

**AN EXPRESSION THAT IS VALID FROM CONTINUUM TO
FREE MOLECULAR REGIME FOR THE FLOW-RATE
THROUGH A LONG CHANNEL**

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Abstract. One considers the flow of a gas through a 2D or axisymmetric microchannel. The objective is to find an expression of the mass-flow rate as a function of pressures at both channel ends, gas properties and gas-surface interaction. Previous expressions are reminded that take into account rarefaction effects through terms of 1st and 2nd order in Knudsen number, added to the Poiseuille formula. The paper emphasizes on the correct evaluation of the additional terms. Then the expression of the flow rate in the free molecular regime is presented, based on a numerical simulation at a molecular level. Finally, an interpolation formula is proposed for the intermediate (transitional) regime. It fits with both previous approaches and does not require any additional adjustment.

1. INTRODUCTION

Under usual conditions, the flow of a gas through a two-dimensional or axisymmetric channel is governed by Navier-Stokes (NS) equations. The implicit hypothesis in this approach is that of a local thermodynamic equilibrium. Molecules that are present in a small volume (i.e. a volume whose dimensions are much smaller than the transverse dimension H of the channel) have enough collisions between themselves to form an equilibrium population. The thermal speed of molecules is governed by a distribution function close to a Maxwellian one. The transverse distribution of flow velocity and the flow rate through the channel are given by the well-known Poiseuille solution. This approach fails when the molecular mean free path λ is not small compared with H . This is a so-called rarefaction effect and it can be encountered in microchannels, characterized by very small dimensions.

If the Knudsen number ($Kn = \lambda/H$) remains rather small (say $Kn < 0.4$), rarefaction can be taken into account by introducing changes into the NS approach. One can introduce a velocity slip at the wall and/or introduce a non-Newtonian behavior of the gas through additional dissipation terms. The approach remains a continuum one. The resulting changes in the expression of the channel flow rate will be presented.

When Kn is very large (say $Kn > 30$), intermolecular collisions are much less frequent than the molecule-wall collisions and they play a negligible role. This is true also for transport properties (including viscosity), as they are based on collisional properties. A statistical approach, suited to this regime, will be presented.

Finally a method will be presented to estimate the flow rate through a microchannel for intermediate values of Kn . It is based on an interpolation between both extreme approaches, similar the *bridging methods* used for hypersonic rarefied flows.

2. CONTINUUM APPROACH

One considers the isothermal flow at temperature T through a rectangular microchannel of length L , width D and depth H ($L \gg D \gg H$). Considering the problem as a two-dimensional one, we write the flow rate induced by a difference between end pressures as¹

$$q = \left[\frac{D H^3 p_{out}^2}{24 \mu R T L} \times (r_p^2 - 1) \right] \times [1 + A_1 Kn_{out} + A_2 Kn_{out}^2], \quad (1)$$

where the first factor is the Poiseuille flow rate, subscript *out* refers to outlet conditions, r_p is the ratio of end pressures ($r_p = p_{in}/p_{out}$), μ is the gas viscosity at temperature T , R is the perfect-gas constant per unit-mass, Kn_{out} is the Knudsen number λ_{out}/H , where the mean free path is estimated in the downstream conditions. Coefficients A_1 and A_2 introduce 1st and 2nd order corrections to the Poiseuille expression, respectively.

2.1. First-order correction

The first-order correction ($A_1 Kn_{out}$) originates from the non-zero longitudinal gas velocity u_w along the wall. A non-rigorous but simple interpretation of this so-called *velocity slip* follows. Assume perfect accommodation of molecules at the wall. In the immediate vicinity of the wall, half of the molecules come directly from the wall and have thus a mean longitudinal velocity equal to zero. The other half come from the bulk of the flow and more specifically from a distance of the order of λ , where the longitudinal velocity is approximately $u_w + \lambda(\partial u/\partial y)_w$. Here y denotes the distance from the wall. Thus the mean velocity at the wall is

$$u_w = \frac{1}{2} \left[0 + \left(u_w + \lambda \left[\frac{\partial u}{\partial y} \right]_w \right) \right], \text{ resulting in } u_w = \lambda \left[\frac{\partial u}{\partial y} \right]_w. \quad (2)$$

