

Non-Isothermal Gas Flow through a Rectangular Microchannels

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ABSTRACT

The mass flow rate of a rarefied gas through a long rectangular channel caused by both pressure and temperature differences has been calculated applying the S model kinetic equation. The calculations have been carried out in the wide ranges of the four parameters determining the solution of the problem: the gas rarefaction, the height-to-width ratio of the channel, the pressure ratio on the channel ends and the analogous temperature ratio. First, the Poiseuille flow and the thermal creep have been calculated as a function of the local rarefaction parameter assuming the pressure and the temperature gradients to be small. Then, the total mass flow rate has been calculated for the temperature ratio equal to 3.8 and for two values of the pressure ratio: 1 and 100.

Keywords: Microchannel, Rarefied gas, Poiseuille flow, Thermal creep, Mass flow rate

INTRODUCTION

For further perfection of microfluidics it is necessary to develop precise numerical methods of calculation of fluid flows through microchannels of different forms. Since the size of the microsystems has the order of the molecular mean free path, the continuum mechanics equations are not applicable to such type of the flows. To take into account the gas rarefaction the flows must be calculated by the methods of the rarefied gas dynamics [1]–[5]. This approach allows us to regard the whole range of the gas rarefaction from the free molecular (collisionless) regime to the hydrodynamic (continuum) regime.

There are some specific phenomena in rarefied gases that disappear in the continuous medium limit. One of them is the so-called thermal creep, i.e. the gas flows caused by a temperature gradient. This phenomenon can be significant and must be taken into account in practical calculations.

From the viewpoint of non-equilibrium thermodynamics [6] the thermal creep is a cross effect. It should be noted that many cross effects arising in rarefied gases and pointed out in the papers [7] must be taken into account in calculations of microfluidics. Moreover, many

of these phenomena can be used to create new types of microfluidics such as pumps, valves etc.

Many elements of microsystems have a rectangular cross section, as is shown in Fig. 1. To calculate the mass flow rate through a channel of arbitrary length ℓ and width b one has to consider the three-dimensional rarefied gas flow. Because of great numerical difficulties this problem was not solved yet in the wide range of the gas rarefaction.

If we assume the channel length to be essentially larger than its width and height, i.e. $\ell \gg a$ and $\ell \gg b$, the end effects can be neglected. In this case the flow becomes two-dimensional and the problem can be solved by modest computational efforts. Some data on such gas flow are available in the papers [8], [9], where the Bhatnagar Gross Krook model equation [10] was applied. An analysis made in the review [5] shows that this equation is not appropriate for non-isothermal rarefied gas flows. The paper [11] also contains data on the unsteady slip flow through a long rectangular channel. But there are no data on the mass flow rate.

The aim of the present work is to calculate the mass flow rate through a long rectangular channel caused by both pressure and temperature gradients over the wide ranges of the gas rarefaction and the ratio a/b .

Consider a channel created by two parallel plates fixed at $y' = \pm a/2$ and two more parallel plates placed at $z' = \pm b/2$ as shown in Fig. 1. Without loss the generality we consider that $a \leq b$. Moreover, we assume the channel length ℓ to be essentially larger than its width, i.e. $\ell \gg b$. The channel connects two reservoirs containing the same gas. The pressure P_1 and the temperature T_1 are maintained in the left reservoir, while the other values of the pressure P_2 and the temperature T_2 are maintained in the right one. We are going to calculate the mass flow rate M , which is defined as the quantity of mass passing through a cross section of the channel per unity of time.

The solution of the problem is determined by the following parameters: the pressure ratio P_2/P_1 , the temperature ratio T_2/T_1 , the height-to-width ratio a/b , and the rarefaction parameter (inverse Knudsen number) defined as

$$\delta = \frac{\sqrt{\pi} a}{2 \lambda}. \quad (1)$$

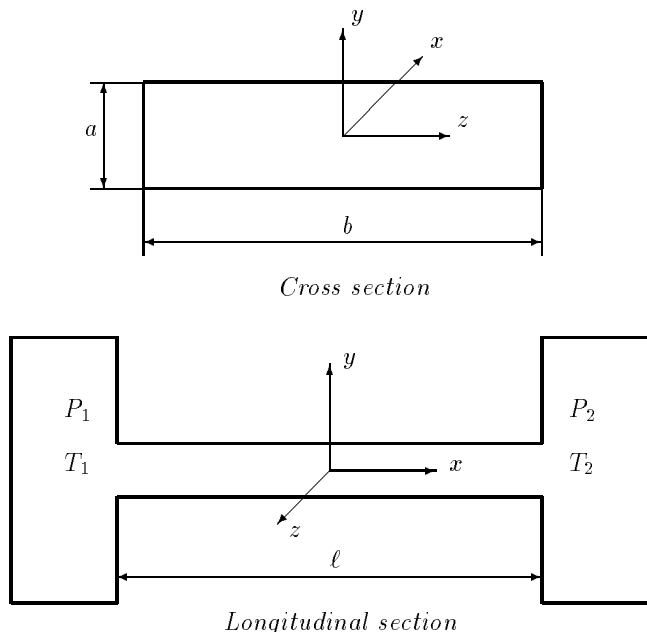


Figure 1: Sketch of the channel and coordinates

Here, λ is the molecular mean free path, which can be calculated via the shear viscosity μ as

$$\lambda = \frac{\mu}{P} \left(\frac{\pi k T}{2m} \right)^{1/2}, \quad (2)$$

where m is the molecular mass, and k is the Boltzmann constant. Substituting (2) into (1) the rarefaction parameter is calculated directly via the pressure P , the temperature T and the viscosity as

$$\delta = \frac{aP}{\mu} \left(\frac{m}{2kT} \right)^{1/2}. \quad (3)$$

If the dependence of the viscosity on the temperature $\mu = \mu(T)$ is known, it can be said that the rarefaction parameter δ is determined by the pressure and temperature only, i.e. $\delta = \delta(P, T)$.

