Variational derivation of thermal slip coefficients on the basis of the Boltzmann equation for hard-sphere molecules and Cercignani-Lampis boundary conditions: Comparison with experimental results

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In the present paper, a variational method is applied to solve the Boltzmann equation based on the true linearized collision operator for hard-sphere molecules and the Cercignani-Lampis boundary conditions. This technique allows us to obtain an explicit relation between the first- and second-order thermal slip coefficients and the tangential momentum and normal energy accommodation coefficients, defined in the frame of the Cercignani-Lampis scattering kernel. Comparing the theoretical results with the experimental data from *Yamaguchi et al.*, J. Fluid Mech., **795**, 690 (2016), a pair of accommodation coefficients has been extracted for each noble gas considered in the experiments. Then, these values have been used to compute, by means our variational technique, the temperature-driven mass flow rates and the outputs have been compared with the measurements for Helium, Neon and Argon. Good agreement has been obtained between the theoretical and the experimental data, within the range of validity of the proposed second-order slip model. For all the gases analyzed, the tangential accommodation coefficient is found to be much larger than the normal energy coefficient. The general trend, according to which, by increasing the molecular weight of the different gases, the values of both accommodation coefficients also increase, is confirmed in this study.

I. INTRODUCTION

Accurate modeling of gas-surface interaction is very important for external rarefied gas flows, such as those around shuttles and satellites, as well as for internal rarefied or small-scale flows, like those in micro-electro-mechanical systems or in gas shale reservoirs, both characterized by large surface area to volume ratios. The rarefaction level of a gas can be quantified by the rarefaction parameter, i.e. the ratio between a characteristic dimension of a flow and the molecular mean free path of a gas. The most reliable description of rarefied gas flows is provided by the Boltzmann equation (BE)[1]. The boundary conditions for the BE must be formulated on a probabilistic ground, by specifying the relation between the velocity distribution function of the reflected and the incident gas molecules on the solid surface, the so-called scattering kernel[1]. In the case of low rarefaction level, the gas flow can be still simulated in the frame of the continuum modeling based on the Navier-Stokes-Fourier system[2] or on higher-order expansions as the 13 moment equations (R13)[3]. However, the implementation of special boundary conditions, like the velocity slip and temperature jump on gas-solid interfaces, is necessary to take into account the rarefaction effects. All these conditions involve the viscous-slip, the thermal-slip and the temperature-jump coefficients, which depend on the gas-solid surface interaction through the accommodation coefficients. Different scattering kernels can be found in the literature: Maxwell[4], Cercignani-Lampis (CL)[5], Epstein[6], Klinc & Kuščer[7,8], Dadzie-Méolans[9] and some others. These proposed models have one or several adjustable parameters that can be associated with the accommodation processes of physical quantities. For example, the Cercignani-Lampis model includes two parameters: the accommodation coefficient of the tangential momentum, α_t, and the accommodation coefficient of the kinetic energy due to the normal velocity, α_n. However, the most popular and easy to use scattering kernel is the Maxwell model, characterized by only one parameter α, which is the accommodation coefficient of all molecular properties. Therefore, in general, one can associate α either with the accommodation of the tangential momentum or with the accommodation of energy. Despite this ambiguous interpretation, the Maxwell model has been successfully applied to describe various isothermal flows driven by a pressure gradient, both at the microscale and at low-pressures[10–15]. In fact, in this case, when the temperature of the system is kept constant, the momentum exchange mechanism assumes a dominant role and the accommodation coefficient can be identified with the tangential momentum

accommodation coefficient (TMAC)[16]. In a different situation, when only an exchange of energy takes place between a gas and a surface, without the macroscopic gas motion, the thermal or energy accommodation coefficient is introduced in the frame of the Maxwell model, to characterize the peculiarity of this type of interaction[17–21]. However, for the majority of gas flows, where exchanges of both momentum and energy exist, i.e. pressure and temperature gradients are present at the same time, the interpretation of this single coefficient becomes problematic. In all these cases, one can resort to the Cercignani-Lampis scattering kernel which contains two different adjustable parameters: α_t and α_n.

Several attempts have been made to extract, for different gases, both the tangential momentum, α_t, and the normal energy, α_n, accommodation coefficients simultaneously, see Refs. [22], [23]. The author of Ref. [22] used the experimental data given in Ref. [11] to obtain the accommodation coefficient of the tangential momentum from the Poiseuille flow and then, that related to the normal energy from the measurements of the thermomolecular pressure difference for the same gas[24]. But it was not possible to find a pair of coefficients that could fit both experiments. The authors of Ref. [23] solved numerically the linearized Boltzmann equation with the Lennard-Jones intermolecular potential and the Cercignani-Lampis boundary conditions, to calculate the temperature-driven mass flow rate and the thermomolecular pressure difference, and compared their outputs with the experimental data provided in Ref. [25]. But again, it was not possible to find values of α_t and α_n for the same gas, with which to describe these phenomena. However, in both papers, the accommodation coefficients have been selected by the trial and error method.

The main objective of this work is to improve the fundamental understanding of the gas-surface interaction. To this end, a variational approach has been used to obtain asymptotic near-continuum solutions of the linearized Boltzmann equation for hard-sphere molecules, in order to provide analytical expressions for the first- and second-order thermal slip coefficients. The Cercignani-Lampis boundary conditions have been considered in order to take into account the influence of the tangential momentum α_t and the normal energy α_n accommodation coefficients on the slip parameters. The theoretical results have been compared with the experimental data reported in Ref. [25] for five different noble gases and, for each of them, the accommodation coefficients α_t and α_n have been extracted. Then, these values have been used to evaluate the temperature-driven mass flow rate, by means of our variational technique. A comparison with the experimental measurements

reveals a fairly good agreement within the range of validity of the proposed second-order slip model.

II. THE POISEUILLE AND THERMAL-CREEP PROBLEMS: MATHEMATICAL FORMULATION

Let us consider two parallel infinite plates separated by a distance d and a monatomic gas flowing between them due to longitudinal gradients of pressure and temperature. In the $(x,\, z)$ plane, the z axis coincides with the direction of the fluid motion, while the two walls are fixed at $x = \pm d/2$. If the pressure and temperature gradients are taken to be small, it can be assumed that the velocity distribution of the flow is nearly the same as that occurring in an equilibrium state. This means that the Boltzmann equation can be linearized about a Maxwellian f_0 by putting[26],[27]

$$f(x, z, \mathbf{c}) = f_0 \left[1 + kz + \left(c^2 - \frac{5}{2} \right) \tau z + h(x, \mathbf{c}) \right] \tag{1}$$

where $f(x, z, \mathbf{c})$ is the distribution function for the molecular velocity $\mathbf{c}$ expressed in units of $(2RT)^{1/2}$ (with R being the specific gas constant and T being the equilibrium temperature) and $h(x, \mathbf{c})$ is the small perturbation on the basic equilibrium state. The above mentioned Maxwellian is given by

$$f_0(\mathbf{c}) = \frac{\rho_0}{\pi^{3/2}} \exp(-c^2) \tag{2}$$

where ρ_0 is the equilibrium gas density and

$$k = \frac{1}{p} \frac{\partial p}{\partial z}, \quad \tau = \frac{1}{T} \frac{\partial T}{\partial z} \tag{3}$$