More correct expressions of the velocity slip have been proposed. They are presented and discussed, e.g. by Barber and Emerson² who write

$$u_w = \alpha_1 \times \left[\frac{2-a_u}{a_u} \right] \times \lambda \left[\frac{\partial u}{\partial y} \right]_w \text{ with } \alpha_1 = 1.016 \times \frac{2}{\sqrt{\pi}} \cong 1.1466 \quad (3)$$

Additional terms should be introduced for a non-isothermal flow and for a wall that presents a curvature rather than being plane. a_u is the accommodation coefficient for tangential momentum accommodation. α_1 is absent from the simple expression (Eq.2) and comes from kinetic considerations. This coefficient is a source of difficulty:

- The 1.016 factor is replaced by 0.98737 by some authors, due to a different approach for solving the Boltzmann equation;
- It has been established for full accommodation ($a_u = 1$) and may depend on a_u in the case of partial accommodation;
- It has been established for *rigid-sphere* molecules, i.e. for a gas whose viscosity varies with temperature as $\mu \sim T^{1/2}$.

- Many authors just take $\alpha_1 = 1$.

As the accommodation coefficient is often obtained by fitting, based on experimental flow rates, a change in α_1 results in a different conclusion as to the accommodation coefficient. Barber and Emerson² show that experiments by Colin *et al.*³ are interpreted by an accommodation coefficient $a_u = 0.93$ if α_1 is taken equal to 1 or by a nearly full accommodation ($a_u = 0.998$) if α_1 is taken equal to 1.1466.

Furthermore the definition of the mean free path is somewhat confusing. Bird⁴ demonstrate that for a VHS (Variable Hard Sphere) gas, the viscosity law looks like $\mu \sim T^\omega$ and the mean free path is related to the macroscopic parameters of the flow by

$$\lambda = K(\omega) \times \frac{\mu(T)}{\rho \times (2\pi RT)^{1/2}} \text{ with } K(\omega) = \frac{2(7-2\omega)(5-2\omega)}{15}, \quad (4)$$

where ρ is the density. For $\omega = 1/2$, one finds the rigid-sphere expression

$$\lambda = \frac{16}{5} \frac{\mu(T)}{\rho \times (2\pi RT)^{1/2}} \quad (5)$$

which differs slightly from that of Chapman, valid also for rigid spheres, but with a different definition of the mean free path

$$\lambda = \frac{\mu(T)}{\rho} \left(\frac{\pi}{2RT} \right)^{1/2} \quad (6)$$

By extension, Eq. 4 can be used for any viscosity law (e.g. a Sutherland's law), if ω is considered as the exponent of a local power-law viscosity, fitted at temperature T : $\omega = (d\mu/dT)/(\mu/T)$. Many authors use Eq. 6 rather than Eq. 4, whatever the viscosity law, which, in the worst case induces an error by a factor 1.6 on the mean free path and on the Knudsen number. Therefore, it is essential to know how the mean free path has been calculated when using results found in the literature.

If Eq. 3 is retained for the velocity slip, one can integrate the transverse velocity profile across the channel section as a function of the longitudinal pressure gradient dp/dx to get the flow rate. Then pressure can be integrated along the channel for a given flow rate. Coefficient A_1 in Eq. 1 is then found as

$$A_1 = 12\alpha_1(\omega, a_u) \times [(2 - a_u)/a_u]/[r_p + 1]. \quad (7)$$

As explained before, α_1 is close to unity, but depends actually on both ω and a_u .

2.1. Second-order correction

A number of authors proposed to introduce a second-order term in the expression of the velocity slip. Assuming full accommodation and a rigid-sphere gas, Hadjiconstantinou⁵ writes the velocity slip as

$$u_w = \alpha_1 \times \lambda \left(\frac{\partial u}{\partial y} \right)_w - \alpha_2 \times \lambda^2 \left(\frac{\partial^2 u}{\partial y^2} \right)_w \quad (8)$$

where he takes $\alpha_1 = 1.11$ (see discussion above) and $\alpha_2 = 0.61$.

Barber and Emerson² as well as Karniadakis *et al.*⁶ present tables of α_1 and α_2 values proposed by different authors. α_2 is either a constant or a function of Prandtl number and of the specific heat ratio. Its value varies from -0.5 to 1.309. In all cases, the transverse velocity profile can be integrated and the value of α_2 determines the value of A_2 in Eq.1 :

$$A_2 = 24\alpha_2 \times \ln r_p / (r_p^2 - 1). \quad (9)$$

In particular, the value $\alpha_2 = 9/8$ proposed by Deissler⁷ results in

$$A_2 = 27 \times \ln r_p / (r_p^2 - 1), \quad (10)$$

which makes Eq.1 reproduce experimental flow rates obtained by Aubert and Colin⁸ in the range $Kn_{\text{out}} < 0.25$.

