zeta_n} = \exp(-2U\tilde{\psi}_\chi) \left[\Omega_1^{(0)} + \left(\zeta_1^2 + \zeta_\rho^2 - \frac{3}{2} \right) \Theta_1^{(0)} - \varphi_1^{(0)} \right] + \mathcal{I}_{TJ}, \quad (\text{A2a})$$

$$\Omega_1^{(0)}(\eta) = \int_{\mathbb{R}^3} \varphi_1^{(0)} E \, d\boldsymbol{\zeta}, \quad \Theta_1^{(0)}(\eta) = \int_{\mathbb{R}^3} \frac{2}{3} \left(\zeta_1^2 + \zeta_\rho^2 - \frac{3}{2} \right) \varphi_1^{(0)} E \, d\boldsymbol{\zeta}, \quad (\text{A2b})$$

$$\mathcal{I}_{TJ} = -U \frac{d\tilde{\psi}_\chi}{d\eta} \left(3\zeta_n^2 + \zeta_\rho^2 - \frac{5}{2} - 2\eta\zeta_n \right) + [\exp(-2U\tilde{\psi}_\chi) - 1] \zeta_n \left(\zeta_n^2 + \zeta_\rho^2 - \frac{5}{2} \right), \quad (\text{A2c})$$

$$\varphi_1^{(0)} = -2\sqrt{\pi} \int_{\zeta_n < 0} \zeta_n \varphi_1^{(0)} E \, d\boldsymbol{\zeta} - (\zeta_n^2 + \zeta_\rho^2 - 2) c_1^{(0)} + \zeta_n \left(\zeta_n^2 + \zeta_\rho^2 - \frac{5}{2} \right) \quad (\eta = 0, \zeta_n > 0), \quad (\text{A2d})$$

$$\varphi_1^{(0)} \rightarrow 0 \quad (\eta \rightarrow \infty), \quad (\text{A2e})$$

where $\varphi_1^{(0)} = \varphi_1^{(0)}(\eta, \zeta_n, \zeta_\rho)$ is the unknown function. This problem corresponds to the *temperature jump* under the presence of a near-wall potential field.

The Knudsen-layer problem that determines $b_1^{(1)}$ and $Y_1^{(1)}$ is summarized as

$$\zeta_n \frac{\partial \varphi_1^{(1)}}{\partial \eta} - U \frac{d\tilde{\psi}_\chi}{d\eta} \frac{\partial \varphi_1^{(1)}}{\partial \zeta_n} = \exp(-2U\tilde{\psi}_\chi)(2Y_1^{(1)} - \varphi_1^{(1)}) + \mathcal{I}_{SS}, \quad (\text{A3a})$$

$$Y_1^{(1)}(\eta) = \frac{1}{2} \int_{\mathbb{R}^3} \zeta_\rho^2 \varphi_1^{(1)} E \, d\boldsymbol{\zeta}, \quad (\text{A3b})$$

$$\mathcal{I}_{SS} = -2U \frac{d\tilde{\psi}_\chi}{d\eta} + [\exp(-2U\tilde{\psi}_\chi) - 1] 2\zeta_n, \quad (\text{A3c})$$

$$\varphi_1^{(1)} = -2b_1^{(1)} + 2\zeta_n \quad (\eta = 0, \zeta_n > 0), \quad (\text{A3d})$$

$$\varphi_1^{(1)} \rightarrow 0 \quad (\eta \rightarrow \infty), \quad (\text{A3e})$$

where $\varphi_1^{(1)} = \varphi_1^{(1)}(\eta, \zeta_n, \zeta_\rho)$ is the unknown function. This problem corresponds to the *shear slip* under the presence of a near-wall potential field.

We expect that solutions to Eqs. (A1), (A2), and (A3) can be found only when the unknown coefficients $c_1^{(0)}$, $b_1^{(1)}$, and $b_1^{(2)}$ take particular values. Therefore, if we could find the solutions, then $c_1^{(0)}$, $b_1^{(1)}$, and $b_1^{(2)}$ are determined simultaneously. It should be noted that the existence and uniqueness of the solution for the Knudsen-layer problem, formulated for the Boltzmann equation, is mathematically proved for the cases without the potential [69,70].

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