with p and T being the local gas pressure and temperature, respectively. Using Eq. (1), the steady linearized Boltzmann equation reads as

$$c_x \frac{\partial h}{\partial x} + k c_z + \tau c_z \left(c^2 - \frac{5}{2} \right) = Lh \tag{4}$$

where Lh is the linearized collision operator. In general, it is difficult to manage the Boltzmann operator L as such. Therefore, simplified kinetic models of the exact collision integral are widely used in practice, for both analytical computations and numerical simulations. Because of its simplicity, the Bhatnagar, Gross, and Krook (BGK) model is

one of the most popular of these kinetic models, although it is known to have a serious flaw: it leads to a wrong Prandtl number (i.e. the dimensionless ratio of viscosity and thermal conductivity)[28]. This difficulty can be dealt with, when one works in the linearized framework, since viscosity and temperature effects are then decoupled and either viscosity or thermal conductivity can be fixed to a correct value. However, if one wants to analyze, at the same time, the Poiseuille and thermal-creep problems, where the mass and heat fluxes are due to the combined effects of the pressure and temperature gradients, the BGK can not provide simultaneously accurate results[27]. Thus, one can resort to a more refined kinetic model such as the one proposed by Shakhov (S-model)[29],[30]. But still, the S-model does not include any information about the interaction potential between the gas molecules, while some phenomena related to the thermal-creep problem are very sensitive to the intermolecular force laws[27],[2]. Therefore, in the current investigation, we analyze the Poiseuille and thermal-creep flows on the basis of the exact linearized collision operator for hard-sphere molecules, in order to obtain a better approximation of real-gas behaviors[1]. The boundary conditions for Eq. (4) have the following general form

$$h^+ = Kh^- \tag{5}$$

where $h^\pm$ are the restrictions of the function h, defined on the boundary, to positive (negative) values of c_x (that is, h^+ and h^- concern, respectively, the reemitted and the impinging molecules on the boundaries). The explicit form of the operator K in Eq. (5) depends on the scattering kernel used. Most of the works in rarefied gas dynamics are based on the implementation of the classical Maxwell gas-surface interaction law, characterized by a single accommodation coefficient α, while in practice, every physical quantity (i.e. momentum and energy) should have its own accommodation coefficient. In the literature, there are many data related to rarefied gas flows between two parallel plates that can be accurately reproduced on the basis of the Boltzmann equation and the Maxwell model of boundary conditions. This is especially true for isothermal gas flows. However, recent measurements of the thermal creep flow through microchannels have revealed that it is very difficult to extract from the experimental data only one accommodation coefficient, which allows one to describe all flow properties[25]. Therefore, in order to include a more realistic physical description of the gas-surface interaction, in the current investigation, we will focus on the Cercignani-Lampis (CL) scattering kernel[5]. This model is based on two different adjustable parameters: α_t, which is the accommodation coefficient of the

tangential momentum and α_n, which is the accommodation of the kinetic energy owing to the velocity normal to the bounding walls. In this case, the boundary conditions (5) can be written as

$$h^+(-(d/2)\mathrm{sgn}c_x, \mathbf{c}) = \int_{c'_x<0} R_{CL}(-\mathbf{c} \to -\mathbf{c}')\; h^-(-(d/2)\mathrm{sgn}c_x, \mathbf{c}')\; d\mathbf{c}' \tag{6}$$

where

$$R_{CL}(\mathbf{c}' \to \mathbf{c}) = \frac{2c_x}{\pi\alpha_t\alpha_n(2-\alpha_t)} \exp\left\{ -\frac{[\mathbf{c}_t - (1-\alpha_t)\mathbf{c}'_t]^2}{\alpha_t(2-\alpha_t)} \right\} \times \exp\left\{ -\frac{[{c_x}^2 + (1-\alpha_n){c'_x}^2]}{\alpha_n} \right\} I_o\left(\frac{2\sqrt{1-\alpha_n}}{\alpha_n} c_x c'_x \right) \tag{7}$$

with $\mathbf{c}_t = (c_y, c_z)$ being the two-dimensional vector of the tangential molecular velocity and I_o the modified Bessel function of first kind and zeroth order. The CL model recovers, as limiting cases, the specular reflection (for $\alpha_t = \alpha_n = 0$) and the diffuse re-emission (for $\alpha_t = \alpha_n = 1$). Moreover, it includes the back scattering ($\mathbf{c} = -\mathbf{c}'$) when $\alpha_t = 2$ and $\alpha_n = 0$.

The pressure and temperature gradients cause a gas flow and heat transfer in the z-direction. Therefore, once the deviation h from the equilibrium distribution is known, the bulk velocity of the gas $v_z(x)$ and the heat flux $q_z(x)$ can be calculated as

$$v_z(x) = \pi^{-\frac{3}{2}} \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} e^{-c^2} c_z h(x, \mathbf{c})\, d\mathbf{c} \tag{8}$$

$$q_z(x) = \pi^{-\frac{3}{2}} \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} e^{-c^2} c_z \left(c^2 - \frac{5}{2}\right) h(x, \mathbf{c})\, d\mathbf{c}. \tag{9}$$

Hence, the mass $\dot{M}$ and heat flow rate $\dot{Q}$ (per unit time through unit thickness) are given by

$$\dot{M} = \rho \int_{-d/2}^{d/2} v_z(x) dx \tag{10}$$

$$\dot{Q} = \int_{-d/2}^{d/2} q_z(x) dx \tag{11}$$

where ρ is the gas density.

III. THE VARIATIONAL METHOD OF SOLUTION

To apply the variational formulation, we shall rewrite Eq. (4) in the following symbolic form:

$$(D - L)h = S \tag{12}$$

where $Dh = c_x \dfrac{\partial h}{\partial x}$ and $S = -c_z k - c_z \left(c^2 - \frac{5}{2} \right) \tau$. Using the variational principle described in Refs. [31], [32], we introduce the following functional J of the test function $\tilde{h}$:

$$J(\tilde{h}) = ((\tilde{h}, P(D\tilde{h} - L\tilde{h}))) - 2((PS, \tilde{h})) + (\tilde{h}^+ - K\tilde{h}^-, P\tilde{h}^-)_B, \tag{13}$$

where P is the parity operator in velocity space, defined by $P[h(\mathbf{c})] = h(-\mathbf{c})$, while $((,))$, $(,)_B$ denote two scalar products:

$$((h, g)) = \pi^{-3/2} \int_{-d/2}^{+d/2} \int_{-\infty}^{+\infty} \exp(-c^2) h(x, \mathbf{c}) g(x, \mathbf{c}) \, d\mathbf{c} dx \tag{14}$$

$$(h^\pm, g^\pm)_B = \pi^{-3/2} \int_{\partial\Omega} \int_{c_x > 0} c_x \exp(-c^2) h^\pm(\mathbf{c}) g^\pm(\mathbf{c}) \, d\mathbf{c} d\sigma \, . \tag{15}$$

In the one-dimensional case, the integration over the boundary $\partial\Omega$ reduces to the sum of the terms at $x = \pm d/2$.

