Variational Approach to Gas Flows in Microchannels on the basis of the Boltzmann Equation for Hard-Sphere Molecules

Carlo Cercignani[1] and Silvia Lorenzani[1,*]

*Corresponding author: Tel.:++39 02 23994566; Email: silvia.lorenzani@polimi.it
1: Dipartimento di Matematica, Politecnico di Milano, Milano, Italy

Abstract

The objective of the present paper is to provide an analytic expression for the first- and second-order velocity slip coefficients. Therefore, gas flow rates in microchannels have been rigorously evaluated in the near-continuum limit by means of a variational technique which applies to the integrodifferential form of the Boltzmann equation based on the true linearized collision operator. The diffuse-specular reflection condition of Maxwell's type has been considered in order to take into account the influence of the accommodation coefficient on the slip parameters. The polynomial form of Knudsen number obtained for the Poiseuille mass flow rate and the values of the second order velocity slip coefficients found on the basis of our variational solution of the linearized Boltzmann equation for hard-sphere molecules are analyzed in the frame of potential applications of classical continuum numerical tools (as lattice Boltzmann methods) in simulations of microscale flows.

Key words:
Linearized Boltzmann collision operator, variational method, slip coefficients.

1. Introduction

Since rarefied gas flows occur in many micro-electro-mechanical systems (MEMS), a correct prediction of these flows is important to design and develop MEMS. In spite of their apparently complex structure, the basic constituent of a real MEMS device is the microchannel, the region between two parallel plates that can reveal many specific features of the low speed internal flows in microdevices. The pressure distribution along these microchannels and the flow rates across them are found to deviate from the linear distribution of the Poiseuille flow. Therefore, an important aspect of the matter is to have an approximate closed form solution for the flow rate of plane Poiseuille flow in order to use it in applications when low working pressures impose corrections due to gas rarefaction effects. In order to develop an accurate formula directly from kinetic theory, there is a particularly useful technique, the variational method proposed in [4], which applies to the integrodifferential form of the Boltzmann equation and can be used for any linearized Boltzmann model. In the literature, the variational formulation has been the most cited method of analysis for the kind of approaches where corrected parameters, employed in classical continuum numerical tools, have been computed via kinetic theory.

In recent years, there has been considerable success in the implementation of second-order slip boundary conditions to extend the Navier-Stokes equations (which are significantly more efficient compared to molecular-based approaches) into the transition regime. Unfortunately, no consensus has been reached yet on the correct form of higher-order velocity slip coefficient.

In the current investigation, the variational technique is used to compute the flow rate of plane Poiseuille flow, by considering the true linearized Boltzmann collision operator and general boundary conditions of Maxwell's type. The variational approach permits to write down simple approximate equations to be used in classical hydrodynamic numerical tools in order to extend the continuum description even beyond the slip regime.

2. The variational approach to plane Poiseuille flow

Let us consider two plates separated by a distance d and a gas flowing parallel to them, in the z direction, due to a pressure gradient. Both boundaries are held at a constant temperature T_0. If the pressure gradient is 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

$$f = f_0(1 + h) \tag{1}$$

where $f(x, z, \mathbf{c})$ is the distribution function for the molecular velocity $\mathbf{c}$ expressed in units of $(2RT_0)^{1/2}$ (R being the gas constant), x is the coordinate normal to the plates and $h(x, \mathbf{c})$ is the small perturbation upon the basic equilibrium state. The above mentioned Maxwellian is given by

$$f_0(z, \mathbf{c}) = (1 + kz)\rho_0\pi^{-\frac{3}{2}} \exp(-c^2) \tag{2}$$

where ρ_0 is the density on the boundaries and

$$k = \frac{1}{p}\frac{\partial p}{\partial z} = \frac{1}{\rho}\frac{\partial \rho}{\partial z}$$

with p and ρ being the gas pressure and density, respectively. Using Eq. (1), the steady linearized Boltzmann equation reads as [3]