Hadjiconstantinou⁹ reminds that the velocity slip u_w is a boundary condition associated to NS equations to make the latter describe correctly the flow where they are valid, i.e. in the bulk of the flow, but not necessarily in the vicinity of the wall. In the Knudsen layer (of thickness $\cong \lambda$) the gas is in strong non-equilibrium and NS equations fail to give the physical velocity (Figure 1). By integrating the NS velocity profile across the channel, one gets an error on the flow rate. The error is second-order in Kn and does not affect the first-order approximation. According to Hadjiconstantinou α_2 should be replaced by $\alpha_2 - \xi$ in the expression of A_2 , with $\xi = 0.296$ for a rigid-sphere gas. Hence

$$A_2 = 24(\alpha_2 - \xi) \times \ln r_p / (r_p^2 - 1). \quad (11)$$

In other terms, the determination of the second-order coefficient from experimental data results in $\alpha_2 - \xi$ rather than in α_2 .

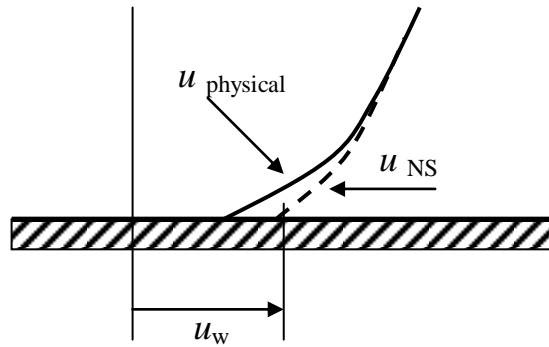


Figure 1. Velocity slip at the wall

A number of questions remain open:

- How to modify α_2 in the case of partial accommodation? Karniadakis et al.⁶ affect both the first-order and the second-order terms by the factor $(2 - a_u)/a_u$ in Eq.8.
- What is the value of ξ for a gas other than a rigid-sphere one?

Another interpretation of the second-order term in Eq.8 is proposed by Elizarova and Sheretov¹⁰. They consider that in a strong non-equilibrium situation, the gas does not behave as a Newtonian one. Accordingly they introduce additional dissipation terms in NS equations. The resulting equations, referred to as *quasigasodynamic* (QGD) or *quasihydrodynamic* (QHD) system can be applied to a microchannel, associated to first-order velocity slip. They obtain an expression of the flow rate identical to Eq.1, with

$$A_2 = \left[\frac{48\pi}{K(\omega)^2 Sc} \right] \times \frac{\ln r_p}{r_p^2 - 1}, \text{ where } Sc \text{ is the Schmidt number}^4 \text{ } Sc = \frac{5}{7-2\omega}. \quad (12)$$

Although based on a totally different interpretation, Eq.12 results to a value of A_2 that is nearly equal to that given by Eq.9 with Deissler condition and leads to the same good agreement with experimental results.

To conclude this section, Eq.1 reproduces the correct flow rate in the range ($Kn_{\text{out}} < 0.25$ or even $Kn_{\text{out}} < 0.4$). However, for the first-order term, the value of α_1 must be consistent with the definition of the mean free path. Otherwise, a_u loses its physical meaning.

The second-order term accounts potentially for different phenomena and it is probably unrealistic to get it from theoretical considerations based on Taylor developments. This is because in the Kn range where the corrections would have some interest, the sum of first- and second-order terms are much larger than the Poiseuille term. Thus A_2 can be considered as purely phenomenological and be written as

$$A_2 = B(\omega, a_u) \times \ln r_p / (r_p^2 - 1), \quad (13)$$

where B is a function of ω and a_u to be fitted to experiment.