The functional $J(\tilde{h})$ attains its minimum value when $\tilde{h} = h(x, \mathbf{c})$ solves Eq. (12) with appropriate boundary conditions. If we let $\tilde{h} = h$, Eq. (13) gives:

$$J(h) = -((PS, h)) = -k \int_{-d/2}^{d/2} v_z(x) dx - \tau \int_{-d/2}^{d/2} q_z(x) dx = -k \frac{\dot{M}}{\rho} - \tau \dot{Q}. \tag{16}$$

Thus, the stationary value of J has a direct connection with the quatities of physical interest for the problem at hand. Within the framework of a linearized analysis, the mass and heat flow rates, per unit width, can be expressed by the sum of the Poiseuille and thermal-creep contributions:

$$\dot{M} = d^2 \, p \, [-G_p \, k + G_T \, \tau] \tag{17}$$

$$\dot{Q} = \frac{d^2}{2} \, p \, [Q_p \, k - Q_T \, \tau] \tag{18}$$

where G_p, G_T, Q_p and Q_T are dimensionless coefficients (defined to be always positive) that represent the Poiseuille coefficient, the thermal-creep coefficient, the mechanocaloric coefficient and the reduced heat flux, respectively. In the papers [33], [34], [35], it was proven that the cross coefficients G_T and Q_p obey the Onsager relation:

$$G_T = Q_p. \tag{19}$$

Since the purpose of the present investigation is to provide an analytic expression for the slip coefficients, it is sufficient to consider asymptotic results (near-continuum) for mass flow rates. Therefore, the following simplified test function has been used to evaluate Eq. (13):

$$\tilde{h}(x,\mathbf{c}) = 2Ac_z(x^2 - 2xc_x\theta + 2{c_x}^2\theta^2) + 2c_z\left(C - \frac{k\theta}{2}\right) - B\tau\theta c_z\left(c^2 - \frac{5}{2}\right) \tag{20}$$

where A, B and C are adjustable constants to be varied in order to obtain the best value of $J(\tilde{h})$ and θ is a length parameter that will be specified in the following. To obtain the test function (20), the solution of the BGK-Boltzmann equation, in integral form, has been considered, where the bulk velocity profile has been approximated by

$$\tilde{v}_z(x) = Ax^2 + C \tag{21}$$

with the adjustable constants A and C being represented as:

$$A = A_p + A_T, \quad C = C_p + C_T \tag{22}$$

due to the linear superposition of the Poiseuille and thermal-creep effects. Further and more precise details, related to the derivation of the test function, have been reported in a paper in preparation. It is worth noting that the trial function (20) exhibits an analogous dependence on x and $\mathbf{c}$ as the asymptotic form of the test function obtained in [33] via the use of the well-known Chapman-Enskog procedure.

Let us now rescale all variables appearing in Eq. (20) as follows:

$$\delta = \frac{d}{\theta}, \quad A = \frac{A}{\theta^2}. \tag{23}$$

If one substitute $\tilde{h}$, given by (20), in Eq. (13) and splits the constants as in (22), with the following normalization

$$\hat{A}_p = \frac{A_p}{(k\theta)}, \quad \hat{C}_p = \frac{C_p}{(k\theta)}, \quad \hat{A}_T = \frac{A_T}{(\tau\theta)}, \quad \hat{C}_T = \frac{C_T}{(\tau\theta)} \tag{24}$$

the functional $J(\tilde{h})$ is reduced to the sum of three functionals: $J^{(1)}(\tilde{h}), J^{(2)}(\tilde{h}), J^{(3)}(\tilde{h})$, simply grouping together the terms proportional to $(k\theta)^2$, $(\tau\theta)^2$ and $(k\theta)(\tau\theta)$, respectively. Each functional is a polynomial of the second order with respect to the constants A_p, A_T, B, C_p, C_T, that are to be determined:

$$J^{(1)}(\tilde{h})/(k\theta)^2 = (\sqrt{\pi})^{-1} \times \left\{ \frac{c_{11}}{2} A_p^2 + \frac{c_{22}}{2} C_p^2 + c_{12} A_p C_p - c_1 A_p - c_2 C_p + \frac{1}{2}(c_2 - c_{22}/4) \right\}, \quad (25)$$

$$J^{(2)}(\tilde{h})/(\tau\theta)^2 = (\sqrt{\pi})^{-1} \times \left\{ \frac{c_{11}}{2} A_T^2 + \frac{d_{22}}{2} B^2 + \frac{c_{22}}{2} C_T^2 + + d_{12} A_T B + c_{12} A_T C_T - d_1 A_T - d_2 B + d_{23} B C_T \right\}, \quad (26)$$

$$J^{(3)}(\tilde{h})/[(k\theta)(\tau\theta)] = (\sqrt{\pi})^{-1} \times \left\{ c_{11} A_p A_T + c_{22} C_p C_T + c_{12}(A_p C_T + A_T C_p) - d_1 A_p - c_1 A_T - c_2 C_T + d_{12} A_p B + d_{23} B C_p - \frac{d_{23}}{2} B \right\}. \quad (27)$$

The explicit expressions for the coefficients appearing in Eqs. (25)-(27) are reported in Appendix A. The derivatives of $J^{(1)}(\tilde{h})/(k\theta)^2$, $J^{(2)}(\tilde{h})/(\tau\theta)^2$, $J^{(3)}(\tilde{h})/[(k\theta)(\tau\theta)]$, with respect to A_p, A_T, B, C_p, C_T vanish in correspondence of the optimal values of these constants. The resulting expressions for the minimum of these functionals are

$$min \frac{J^{(1)}(\tilde{h})}{(k\theta)^2} = (8\sqrt{\pi})^{-1} \left[c_{11} c_{22} - c_{12}^2 \right]^{-1} \left[8 c_{12} c_1 c_2 - 4 c_1^2 c_{22} + c_{12}^2 (c_{22} - 4 c_2) - c_{11} (c_{22} - 2 c_2)^2 \right] \quad (28)$$

$$min \frac{J^{(2)}(\tilde{h})}{(\tau\theta)^2} = (2\sqrt{\pi})^{-1} \left[c_{11} c_{22} d_{22} - d_{12}^2 c_{22} - c_{11} d_{23}^2 + 2 c_{12} d_{12} d_{23} - c_{12}^2 d_{22} \right]^{-1} \times \left[-d_1^2 d_{22} c_{22} - c_{11} d_2^2 c_{22} + 2 d_1 d_{12} d_2 c_{22} + d_1^2 d_{23}^2 - 2 d_1 c_{12} d_2 d_{23} + c_{12}^2 d_2^2 \right] \quad (29)$$

$$min \frac{J^{(3)}(\tilde{h})}{(k\theta)(\tau\theta)} = (2\sqrt{\pi})^{-1} \left[c_{11} c_{22} d_{22} - d_{12}^2 c_{22} - c_{11} d_{23}^2 + 2 c_{12} d_{12} d_{23} - c_{12}^2 d_{22} \right]^{-1} \times \left[-d_1 c_{12} d_{23}^2 + 2 c_1 d_1 d_{23}^2 - d_2 c_{11} c_{22} d_{23} + 2 c_2 d_2 c_{11} d_{23} + d_2 c_{12}^2 d_{23} - 2 c_1 d_2 c_{12} d_{23} + d_1 c_{22} d_{12} d_{23} - 2 c_2 d_1 d_{12} d_{23} - 2 c_1 d_1 c_{22} d_{22} + 2 c_2 d_1 c_{12} d_{22} + 2 c_1 d_2 d_{12} c_{22} - 2 c_2 d_2 c_{12} d_{12} \right]. \quad (30)$$