$$kc_z + c_x\frac{\partial h}{\partial x} = Lh \tag{3}$$

where Lh is the true linearized collision operator. Once the deviation h from the equilibrium distribution is known, the bulk velocity of the gas can be written as follows:

$$q(x) = \pi^{-\frac{3}{2}} \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} e^{-c^2} c_z h(x, \mathbf{c})\, d\mathbf{c} \tag{4}$$

and the flow rate F (per unit time through unit thickness) as:

$$F = \rho\int_{-d/2}^{d/2} q(x)dx \tag{5}$$

Equation (3) can be rewritten in symbolic form as follows:

$$(D - L)h = S \tag{6}$$

where $Dh = c_x\frac{\partial h}{\partial x}$, $S = -kc_z$. The boundary conditions to be matched to Eq. (6) have the general expression [6]:

$$h^+ = Kh^- \tag{7}$$

where the explicit form of the operator K depends on the scattering kernel used. In the following, we will focus upon Maxwell's scattering kernel and specialize the analysis to symmetric gas-wall interactions so that an accommodation coefficient α can be defined. In this case, the boundary conditions can be written as

$$\begin{aligned} h^+(d/2\mathrm{sgn}c_x, \mathbf{c}) = (1-\alpha)\cdot \\ h^-(d/2\mathrm{sgn}c_x, -c_x, c_y, c_z) \end{aligned} \tag{8}$$

Here $h^\pm$ are the restrictions of the function h, defined on the boundary, to positive, respectively negative, values of c_x.

Using the variational principle described in [4], we introduce the following functional J of the test function $\tilde{h}$:

$$\begin{aligned} J(\tilde{h}) &= ((\tilde{h}, P(D\tilde{h} - L\tilde{h}))) - 2((PS, \tilde{h})) + \\ &(\tilde{h}^+ - K\tilde{h}^-, P\tilde{h}^-)_B \end{aligned} \tag{9}$$

where P is the parity operator in velocity space and $((,))$, $(,)_B$ denote two scalar products defined in [6]. The functional $J(\tilde{h})$ attains its minimum value when $\tilde{h} = h(x, \mathbf{c})$ solves Eq. (6) with appropriate boundary conditions. If we let $\tilde{h} = h$, equation (9) gives:

$$J(h) = -((PS, h)) \tag{10}$$

Looking at the definitions (4) and (5), it can be easily shown that the stationary value of J is related to a quantity of physical interest, the flow rate of the gas, through the relation:

$$F = -\frac{\rho}{k}J(h) \tag{11}$$

Since the purpose of the present paper is to provide an analytic expression for the first and second order slip coefficients, it is sufficient to consider asymptotic results (near-continuum) for mass flow rates. Therefore, the following simplified test function, rescaled by the relative gradient pressure k and the length-parameter θ, has been used to evaluate Eq. (9)

$$\begin{aligned} \tilde{h}(x, \mathbf{c}) &= 2c_zA(x^2 - 2xc_x + 2{c_x}^2) + \\ &2c_z(B - 1/2) \end{aligned} \tag{12}$$

which is the same trial function introduced for the Bhatnagar-Gross-Krook (BGK) kinetic model [7] in the near-continuum flow limit. In Eq. (12) A and B are adjustable constants to be varied in order to obtain the best value of $J(\tilde{h})$.

Substituting $\tilde{h}$, given by Eq. (12), in Eq. (9), we obtain the following polynomial of the second order with respect to the constants A and B, that are to be determined

$$J(\tilde{h}) = (\sqrt{\pi})^{-1} \times \left\{ \frac{c_{11}}{2} A^2 + \frac{c_{22}}{2} B^2 + c_{12}AB - c_1 A - c_2 B + \frac{1}{2}(c_2 - c_{22}/4) \right\} \tag{13}$$

where the same symbol $J(\tilde{h})$ has been used to denote the dimensionless quantity $J(\tilde{h})/(k\theta)^2$. The coefficients in nondimensional form are given by