For an axisymmetric microchannel of radius H , Lengrand *et al.*¹ give an expression of the flow rate based on QGD equations

$$q_{\text{QHD}} = \left[\frac{\pi H^4 p_{\text{out}}^2}{16 \mu RTL} \times (r_p^2 - 1) \right] \left[1 + \frac{8\alpha_1}{r_p + 1} \times \frac{2 - a_u}{a_u} Kn_{\text{out}} + \frac{32\pi}{K(\omega)^2 S_c} \times \frac{\ln r_p}{r_p^2 - 1} Kn_{\text{out}}^2 \right]. \quad (14)$$

The factor α_1 in the first-order term was absent in Ref.1 and has been introduced here according to the above discussion.

More generally, any second-order approach leads to

$$q = \left[\frac{\pi H^4 p_{\text{out}}^2}{16 \mu RTL} \times (r_p^2 - 1) \right] [1 + A_1 Kn_{\text{out}} + A_2 Kn_{\text{out}}^2]. \quad (15)$$

In both the rectangular and axisymmetric configuration, the Poiseuille flow rate is proportional to the difference of the squared end pressures.

2. FREE MOLECULAR APPROACH

One considers a microchannel that joins two reservoirs. The free molecular regime corresponds to conditions when the mean free paths in both reservoirs are much larger than the transverse dimensions of the microchannel. The gas in each reservoir is considered to be at rest in thermodynamic equilibrium under pressures p_{in} , p_{out} and temperatures T_{in} , T_{out} . The local properties of the gas in the channel do not play any role in the process. Even if pressure and temperature can be defined along the channel, each molecule behaves independently of the other ones and has no collision with them. It is thus unrealistic to describe the free molecular flow by such quantities as the pressure gradient dp/dx or by a local property such as viscosity. In contrast, a molecular description is possible. Here we summarize an approach¹, based on an example given by Bird⁴.

A gas molecule that enters the channel at one end will collide one or more times with the channel wall and will exit through the other end with probability P and through the same end with probability $1 - P$. In an equilibrium gas at rest, the number of molecules crossing the unit-area per unit-time is

$$\dot{N} = n(2RT)^{1/2} / (2\pi^{1/2}), \quad (16)$$

where n is the number density. This formula is used to estimate the number flux entering both channel ends. Multiplying by the molecular mass and by the channel area yields the mass flow

L/H	$a = 1$	$a = 0.5$	$a = 0.2$	$a = 0.1$	$a = 0.01$
1.00E-02	9.95E-01	9.97E-01	9.99E-01	1.00E+00	1.00E+00
3.00E-02	9.86E-01	9.93E-01	9.97E-01	9.99E-01	1.00E+00
1.00E-01	9.52E-01	9.76E-01	9.90E-01	9.95E-01	1.00E+00
3.00E-01	8.71E-01	9.33E-01	9.72E-01	9.86E-01	9.99E-01
1.00E+00	6.84E-01	8.20E-01	9.17E-01	9.56E-01	9.95E-01
3.00E+00	4.57E-01	6.41E-01	8.08E-01	8.88E-01	9.86E-01
1.00E+01	2.41E-01	4.05E-01	6.12E-01	7.41E-01	9.57E-01
3.00E+01	1.16E-01	2.26E-01	4.01E-01	5.43E-01	8.92E-01
1.00E+02	4.72E-02	1.02E-01	2.11E-01	3.20E-01	7.49E-01
3.00E+02	1.94E-02	4.52E-02	1.01E-01	1.68E-01	5.52E-01
1.00E+03	7.06E-03	1.72E-02	4.14E-02	7.30E-02	3.28E-01
3.00E+03	2.72E-03	6.84E-03	1.71E-02	3.14E-02	1.73E-01
1.00E+04	9.71E-04	2.45E-03	6.23E-03	1.18E-02	7.56E-02

Table 1. Probability $P(L/H, a)$ for a molecule to pass through a 2D channel of length L and depth H .
 a is the accommodation coefficient.