Let us now go back to Eq. (16). Since the functional J can be split into three parts and the relations (17) and (18) hold, it is easy to see that the computation of the optimal

value of $J^{(1)}(\tilde{h})/(k\theta)^2$, $J^{(2)}(\tilde{h})/(\tau\theta)^2$, $J^{(3)}(\tilde{h})/[(k\theta)(\tau\theta)]$ (Eqs.(28)-(30)), will lead to an accurate estimate of the Poiseuille coefficient G_p, the thermal-creep coefficient G_T, and the reduced heat flux Q_T:

$$G_p = \frac{2}{\delta^2}\frac{J^{(1)}(h)}{(k\theta)^2}, \tag{31}$$

$$G_T = -\frac{1}{\delta^2}\frac{J^{(3)}(h)}{(k\theta)(\tau\theta)}, \tag{32}$$

$$Q_T = \frac{2}{\delta^2}\frac{J^{(2)}(h)}{(\tau\theta)^2}. \tag{33}$$

IV. THERMAL SLIP COEFFICIENTS

The variational method is a powerful technique for finding approximate closed-form solutions to the Boltzmann equation. In particular, this approach has proved useful in computing parameters to be employed in classical hydrodynamical equations, when low working pressures impose corrections due to gas rarefaction effects. A typical example is the derivation of slip coefficients needed to modify the boundary conditions associated with the Navier-Stokes equations. For pressure-driven flows, assuming a first-order boundary condition at a flat wall, in the isothermal case, the slip velocity reads as

$$v_s = \sigma_p \lambda \left(\frac{\partial v}{\partial x}\right)_w, \tag{34}$$

where σ_p is the viscous-slip coefficient, λ is the mean free path of the molecules and the gas-velocity gradient is evaluated at the wall. Likewise, for thermal-driven flows, one can write the following first-order slip boundary condition on a flat wall:

$$v_s = \sigma_T \frac{\mu}{\rho T}\left(\frac{\partial T}{\partial z}\right)_w, \tag{35}$$

where σ_T is the thermal slip coefficient, μ is the gas viscosity, and the temperature gradient is evaluated at the wall. Both the viscous and thermal slip coefficients can be calculated indirectly, by extracting them from asymptotic near-continuum solutions for the Poiseuille and thermal-creep flows, respectively. Concerning the viscous slip coefficients, by this time, it is generally accepted that the classical hydrodynamical equations

can supply realistic results well beyond the slip region, provided that higher-order boundary conditions are employed. In particular, the variational principle introduced in Section III has been used to predict first- and second-order viscous slip coefficients on the basis of the linearized Boltzmann equation for hard-sphere molecules with the Maxwell[36] as well as the Cercignani-Lampis boundary conditions[37]. Then, the variational outputs have been compared with recent experimental results, revealing a very good agreement[38],[39]. On the contrary, the reliability of a higher-order solution for the temperature-driven mass flow rate and the existence of a 'second-order' thermal slip coefficient (where we indicate with 'second-order' a term of next-order with respect to the leading one) have not yet been well assessed. Therefore, in the following, we will focus on the derivation of the asymptotic near-continuum solution for the thermal-creep mass flow, by means of the variational technique presented in Section III, in order to predict thermal slip coefficients. The present investigation is mostly guided by the desire to interpret some recent experimental studies[25] and to define the upper limit in the Knudsen number, within which a second-order description of the flow accurately holds.

A. Theoretical derivation

When the linearized Boltzmann equation for hard-sphere molecules is considered and the Cercignani-Lampis scattering kernel is used to describe the gas-wall interaction, Eqs. (30) and (32) give in the limit $\delta >> 1$,

$$G_T = \frac{\sigma_1}{\delta} + \frac{\sigma_2}{\delta^2} + \cdots \tag{36}$$

where

$$\sigma_1 = \left[64\hat{J}_4\left(\frac{2\hat{J}_1}{\pi^{3/2}}+1\right)\right]^{-1}\left[16\left(5\hat{J}_1 - 10\hat{J}_3 + 2\hat{J}_4\right) + 10\,\pi^{3/2}\left(\alpha_t + \alpha_n - \alpha_t\alpha_n + 4\right)\right], \tag{37}$$

$$\sigma_2 = [2\sqrt{\pi}\mathcal{A}]^{-1}\left[\frac{\mathcal{B}\mathcal{C}}{\mathcal{A}} - \mathcal{E}\right], \quad \mathcal{A} = \frac{32\,\hat{J}_4\,\alpha_t}{3\sqrt{\pi}}\left[\frac{2\hat{J}_1}{\pi^{3/2}}+1\right], \tag{38}$$

$$\begin{aligned}\mathcal{B} = &-\frac{128}{\pi}\hat{J}_4\alpha_t(1-\alpha_t)\left[\mathcal{F}_0\alpha_n + \mathcal{F}_1(1-\alpha_n)\right] - 8\alpha_t\hat{J}_4\left[\frac{4}{\pi}+\alpha_t\right] \\ &+ \frac{16}{3}\sqrt{\pi}\alpha_t\left[\alpha_n + 7\,\alpha_t + 2\,\alpha_t^3 - 6\,\alpha_t^2 - \alpha_t\,\alpha_n\right]\left[\frac{2\hat{J}_1}{\pi^{3/2}}+1\right],\end{aligned} \tag{39}$$

$$\mathcal{C} = -\frac{16}{3}\alpha_t\left[5\,\hat{J}_1 - 10\,\hat{J}_3 + 2\,\hat{J}_4\right] - \frac{10}{3}\pi^{3/2}\alpha_t\left[\alpha_t + \alpha_n - \alpha_t\,\alpha_n + 4\right], \tag{40}$$

$$\mathcal{E} = -32\sqrt{\pi}\alpha_t\left[5\,\hat{J}_3 - \hat{J}_4\right] + 160\pi\alpha_t(1-\alpha_t)\left[\mathcal{F}_0\alpha_n + \mathcal{F}_1(1-\alpha_n)\right] + 10\pi^2\alpha_t \times \left[2\,\alpha_t + \alpha_n - \alpha_t\,\alpha_n\right] - \frac{32}{3}\pi\alpha_t\left[\alpha_t - 2\,\alpha_n - 3\,\alpha_t^2 + \alpha_t^3 + 2\,\alpha_t\,\alpha_n - \frac{15}{4}\right], \tag{41}$$

with $\hat{J}_1 = -1.4180$, $\hat{J}_2 = 1.8909$, $\hat{J}_3 = 0.9449$, $\hat{J}_4 = 4.7252$ and $\mathcal{F}_0 = 0.196079$, $\mathcal{F}_1 = 0.247679$. The rarefaction parameter δ has been defined in (23), where θ is conveniently chosen in order to use the same definition as in the experiments described in the next Section. A comparison between the expression (36) and the thermal-driven mass flow rate, obtained by using the Navier-Stokes equations with slip boundary conditions (35)[2], allows one to identify σ_1 with the first-order thermal slip coefficient σ_T, while σ_2 can be referred to as the 'second-order' thermal slip coefficient.