$$c_{11} = -\frac{4}{3}\sqrt{\pi}\delta^3 - \frac{8}{3\pi}\delta^3 \hat{J}_1 + 8\delta^2 - \frac{32}{\pi}\delta \hat{J}_2 - \alpha\left[\frac{\delta^4}{4} - \sqrt{\pi}\delta^3 + 8\delta^2 - 12\sqrt{\pi}\delta + 32\right] \tag{14}$$

$$c_{12} = -\alpha[\delta^2 - 2\sqrt{\pi}\delta + 8] \tag{15}$$

$$c_1 = \frac{\sqrt{\pi}}{6}\delta^3 + 2\sqrt{\pi}\delta - \alpha\left[\frac{\delta^2}{2} - \sqrt{\pi}\delta + 4\right] \tag{16}$$

$$c_{22} = -4\alpha \tag{17}$$

$$c_2 = 2\sqrt{\pi}\delta - 2\alpha \tag{18}$$

where $\delta = d/\theta$ is the rarefaction parameter (inverse Knudsen number) and the symbol J_i stands for integral expressions defined by using the brackets $[\phi, \psi]$:

$$[\phi, \psi] = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} d\mathbf{c}\, e^{-c^2}\phi(c)L\psi \tag{19}$$

with $L\psi$ being the 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: $\lambda = 1/(\sqrt{2}\pi\sigma^2 n)$ (n is the number density). Therefore,

$$L\psi = \frac{1}{4\sqrt{2}\pi^{5/2}\lambda}\int_0^{2\pi} d\epsilon \int_0^{\pi} \sin\Theta d\Theta \cdot \int_{-\infty}^{+\infty} d\mathbf{c_1} e^{-c_1{}^2} V(\psi_1' + \psi' - \psi_1 - \psi) \tag{20}$$

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 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 [2]. The integrals J_1 and J_2 are eight fold integrals:

$$J_1 = [c_x c_z, c_x c_z]$$
$$J_2 = -[c_x{}^2 c_z, c_x{}^2 c_z] \tag{21}$$

where $\hat{J}_i = \frac{2\lambda}{\sqrt{\pi}} J_i$. The derivatives of $J(\tilde{h})$ with respect to A and B vanish in correspondence of the optimal values of these constants. The resulting expression for the minimum of $J(\tilde{h})$ is:

$$minJ(\tilde{h}) = (8\sqrt{\pi})^{-1} \cdot [c_{11}c_{22} - c_{12}^2]^{-1} \cdot [8c_{12}c_1c_2 - 4c_1^2c_{22} + c_{12}^2 \cdot (c_{22} - 4c_2) - c_{11}(c_{22} - 2c_2)^2] \tag{22}$$

Thus, the computation of the optimal value of the functional $J(h)$ (Eq. 22) will lead to an accurate estimate of the flow rate of the gas, which in non-dimensional form reads:

$$Q(\delta) = \frac{F}{-\frac{\rho}{2}kd^2} = \frac{2}{\delta^2}J(h) \tag{23}$$

3. Near continuum solution and slip coefficients

A notable advantage of the variational approach is that it permits to write down simple approximate equations, computed via kinetic theory, to be used in classical hydrodynamic numerical tools in order to extend the continuum description (that is significantly more efficient compared to molecular-based approaches) even beyond the slip regime. In recent years, there has been considerable success in the implementation of second-order slip boundary conditions to extend the Navier-Stokes equations into the transition regime. Assuming a second-order boundary condition at the wall, in the isothermal case, the slip velocity reads:

$$q_s = \pm A_1\lambda\left(\frac{\partial q}{\partial x}\right)_w - A_2\lambda^2\left(\frac{\partial^2 q}{\partial x^2}\right)_w \tag{24}$$

where the gas-velocity gradients are evaluated at the wall. Here λ is the mean free path of the molecules defined as:

$$\lambda = \frac{\mu}{P}\sqrt{\frac{\pi}{2}RT}$$

where μ is the gas viscosity, P is the pressure, T the absolute temperature and R the universal gas constant. In Eq. (24), A_1 and A_2 are the first and second order slip coefficients, respectively. Recent experimental studies [17], [11] have revealed large discrepancies between the experimentally-determined values of A_2 and the theoretical values listed in [1]. The lack of a well-founded value of the second-order slip coefficient makes it difficult to extend slip-flow predictions into the transition regime.