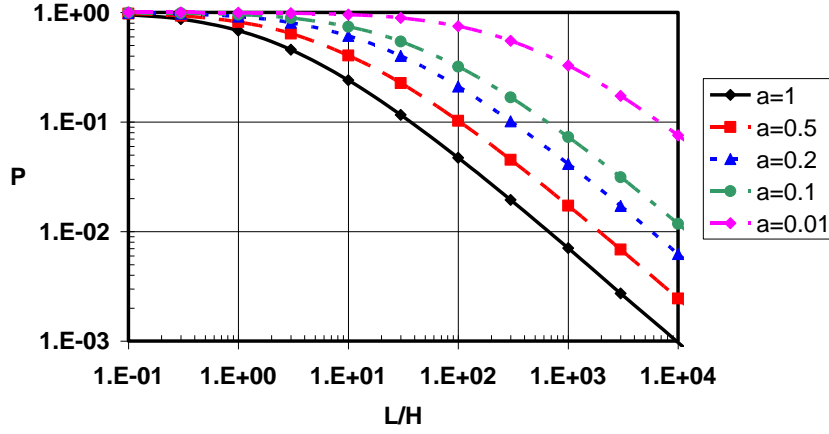


Figure 2. Probability $P(L/H, a)$ for a molecule to pass through a 2D channel of length L and depth H .
 a is the accommodation coefficient.

$$q_{FM} = \frac{PA}{(2\pi)^{1/2}} (\rho_{in}(RT_{in})^{1/2} - \rho_{out}(RT_{out})^{1/2}) = \frac{PA}{(2\pi)^{1/2}} \left(\frac{p_{in}}{(RT_{in})^{1/2}} - \frac{p_{out}}{(RT_{out})^{1/2}} \right) \quad (17)$$

with $A = HD$ for a rectangular channel and $A = \pi H^2$ for an axisymmetric one with radius H .

The transmission probability P is the same in both directions and depends only on channel geometry and gas-surface interaction. For an isothermal flow, Eq.17 reduces to

$$q_{FM} = \frac{p_{out} \times (r_p - 1)}{(2\pi RT)^{1/2}} \times P \times A. \quad (18)$$

The remaining task is the estimation of P . One applies a Monte Carlo method that consists in injecting a large number of molecules through one of the channel ends and observing which end they exit. Each molecule is followed in the calculation and each of its reflections on the wall is treated either as specular (with probability $1 - a$) or as diffuse with full accommodation (with probability a), according to the Maxwell model. With this model, each accommodation coefficient is equal to a including the tangential momentum accommodation coefficient. Thus, we can confuse a and a_u . In computing the trajectory of a molecule and its successive collisions, only the direction of velocity is used and not its value. P is thus independent of gas and wall temperatures. It depends only on L/H and a .

L/H	a=1	a=0.5	a=0.2	a=0.1	a=0.01
1.00E-02	9.95E-01	9.98E-01	9.99E-01	1.00E+00	1.00E+00
3.00E-02	9.85E-01	9.93E-01	9.97E-01	9.98E-01	1.00E+00
1.00E-01	9.53E-01	9.75E-01	9.90E-01	9.95E-01	9.99E-01
3.00E-01	8.70E-01	9.28E-01	9.68E-01	9.82E-01	9.98E-01
1.00E+00	6.72E-01	7.96E-01	8.93E-01	9.37E-01	9.90E-01
3.00E+00	4.21E-01	5.88E-01	7.56E-01	8.41E-01	9.71E-01
1.00E+01	1.91E-01	3.39E-01	5.35E-01	6.67E-01	9.21E-01
3.00E+01	7.68E-02	1.65E-01	3.22E-01	4.59E-01	8.32E-01
1.00E+02	2.52E-02	6.11E-02	1.45E-01	2.41E-01	6.64E-01
3.00E+02	8.75E-03	2.24E-01	5.88E-02	1.09E-01	4.61E-01
1.00E+03	2.67E-03	7.09E-03	1.96E-02	3.86E-02	2.45E-01
3.00E+03	8.87E-04	2.37E-03	6.75E-03	1.38E-02	1.11E-01
1.00E+04	2.58E-04	7.07E-04	2.10E-03	4.29E-03	3.98E-02

Table 2. Probability $P(L/H, a)$ for a molecule to pass through an axisymmetric channel of length L and radius H . a is the accommodation coefficient.