B. Experimental measurements

The authors of Ref. [25] measured the temperature driven mass flow rate through a microchannel with a rectangular cross-section, over a wide range of the gas-rarefaction parameter. A microchannel made of PEEK with a height of $d = 0.22 \pm 0.01\,\mathrm{mm}$, width of $w = 6\,\mathrm{mm}$, and length of $L = 73\,\mathrm{mm}$ was employed. The temperature of the hot reservoir T_H and that of the cold reservoir T_C were maintained to realize two temperature differences ΔT : 1) $T_\mathrm{H} = 347.1 \pm 0.5\,\mathrm{K}$, $T_\mathrm{C} = 289.2 \pm 0.2\,\mathrm{K}$, where $\Delta T = 57.9\,\mathrm{K}$ and 2) $T_\mathrm{H} = 337.0 \pm 0.6\,\mathrm{K}$, $T_\mathrm{C} = 299.6 \pm 0.4\,\mathrm{K}$, where $\Delta T = 37.4\,\mathrm{K}$. Such temperature differences were chosen to have the same mean temperature $T_\mathrm{m} = (T_\mathrm{C} + T_\mathrm{H})/2 = 318\,\mathrm{K}$.

In Ref. [25], only measurements of the thermal-creep flow have been carried out. In this case, the mass flow rate is given by the second term on the right-hand side of Eq. (17), modified as follows, in order to take into account a rectangular channel of width w:

$$\dot{M} = d^2\,p\,w\,G_T\,\frac{1}{T}\frac{dT}{dz}. \tag{42}$$

Since the channel width-to-height ratio is equal to 27.3, the lateral-wall effects can be neglected[40],[41] and one can use for the dimensionless thermal-creep coefficient G_T the expression obtained for a gas flowing between two parallel plates separated by a distance

d. In the expression (42), G_T is a function of the local rarefaction parameter δ. Since in the experiments the variation of δ along the channel is not so large, it can be assumed that $G_T(\delta)$ is well approximated by $G_T(\delta_{\rm m})$, where the mean rarefaction parameter $\delta_{\rm m}$ is calculated using the mean temperature $T_{\rm m}$:

$$\delta_{\rm m} = \frac{p\,d}{\mu(T_{\rm m})\sqrt{2RT_{\rm m}}}. \tag{43}$$

In Ref. [25] (Table 1) the experimentally determined values of G_T have been reported as function of $\delta_{\rm m}$, for different noble gases.

Beyond the mass flow rates, the experimental data presented in Ref. [25] have been used to extract the thermal slip coefficients. By solving the Stokes equation, with the first-order thermal slip boundary condition (35), the mass flow rate reads:

$$\dot{M} = \sigma_T\, d\, w \frac{\mu}{T}\frac{dT}{dz}. \tag{44}$$

Let us assume the following dependence of the gas viscosity μ on temperature T[42]:

$$\mu = \mu_{\rm ref}\left(\frac{T}{T_{\rm ref}}\right)^{\omega} \tag{45}$$

where $\mu_{\rm ref}$ is the viscosity coefficient at the temperature $T_{\rm ref}$ and ω is the viscosity index. Inserting (45) in (44), one obtains:

$$\dot{M} = \sigma_T\, d\, w \frac{\mu_{\rm ref}}{T_{\rm ref}^{\omega}}\mathcal{F} \tag{46}$$

where

$$\mathcal{F} = T^{\omega-1}\frac{dT}{dz}. \tag{47}$$

Since the temperature profile along the channel was not measured in the experiments, the term $\mathcal{F}$ in (46) has been substituted by its mean value, $\overline{\mathcal{F}}$, calculated by integrating (47) along the channel:

$$\overline{\mathcal{F}} = \frac{T_{\rm H}^{\omega} - T_{\rm C}^{\omega}}{\omega\, L}. \tag{48}$$

Therefore, taking into account (46) and (48), the first-order thermal slip coefficient can be extracted from the experimental measurements of the mass flow rate as follows:

$$\frac{\dot{M}}{\dot{M}_{\rm ref}} = \sigma_1^{\rm exp} \tag{49}$$

where

$$\dot{M}_{\rm ref} = \frac{d\, w\, \mu_{\rm ref}}{T_{\rm ref}^{\omega}} \frac{(T_{\rm H}^{\omega} - T_{\rm C}^{\omega})}{\omega\, L}. \tag{50}$$

In Eq. (49) we have indicated with $\sigma_1^{\rm exp}$ the first-order thermal slip coefficient σ_T to highlight that it is the experimentally-determined value. The experimental data reveal that the value of $\sigma_1^{\rm exp}$, for different gases, can be considered to be independent of the rarefaction parameter $\delta_{\rm m}$ and of the temperature difference ΔT.

In order to extract a second-order slip coefficient from the measurements, and mostly to improve the accuracy of the first order coefficient extraction, one can resort to Eq. (42) with G_T given by its asymptotic expression (36):

$$G_T \simeq \frac{\sigma_1^{\rm exp}}{\delta} + \frac{\sigma_2^{\rm exp}}{\delta^2}. \tag{51}$$

In Eq. (51), we have renamed the two coefficients σ_1, σ_2, appearing in (36), with $\sigma_1^{\rm exp}$ and $\sigma_2^{\rm exp}$ to highlight that the latter are experimentally-determined coefficients. Integrating along the channel the resulting expression (by using the property of mass conservation) with μ given by (45) and δ substituted by its mean value $\delta_{\rm m}$ (43), one obtains:

$$\dot{M} = \dot{M}_{\rm ref} \left[\sigma_1^{\rm exp} + \frac{\sigma_2^{\rm exp}}{\delta_{\rm m}} \sigma + \mathcal{O}\left(\frac{1}{\delta_{\rm m}^2}\right) \right] \tag{52}$$

where $\dot{M}_{\rm ref}$ is reported in (50) and

$$\sigma = \frac{[T_{\rm H}^{2\omega+0.5} - T_{\rm C}^{2\omega+0.5}]}{[(2\omega+0.5) T_{\rm m}^{\omega+0.5}]} \frac{\omega}{[T_{\rm H}^{\omega} - T_{\rm C}^{\omega}]}. \tag{53}$$

Since it was found that the constant σ is quite close to unity, the measured data on the mass flow rate can be fitted in the form:

$$\frac{\dot{M}}{\dot{M}_{\rm ref}} = \sigma_1^{\rm exp} + \frac{\sigma_2^{\rm exp}}{\delta_{\rm m}} \tag{54}$$

where $\sigma_1^{\rm exp}$ and $\sigma_2^{\rm exp}$ are the experimentally-determined first- and second-order thermal slip coefficients, respectively. The asymptotic formula (52) allows one to predict the mass flow rate also in the early transition regime. Therefore, the fitting procedure has been carried out in the range of $\delta_{\rm m} = [3, 40]$. The validity of this interval has been assessed

in the next Section, on the basis of our theoretical computations. The values of $\sigma_1^{\rm exp}$ and $\sigma_2^{\rm exp}$ are listed in Ref. [25] (Table 3), for both $\Delta T = 57.9\,{\rm K}$ and $\Delta T = 37.4\,{\rm K}$, and for five different noble gases: Helium (He), Neon (Ne), Argon (Ar), Krypton (Kr) and Xenon (Xe).