The asymptotic near-continuum solution for the Poiseuille mass flux obtained by means of our variational technique can be used to predict slip coefficients. When the true linearized Boltzmann collision operator is used, Eqs. (12), (22) and (23) give in the limit $\delta \to \infty$:

$$Q = \frac{\delta}{\sigma_0} + \sigma_1 + \frac{\sigma_2}{\delta} + \cdots \tag{25}$$

where:

$$\sigma_0 = (4\sqrt{\pi})^{-1}\cdot\left[\frac{96}{\pi}\hat{J}_1 + 48\sqrt{\pi}\right] \tag{26}$$

$$\mathcal{A} = \frac{32}{3\pi}\hat{J}_1 + \frac{16}{3}\sqrt{\pi} \tag{27}$$

$$\mathcal{B} = \mathcal{A}^{-1}\cdot\left[\frac{128}{\pi}\hat{J}_2 - 16\sqrt{\pi}\alpha\right] \tag{28}$$

$$\mathcal{C} = \mathcal{A}^{-1}\cdot[-4\pi\alpha + 16\alpha - 32] \tag{29}$$

$$\mathcal{D} = \frac{128}{3}\hat{J}_1 - \frac{32}{3}\pi^{3/2}\alpha + \frac{64}{3}\pi^{3/2} \tag{30}$$

$$\mathcal{E} = \frac{256}{3}\pi\alpha - 128\pi \tag{31}$$

$$\sigma_1 = [4\sqrt{\pi}\alpha\mathcal{A}]^{-1}\cdot[\mathcal{D} - 16/9\pi\alpha\mathcal{C}] \tag{32}$$

$$\sigma_2 = [4\sqrt{\pi}\alpha\mathcal{A}]^{-1}\cdot[\mathcal{E} + 16/9\pi\alpha\mathcal{C}^2 - 16/9\pi\alpha\mathcal{B} - \mathcal{C}\mathcal{D}] \tag{33}$$

Table 1: First- and second-order slip coefficients obtained on the basis of our variational solution of the linearized Boltzmann equation for hard-sphere molecules, for different values of the accommodation coefficient α.

	A_1	A_2
$\alpha = 1.$	1.1209	0.2347
$\alpha = 0.5$	3.1533	−0.0090
$\alpha = 0.1$	18.9108	−0.1831

with $\hat{J}_1 = -1.4180$, $\hat{J}_2 = 1.8909$. σ_1 and σ_2 are related to the first and second order slip coefficients, respectively. Rewriting Eq. (25) in terms of deviations from the continuum solution, one obtains:

$$S = Q/(\delta/\sigma_0) = 1 + \left[\tfrac{2}{\sqrt{\pi}}(\sigma_0\sigma_1)\right]K_n + \left[\tfrac{4}{\pi}(\sigma_0\sigma_2)\right]{K_n}^2 \tag{34}$$

where the Knudsen number K_n is given by $K_n = \sqrt{\pi}/(2\delta)$.

A comparison with the solution of the Navier-Stokes equations obtained by using the boundary condition (24) [17]

$$S \simeq 1 + 6A_1K_n + 12A_2{K_n}^2 \tag{35}$$

gives:

$$A_1 = \frac{\sigma_0\sigma_1}{3\sqrt{\pi}} \tag{36}$$

$$A_2 = \frac{\sigma_0\sigma_2}{3\pi} \tag{37}$$

The first-(A_1) and second-order (A_2) slip coefficients, obtained on the basis of our variational solution of the linearized Boltzmann equation for hard-sphere molecules, are given in Table 1, for several values of the accommodation coefficient α.

The values of the first-order slip coefficient A_1 are in very good agreement with the ones obtained in [19] through a numerical solution of the linearized Boltzmann equation for hard sphere molecules. On the contrary, the estimate we obtain for A_2 seems inconsistent with available theoretical models listed in [1], while it is very close to the values obtained in recent experimental studies (see Table 2), where the slip coefficients were computed starting from mass flow rate measurements.