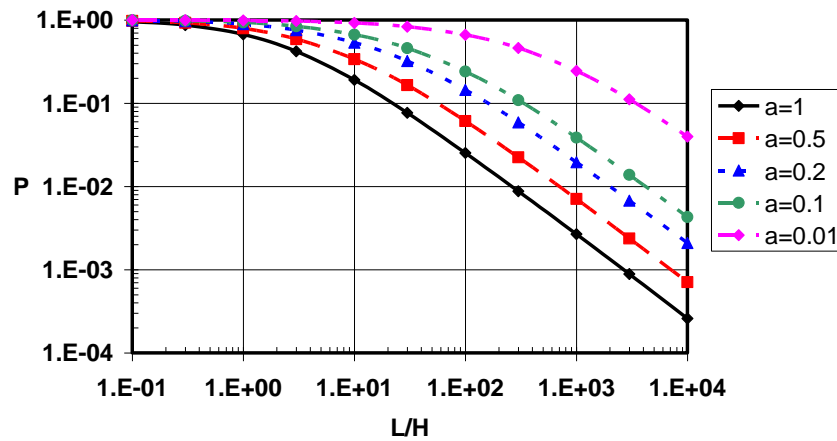


Figure 3. Probability $P(L/H, a)$ for a molecule to pass through an axisymmetric channel of length L and radius H . a is the accommodation coefficient.

The calculation has been carried out for a number of combinations $(L/H, a)$ and the corresponding values of P are given in Table 1, and Figure 2 for a rectangular or 2D channel and in Table 2 and Figure 3 for an axisymmetric channel. In both cases, the transmission probability tends to zero as $(L/H)^{-1}$ when $L/H \rightarrow \infty$. This behavior is the same as in the continuum regime, but it is obtained only for "very long" channels.

In both the rectangular and axisymmetric configuration, the free molecular flow rate is proportional to the difference between end pressures, in contrast with the Poiseuille solution.

2. TRANSITIONAL REGIME

A method that has been widely used for solving aerothermodynamic problems in rarefied conditions is the so-called *bridging method*. It allows one to estimate an overall quantity in a regime intermediate between the continuum and the free molecular regimes. For illustration purpose, assume that we want to estimate the drag coefficient C_D of a space vehicle. A first calculation based on a continuum approach results in a value $C_{D,C}$. A second calculation under free molecular assumption results in a value

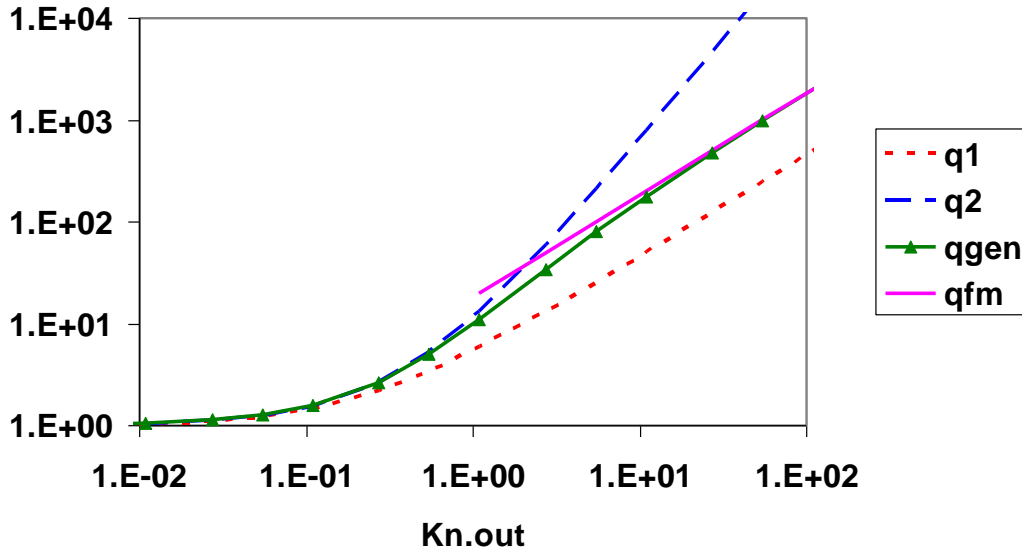


Figure 3. Comparison of different approaches for the flow rate through a rectangular channel. The flow rate is reduced by the Poiseuille value. Flow conditions are given in the text.

$C_{D,FM}$. An interpolation (bridging) function, supposedly universal for a given geometry is applied to obtain C_D from $C_{D,C}$ and $C_{D,FM}$.