V. RESULTS AND DISCUSSION

To test the reliability of our variational approach, we list in Table I the values of the first-order slip coefficient σ_1, computed by using Eq. (37), along with the results for the thermal slip coefficient reported in Ref. [2] (Table 10) as deduced from a strictly numerical solution of the linearized Boltzmann equation for rigid-sphere collisions[43] and of the S-model[44],[22]. As shown in the table, the agreement between the three methods of solution is fairly good. The variational outputs overstate those derived from the linearized Boltzmann equation (the relative error lies within 10%) and understate the findings obtained through the S-model (the relative error lies within 5%), for each value of the accommodation coefficients, α_t and α_n. The better agreement between the variational results and those obtained on the basis of the S-model is likely related to the different numerical approximations involved in solving the true linearized Boltzmann equation and a simplified kinetic model. In both references [43], [44], the scattering kernel is written in the expanded form, originally given by Pekeris-Alterman[45]. But, while for rigid-sphere collisions the component functions k_n, appearing in the series representation of the scattering kernel, are required for all n, the S-model is obtained in closed-form by putting $k_n = 0$ for $n > 1$. Therefore, a truncated version of the scattering kernel has been considered for the numerical solution of the linearized Boltzmann equation reported in [43]. Furthermore, the author of Ref. [43] pointed out that additional numerical work was required to implement the Cercignani-Lampis boundary conditions, leading to a significantly more intensive computation, due to the numerical evaluation of repeated integrals. On the contrary, in the present paper, the variational method has been used to solve the true linearized Boltzmann equation for hard-sphere molecules without approximation in its form. Even the integrals specific to the CL-boundary conditions have been computed analytically. The only approximation involved in our analysis is related to the test-function. However, it is worth mentioning that there exist several basic theorems which allow to perform a good choice. In our context, then, this choice is even simpler since the func-

tions which need to be approximated by trial functions are solutions of physically realistic problems and especially in their asymptotic forms can be immediately obtained via the use of the Chapman-Enskog procedure or via the solution of the Boltzmann equation in integral form based on a simplified kinetic model. It is worth noting that in the review paper [2], the author recommends to use, for practical calculations in the case of diffuse re-emission, the following value of the thermal-slip coefficient $\sigma_1 = 1.1$, which is identical to the value obtained through our variational computations, when $\alpha_t = \alpha_n = 1$. Finally, it is important to underline that the use of rigid spheres does not represent a limitation with respect to the generality of the results, since in the range of the gas rarefaction considered here, $\delta \geq 3$, the influence of the intermolecular interaction potential is very small[23].

Since the present investigation is mostly guided by the desire to interpret some recent experimental studies[25], where the thermal slip coefficients were computed starting from mass flow rate measurements, in Table II we list the experimental estimates for σ_1 and σ_2 (see Section IV B). We have also included in Table II the first- and second-order thermal slip coefficients computed on the basis of our variational technique applied to the linearized Boltzmann equation for a hard-sphere gas, for specific values of the accommodation coefficients, α_t and α_n, chosen to provide results as close as possible to the experimental measurements. As revealed by the table, the agreement between our variational outputs and the experimental data is quite good, for each of the five noble gases considered. This outcome assumes particular relevance, since the experimental measurements presented in [25] and summarized in Section IV B had not yet received a satisfactory explanation on the basis of the theoretical findings obtained by the linearized Boltzmann equation, in the frame of Maxwell's model for boundary conditions.

Looking at the data reported in Table II, one can infer that, by increasing the molecular weight of the different gases, the values of both accommodation coefficients, α_t and α_n, also increase. The same trend has been already pointed out in Ref. [2] (Table 6) for the values of α_t extracted from the experimentally-determined first-order viscous slip coefficients. Since the exact domain of the existence of the slip flow regime is still a debated issue, our variational analysis can be considered a useful tool in order to define the upper limit in the rarefaction parameter, within which a second-order description of the flow accurately holds. To this end, the variational calculations showing the dimensionless thermal-creep mass flow rate G_T, computed through the truncated formula (36), versus the rarefaction

TABLE I. The first-order thermal slip coefficient σ_1 for the CL boundary conditions. Comparison between our outputs (variational method applied to the Boltzmann equation for a hard-sphere gas (Var.(HS)), the numerical results based on the S-model[44],[22] and those obtained by a direct solution of the linearized Boltzmann equation with hard spheres molecules (Num.(HS))[43].

α_t		$\alpha_n = 0.25$	$\alpha_n = 0.5$	$\alpha_n = 0.75$	$\alpha_n = 1.$
0.5	S − model[44], [22]	1.034	1.081	1.127	1.172
	Var.(HS)	0.971	1.018	1.065	1.111
	Num.(HS)[43]	0.915	0.954	0.991	1.028
0.75	S − model[44], [22]	1.107	1.129	1.152	1.174
	Var.(HS)	1.041	1.065	1.088	1.111
	Num.(HS)[43]	0.964	0.982	1.001	1.019
1.	S − model[44], [22]	1.175	1.175	1.175	1.175
	Var.(HS)	1.111	1.111	1.111	1.111
	Num.(HS)[43]	1.018	1.018	1.018	1.018
1.25	S − model[44], [22]	1.240	1.219	1.197	1.175
	Var.(HS)	1.182	1.158	1.135	1.111
	Num.(HS)[43]	1.071	1.053	1.035	1.017
1.5	S − model[44], [22]	1.305	1.264	1.221	1.177
	Var.(HS)	1.252	1.205	1.158	1.111
	Num.(HS)[43]	1.114	1.080	1.044	1.008

parameter δ, are presented in Table III.

Our theoretical findings are compared with the numerical results obtained in Ref. [23] (Table 1) on the basis of the linearized Boltzmann equation for hard-spheres and of the S-model[46]. As revealed by Table III, the validity of the second-order slip model, given by Eq. (36), extends up to $\delta \simeq 3$, if one wants that the error lies within 10% for all values of

TABLE II. Experimental estimates for the first- (σ_1) and second-order (σ_2) slip coefficients[25]. Our variational outputs (Var.(HS)), based on the linearized Boltzmann equation for a hard-sphere gas and CL boundary conditions, are also included for specific values of the accommodation coefficients (α_t, α_n), chosen to provide results as close as possible to the experimental measurements.

	Experiments[25]		Var.(HS)				
	$\sigma_1^{\rm exp}$	$\sigma_2^{\rm exp}$	σ_1	σ_2	α_t	α_n	$\Delta_{\rm max}$
He	1.006 ± 0.020	-1.147 ± 0.113	1.0481	-1.1334	0.8	0.15	4.2%
Ne	0.998 ± 0.029	-1.226 ± 0.172	1.0556	-1.1718	0.8	0.25	5.7%
Ar	1.017 ± 0.057	-1.274 ± 0.406	1.0659	-1.2255	0.83	0.28	4.8%
Kr	1.061 ± 0.053	-1.327 ± 0.400	1.0817	-1.3083	0.88	0.33	1.9%
Xe	1.102 ± 0.085	-1.746 ± 0.626	1.1509	-1.6881	1.16	0.35	4.4%

the accommodation coefficients, α_t and α_n. Once the range of validity of the truncated formula (36) has been assessed, we have reported in Table IV a comparison between the experimental data on the mass flow rate G_T for Helium, Neon and Argon (see Table 1 in [25]) and our variational results obtained by fixing the values of the accommodation coefficients for each gas, as shown in Table II. As revealed by Table IV, the agreement between the theoretical outputs and the experimental measurements is fairly good, for each gas, with $5 - 10\%$ of error comparable to the experimental accuracy.