Table 2: Experimental and theoretical first- and second-order slip coefficients

	A_1	A_2
Experiments with Nitrogen		
Maurer et al. (2003)	1.30 ± 0.05	0.26 ± 0.1
Experiments with Helium		
Maurer et al. (2003)	1.20 ± 0.05	0.23 ± 0.1
Ewart et al. (2007)	1.26 ± 0.02	0.17 ± 0.02
Present results (α = 1.)	1.1209	0.2347
Present results (α = 0.91)	1.3276	0.1887
Present results (α = 0.87)	1.4323	0.1685

In Table 2 we have reported our theoretical results concerning the slip coefficients for three different values of the accommodation coefficient α to be as close as possible to the experimental measurements.

It is worthwhile to mention that the second-order slip coefficient we obtain for $\alpha = 1.$ (fully-diffusive boundary) by using the linearized Boltzmann equation for hard-sphere molecules is in fair agreement with the value reported in [12] by Hadjiconstantinou who, on the basis of Cercignani's suggestion, modified the BGK-value by an appropriate scaling, taking into account the contributions of the Knudsen layer. A recent work by Lockerby et al. [15] indicates values of the second-order slip coefficient in the range 0.145-0.19, depending on the Prandtl number of the gas but irrespective of the values of the accommodation coefficient. It is worthwhile to underline that with decreasing α, A_2 can become negative, as assumed by some models proposed in the literature [13]. This is a complete new feature arising from our variational analysis of the linearized Boltzmann equation for hard sphere molecules, which has not be found in previous analytical studies of a hard sphere gas [16] and can not be predicted by using kinetic models as the BGK (see Table 3).

A brief remark is in order here concerning the range of validity of Eq. (25). The truncation at the order δ^{-1} in Eq. (25) gives an accurate result for Q when $\delta \geq 10$, for each value of the accommodation coefficient. A comparison with the highly accurate numerical results reported by Siewert in [18] for $\delta = 10.$ and $\alpha = 1., 0.5, 0.1$, shows that the relative error is within 0.3%. This good agreement makes us feel more confident of the reliability of the values obtained for the second-order slip coefficient.

Table 3: First- and second-order slip coefficients obtained by means of our variational solution of the linearized Boltzmann equation based on the Bhatnagar, Gross and Krook (BGK) model, for different values of the accommodation coefficient α.

	A_1	A_2
$\alpha = 1.$	1.1366	0.6926
$\alpha = 0.5$	3.2049	0.4443
$\alpha = 0.1$	19.2596	0.2658

To obtain a comparable accuracy with the same order of approximation for smaller values of δ, higher-order terms in the expansion for Q should be retained and used to modify the σ_2 coefficient (or alternatively the second-order slip coefficient A_2). This is an advantage offered by the variational approach since it permits to write down analytical formulae which can be easily manipulated.

Recently, the asymptotic solution of the BGK model equation for the Poiseuille mass flux ($\delta \to \infty$) has been used in [14], in order to enforce lattice Boltzmann (LB) models to predict slip velocity up to second order in the Knudsen number. Since the hard-sphere model is more appropriate than the BGK equation for describing isothermal flows of real gases, it could be more convenient to use the asymptotic formula (25) in order to adjust free parameters appearing in LB methods in simulations of microscale flows.

4. Conclusions

In the present paper a variational approach has been used to solve the plane Poiseuille problem between two parallel plates in the near continuum flow limit, as an issue of relevance for applications, by considering the true linearized Boltzmann collision operator. According to our variational analysis both the first (A_1) and second order (A_2) slip coefficients depend on the accommodation coefficient α. The estimate we obtain for A_2 seems inconsistent with available theoretical models while it is very close to the values obtained in recent experiments. Moreover, it has been found that with decreasing

α, A_2 can become negative, as assumed by some heuristic models proposed in the literature.

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