In the case of a rectangular microchannel, we know the flow rate expression for $Kn_{out} \rightarrow 0$ (Poiseuille expression) and for $Kn_{out} \rightarrow \infty$. The success of Eq.1 for moderate Knudsen numbers suggests an expression of the flow rate that coincides with Eq.1 when $Kn_{out} \rightarrow 0$ and reduces to Eq.18 when $Kn_{out} \rightarrow \infty$. This is achieved if we replace Eq.1 by

$$q = \left[\frac{D H^3 p_{out}^2}{24 \mu RTL} \times (r_p^2 - 1) \right] \times \left[1 + A_1 Kn_{out} + \frac{A_2 Kn_{out}^2}{1 + \beta K n_{out}} \right]. \quad (19)$$

and take

$$\beta = \frac{B(\omega, a_u)}{24} \times \frac{\ln r_p}{r_p - 1} \times \left[\left(\frac{P(L/H, a_u)}{K(\omega)} \times \frac{L}{H} \right) - \left(\frac{\alpha_1(\omega, a_u)}{2} \times \frac{2 - a_u}{a_u} \right) \right]^{-1}. \quad (20)$$

Here we used Eq.4 to relate λ and μ and we used Eqs. 7 and 13 as expressions for A_1 and A_2 , respectively.

As an example, we consider the flow through a rectangular microchannel. The flowing gas is air at 300 K ($\mu = 1.85 \times 10^{-5}$ Pa.s, $\omega = 0.769$, $R = 287$ J.kg $^{-1}$.K $^{-1}$). The channel has dimensions $H = 10 \mu\text{m}$, $D = 0.15$ mm, $L = 3$ mm. The pressure ratio is $r_p = 2$. Full accommodation is assumed at the wall ($a = a_u = 1$). The ratio L/H is equal to 300 and the probability P is equal to 0.0194. We take $\alpha_1 = 1.146$ and $B = 27$, hence $A_1 = 4.584$ and $A_2 = 6.238$. The pressure p_{out} was varied from 1 to 10^5 Pa to cover the Knudsen number range $5.45 \times 10^{-3} < Kn_{out} < 545$. The reduced flow rate ($q/q_{Poiseuille}$) is plotted in Figure 4 as a function of Kn_{out} . The $q1$ curve corresponds to the first-order correction. It departs from the Poiseuille solution for $Kn_{out} \cong 0.02$. The $q2$ curve corresponds to the second-order correction. It departs from the previous one for $Kn_{out} \cong 0.1 - 0.2$. Equations 19 and 20 correspond to the $qgen$ curve. The latter follows the previous one till $Kn_{out} \cong 0.5$ and should feature the same agreement with experimental data as the second-order correction. Finally the $qgen$ curve merges with the free molecular curve qfm for $Kn_{out} \cong 30$.

For an axisymmetric channel, the same approach is used. The flow rate writes

$$q = \left[\frac{\pi H^4 p_{\text{out}}^2}{16 \mu RTL} \times (r_p^2 - 1) \right] \times \left[1 + A_1 Kn_{\text{out}} + \frac{A_2 Kn_{\text{out}}^2}{1 + \beta K n_{\text{out}}} \right]. \quad (21)$$

with

$$A_1 = \frac{8 \alpha_1(\omega, a_u)}{r_p + 1} \times \frac{2 - a_u}{a_u} \text{ and } A_2 = B(\omega, a_u) \times \frac{\ln r_p}{r_p^2 - 1} \quad (22)$$

and the consistence with the free molecular solution is achieved for

$$\beta = \frac{B(\omega, a_u)}{16} \times \frac{\ln r_p}{r_p - 1} \times \left[\left(\frac{P(L/H, a_u)}{K(\omega)} \times \frac{L}{H} \right) - \left(\frac{\alpha_1(\omega, a_u)}{2} \times \frac{2 - a_u}{a_u} \right) \right]^{-1}. \quad (23)$$

As for the rectangular channel, the expression of B depends on the second-order model. For example, QHD equations result in $B(\omega, a_u) = 32\pi/(K(\omega)^2 Sc)$.

2. CONCLUSION

The expression for the flow rate through a rectangular or axisymmetric channel has been reminded, based on a continuum approach, including first- and second-order corrections to the Poiseuille solution. Emphasis was put on correct estimates of the different terms, as concerns their dependences on viscosity law (ω), gas-surface interaction (a_u), definition of mean free path and physical meaning of velocity slip.

A physically sound molecular approach was applied in the free molecular regime and lead to a qualitatively different solution, the flow rate being proportional to the pressure difference rather than to the difference of squared pressures.

Finally an interpolation formula has been proposed to cover the intermediate (transitional) regime. It requires no additional fitting. It should facilitate the interpretation of past and future experiments.

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