TABLE III. Thermal-creep mass flow rate G_T for the CL- boundary conditions. Comparison between our variational outputs (Var.(HS)), the numerical results based on the S-model[46] and those obtained by a direct solution of the linearized Boltzmann equation with hard spheres molecules (LBE(HS))[23].

δ	α_t		$\alpha_n = 0.25$	$\alpha_n = 0.5$	$\alpha_n = 0.75$	$\alpha_n = 1.$
3.5	0.25	S − model[46]	0.2084	0.2082	0.2083	0.2084
		Var.(HS)	0.2186	0.2145	0.2082	0.1997
	0.5	S − model[46]	0.2055	0.2056	0.2057	0.2058
		Var.(HS)	0.2153	0.2106	0.2049	0.1982
		LBE(HS)[23]	0.201	0.203	0.204	0.206
	0.75	S − model[46]	0.2046	0.2047	0.2048	0.2048
		Var.(HS)	0.2078	0.2047	0.2013	0.1977
	1.0	S − model[46]	0.2046	0.2047	0.2047	0.2047
		Var.(HS)	0.1976	0.1976	0.1976	0.1976
		LBE(HS)[23]	0.202	0.202	0.202	0.202
10.	0.25	S − model[46]	0.08592	0.08997	0.09400	0.09794
		Var.(HS)	0.08533	0.08941	0.09321	0.09673
	0.5	S − model[46]	0.09018	0.09290	0.09556	0.09819
		Var.(HS)	0.08950	0.09198	0.09433	0.09655
		LBE(HS)[23]	0.0834	0.0861	0.0887	0.0912
	0.75	S − model[46]	0.09419	0.09554	0.09684	0.09814
		Var.(HS)	0.09315	0.09430	0.09541	0.09649
	1.0	S − model[46]	0.09808	0.09813	0.09813	0.09813
		Var.(HS)	0.09648	0.09648	0.09648	0.09648
		LBE(HS)[23]	0.0900	0.0900	0.0900	0.0900
20.	0.25	S − model[46]	0.04519	0.04794	0.05066	0.05333
		Var.(HS)	0.04385	0.04663	0.04934	0.05198
	0.5	S − model[46]	0.04830	0.05019	0.05200	0.05380
		Var.(HS)	0.04665	0.04844	0.05020	0.05193
		LBE(HS)[23]	0.0437	0.0454	0.0470	0.0485
	0.75	S − model[46]	0.05111	0.05206	0.05294	0.05383
		Var.(HS)	0.04932	0.05020	0.05106	0.05192
	1.0	S − model[46]	0.05378	0.05383	0.05383	0.05383
		Var.(HS)	0.05192	0.05192	0.05192	0.05192
		LBE(HS)[23]	0.0480	0.0480	0.0480	0.0480
100.	0.25	S − model[46]	0.00938	0.01008	0.01077	0.01144
		Var.(HS)	0.00896	0.00963	0.01030	0.01097
	0.5	S − model[46]	0.01015	0.01064	0.01108	0.01152
		Var.(HS)	0.009635	0.01008	0.01053	0.01097
		LBE(HS)[23]	0.0091	0.0094	0.0098	0.0102
	0.75	S − model[46]	0.01085	0.01110	0.01132	0.01154
		Var.(HS)	0.01030	0.01053	0.01075	0.01097
	1.0	S − model[46]	0.01151	0.01154	0.01154	0.01154
		Var.(HS)	0.01097	0.01097	0.01097	0.01097
		LBE(HS)[23]	0.0101	0.0101	0.0101	0.0101

TABLE IV. Comparison between the measured mass flow rate G_T of Helium, Neon and Argon (Expt.)[25] and our variational outputs (Var.(HS)), based on the linearized Boltzmann equation for a hard-sphere gas and CL boundary conditions. In order to obtain the variational results, the accommodation coefficients α_t, α_n have been fixed, for each gas, as reported in Table II.

	He			Ne			Ar	
δ	Expt.	Var.(HS)	δ	Expt.	Var.(HS)	δ	Expt.	Var.(HS)
3.22	0.204	0.2162	3.14	0.208	0.2173	3.38	0.199	0.2081
3.47	0.196	0.2079	3.48	0.190	0.2065	4.01	0.175	0.1896
3.71	0.188	0.2002	3.83	0.182	0.1957	4.73	0.169	0.1706
4.33	0.178	0.1816	4.18	0.175	0.1854	5.37	0.153	0.1560
4.94	0.156	0.1657	4.52	0.162	0.1762	6.04	0.127	0.1429
5.57	0.140	0.1516	4.87	0.154	0.1673	6.72	0.125	0.1315
6.19	0.132	0.1397	5.24	0.148	0.1587	7.41	0.119	0.1215
6.80	0.130	0.1296	6.09	0.134	0.1417	8.08	0.102	0.1131
7.41	0.115	0.1208	6.94	0.119	0.1277	8.75	0.106	0.1058
8.04	0.107	0.1128	7.83	0.108	0.1157	9.41	0.0989	0.09944
8.67	0.0996	0.10581	8.70	0.099	0.1058	10.1	0.0874	0.09352
9.28	0.0987	0.09978	9.55	0.089	0.09768	11.7	0.0751	0.08215
9.90	0.0918	0.09430	10.4	0.087	0.09066	13.4	0.0698	0.07272
10.5	0.0871	0.08954	11.3	0.077	0.08424	15.1	0.0654	0.06522
11.1	0.0803	0.08522	12.2	0.072	0.07865	16.8	0.0638	0.05911
11.7	0.0800	0.08130	13.1	0.072	0.07375	18.5	0.0533	0.05404
			13.9	0.069	0.06987	20.2	0.0496	0.04976
			14.8	0.059	0.06597	21.8	0.0453	0.04632
			15.7	0.062	0.06248	23.6	0.0393	0.04296
			16.5	0.056	0.05967	25.2	0.0377	0.04037
						26.9	0.0388	0.03793
						28.6	0.0323	0.03577
						30.3	0.0349	0.03384
						31.9	0.0279	0.03221

VI. CONCLUDING REMARKS

In the present study, we have investigated the Poiseuille and thermal-creep problems of a rarefied gas between two parallel plates, by means of a variational technique which applies to the integrodifferential form of the Boltzmann equation, based on the true linearized collision operator and the Cercignani-Lampis scattering kernel of the gas-surface interaction. A second-order slip model for the temperature-driven (thermal-creep) mass flow rate has been proposed on the basis of the variational analysis. In addition, new analytical expressions for the thermal slip parameters have been provided, in terms of the tangential momentum α_t and the normal energy α_n accommodation coefficients. The theoretical results for the first- and second-order thermal slip coefficients have been compared with the experimental data reported in Ref. [25] for five noble gases (Helium, Neon, Argon, Krypton and Xenon) and, for each of them, the accommodation coefficients α_t and α_n have been extracted. Then, these values of α_t and α_n have been used to evaluate the temperature-driven mass flow rates in the frame of our variational analysis and the outputs have been compared with the measurements for Helium, Neon and Argon[25]. The good agreement obtained between the theoretical and the experimental data, within the range of validity of the proposed second-order slip model, suggests that the Cercignani-Lampis boundary conditions, unlike the Maxwell model, can conveniently be used to describe non-isothermal gas flows. Instead, the authors of Ref. [23] came to the opposite conclusion relying on a comparison of their numerical results with the same experimental data[25]. However, the approach used in Ref. [23] to find a pair of accommodation coefficients is different from the method applied in the present paper. In Ref. [23], the accommodation coefficients α_t and α_n have been selected to provide the best agreement between the mass flow rate measurements of thermal creep flow and the numerical calculations, as the rarefaction parameter δ changes. Indeed, the authors of Ref. [23] were unable to obtain values of the accommodation coefficients α_t, α_n that could provide a good agreement with the experimental data of the mass flow rate over a wide range of gas rarefaction. Of course, when a model with more than one free parameter is considered, there may be different combinations of the coefficients that produce equally good results, at least locally. The advantage of the method proposed in the present paper is that the two accommodation coefficients α_t, α_n are preliminarily determined by imposing that the first- and second-order thermal-slip coefficients theoretically derived can

closely reproduce the experimental data. These two constraints allowed us to uniquely determine α_t and α_n, and indeed the match, that we have obtained with the measured values of the temperature-driven mass flow rates for Helium, Neon and Argon, is quite good even beyond the range of validity of the proposed second-order slip model.

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Appendix A: Explicit form of the variational coefficients

In the following we report the explicit expression of the coefficients appearing in Eqs. (25)-(27):

$$\begin{aligned} c_{11} = &-\frac{\delta^4}{4}\alpha_t - \frac{4}{3}\sqrt{\pi}\delta^3 + \sqrt{\pi}\delta^3\alpha_t + 4\delta^2 - 4\delta^2\alpha_t - 4\sqrt{\pi}\delta\alpha_n\alpha_t + 12\sqrt{\pi}\delta\alpha_t + 4\sqrt{\pi}\delta\alpha_n \\ &+ 16\alpha_n\alpha_t - 32\alpha_t - 16\alpha_n - \frac{8}{3\pi}\delta^3\hat{J}_1 - \frac{32}{\pi}\delta\hat{J}_2 + 16\delta^2\mathcal{F}_0\alpha_n(1-\alpha_t) \\ &+ 16\delta^2\mathcal{F}_1(1-\alpha_t)(1-\alpha_n), \end{aligned} \tag{A1}$$

$$c_{12} = -\delta^2\alpha_t + 2\sqrt{\pi}\delta\alpha_t - 8\alpha_t, \quad c_{22} = -4\alpha_t, \tag{A2}$$

$$c_1 = \frac{\sqrt{\pi}}{6}\delta^3 - \frac{\delta^2}{2}\alpha_t + 2\sqrt{\pi}\delta + \sqrt{\pi}\delta\alpha_t - 4\alpha_t, \quad c_2 = 2\sqrt{\pi}\delta - 2\alpha_t, \tag{A3}$$

$$d_{12} = \frac{\delta^2}{4}\alpha_t + \frac{\sqrt{\pi}}{2}\delta\alpha_n\alpha_t - \sqrt{\pi}\delta\alpha_t - \frac{\sqrt{\pi}}{2}\delta\alpha_n - 4\alpha_n\alpha_t + 6\alpha_t + 4\alpha_n + \frac{8}{\pi}\delta\hat{J}_3, \tag{A4}$$

$$d_{22} = -2\alpha_t^3 + 6\alpha_t^2 + \alpha_n\alpha_t - \frac{29}{4}\alpha_t - \alpha_n - \frac{2}{\pi}\delta\hat{J}_4, \tag{A5}$$

$$d_1 = 2\sqrt{\pi}\delta, \quad d_2 = -\frac{5}{2}\sqrt{\pi}\delta, \quad d_{23} = \alpha_t, \tag{A6}$$

where $\mathcal{F}_0 = 0.196079$ and $\mathcal{F}_1 = 0.247679$. In Eqs. (A1), (A4), (A5), the symbol $\hat{J}_i$ stands for integral expressions defined by using the brackets $[\phi, \psi]$,

$$[\phi, \psi] = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} e^{-c^2} \phi(c) L\psi \, d\mathbf{c}, \tag{A7}$$

with $L\psi$ being the linearized Boltzmann collision operator. For hard spheres of diameter σ, the length parameter θ is given by $\theta = \sqrt{2}/(\pi^{3/2}\sigma^2 n)$ and the mean free path λ reads as $\lambda = 1/(\sqrt{2}\pi\sigma^2 n)$ (where n is the number density). Therefore,

$$L\psi = \frac{1}{4\sqrt{2}\pi^{5/2}\lambda} \int_0^{2\pi} d\epsilon \int_0^{\pi} \sin\Theta d\Theta \cdot \int_{-\infty}^{+\infty} e^{-{c_1}^2} V \left(\psi_1' + \psi' - \psi_1 - \psi\right) d\mathbf{c_1}, \tag{A8}$$

where ψ is a function of $\mathbf{c}$, while ψ_1 refers to $\mathbf{c_1}$. V is the relative velocity: $|\mathbf{c} - \mathbf{c_1}|$. $\psi' \equiv \psi(\mathbf{c}')$ and $\psi_1' \equiv \psi(\mathbf{c_1'})$, where $\mathbf{c}'$ and $\mathbf{c_1'}$ are the velocities after collision of two molecules with velocities $\mathbf{c}$ and $\mathbf{c_1}$. The collision geometry, in conjunction with the conservation laws, relates the velocities after collision to the velocities before collision. Thus,

$$c_x' = c_x + (c_{1x} - c_x)\cos^2(\Theta/2) + 1/2 \cdot [V^2 - (c_{1x} - c_x)^2]^{1/2} \sin\Theta \cos\epsilon,$$

$$c_{1x}' = c_{1x} - (c_{1x} - c_x)\cos^2(\Theta/2) - 1/2 \cdot [V^2 - (c_{1x} - c_x)^2]^{1/2} \sin\Theta \cos\epsilon,$$

where Θ is the angle through which the relative velocity has turned and ϵ is the azimuthal angle which the plane containing the relative velocities before and after collision makes with a fixed reference plane. Similar relations exist for the y and z components[42].

The integrals J_1, J_2, J_3, J_4 appearing in Eqs. (A1), (A4), (A5) are eight-fold integrals,

$$\begin{aligned} J_1 &= [c_x c_z, c_x c_z], \quad J_2 = -[{c_x}^2 c_z, c_x {c_z}^2] \\ J_3 &= -[{c_x}^2 c_z, c^2 c_z], \quad J_4 = -[c^2 c_z, c^2 c_z], \end{aligned} \tag{A9}$$

where $\hat{J}_i = \dfrac{2\lambda}{\sqrt{\pi}} J_i$. These integrals have been numerically evaluated using a Monte Carlo integration on an eight-dimensional space. For the validation of the numerical Monte Carlo integrations, we have recalculated the collision integrals reported in Refs. [47], [48], where the results have been obtained by means of the analytical methods developed by Wang Chang and Uhlenbeck[49].

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