It was shown [12], [13] that in a long channel the local pressure and temperature gradients are always small at any ratios P_2/P_1 and T_2/T_1 . Thus, the solution of the problem can be divided on two stages:

In the first stage we assume the local pressure and temperature gradients to be small, i.e.

$$v = \frac{a}{P} \frac{dP}{dx'}, \quad |v| \ll 1, \quad \tau = \frac{a}{T} \frac{dT}{dx'}, \quad |\tau| \ll 1. \quad (4)$$

This allows us to linearize the kinetic equation and to calculate the dimensionless flow rate Q through a cross section defined as

$$Q = \frac{1}{a b P} \left(\frac{2kT}{m} \right)^{1/2} \dot{M}, \quad (5)$$

where $P = P(x')$ is the local pressure in the cross section and $T = T(x')$ is the local temperature in the same section. Since the pressure and temperature gradients are small the reduced flow rate can be decomposed as

$$Q = -Q_P v + Q_T \tau, \quad (6)$$

where the positive coefficients Q_P and Q_T do not depend on the gradients v and τ . The first coefficient Q_P describes the gas flow caused by the pressure gradient. This is the so-called Poiseuille flow. The second coefficient Q_T corresponds to the gas flow caused by the temperature gradient, i.e. the thermal creep.

Finally, the first stage of the problem provides the values of these coefficients as a function of the ratio a/b and of the local rarefaction parameter δ calculated via $P(x')$ and $T(x')$ by (3).

To realize the second stage we need to introduce the other reduced flow rate as

$$G = \frac{\ell}{a^2 b P_1} \left(\frac{2kT_1}{m} \right)^{1/2} \dot{M}. \quad (7)$$

Unlike Q , this reduced flow rate does not depend on the local rarefaction parameter $\delta(x')$, but it is determined by the ratios a/b , P_2/P_1 , T_2/T_1 and by the rarefaction parameter δ_1 corresponding to the pressure P_1 and the temperature T_1 . The coefficient G will be calculated below via the coefficients Q_P and Q_T .

INPUT EQUATION

To calculate the coefficients Q_P and Q_T the linearized Boltzmann equation should be solved. This equation provides reliable numerical data but requires great computational efforts. Although, nowadays it is possible to calculate two-dimensional flows using the exact Boltzmann equation, the model kinetic equations continue to be good tools for practical calculations, because they allow us to reduce essentially the computational efforts. The problem is only to apply an appropriate model equation.

An analysis made in the review [5] shows that for non-isothermal flows of rarefied gases the S model [14] is suitable. In case of stationary flow it reads

$$\mathbf{v} \frac{\partial f}{\partial \mathbf{r}'} = \frac{P}{\mu} \left\{ f^M \left[1 + \frac{2m \mathbf{q}' \mathbf{V}}{15PkT} \left(\frac{mV^2}{2kT} - \frac{5}{2} \right) \right] - f \right\}, \quad (8)$$

where $f(\mathbf{r}', \mathbf{v})$ is the velocity distribution function, f^M is the local Maxwellian, $\mathbf{V} = \mathbf{v} - \mathbf{u}'$, \mathbf{v} is the molecular velocity, \mathbf{r}' is the position vector, \mathbf{u}' is the bulk (hydrodynamic) velocity, and \mathbf{q}' is the heat flow vector. The bulk velocity \mathbf{u}' and the heat flow vector \mathbf{q}' are calculated via the distribution function $f(\mathbf{r}', \mathbf{v})$.

It must be noted that the distribution function $f(\mathbf{r}', \mathbf{v})$ does not consider the internal structure of molecules and describes a state of monoatomic gas. To calculate

Table 1: Poiseuille flow Q_P vs δ and a/b

δ	Q_P			
	$a/b = 1$	$a/b = 0.1$	$a/b = 0.05$	$a/b = 0$
0	0.8387	1.991	2.373	∞
0.001	0.8371	1.978	2.344	4.273
0.01	0.8313	1.910	2.218	3.050
0.02	0.8255	1.860	2.132	2.713
0.05	0.8115	1.763	1.975	2.306
0.1	0.7959	1.671	1.832	2.038
0.2	0.7794	1.573	1.688	1.823
0.5	0.7663	1.465	1.537	1.613
1.	0.7739	1.437	1.493	1.549
2.	0.8175	1.505	1.556	1.606
5.	0.9950	1.882	1.941	2.000
10.	1.323	2.609	2.690	2.772
20.	2.006	4.129	4.262	4.393
40.	3.395	7.214	7.451	7.695

Table 2: Thermal creep Q_T vs δ and a/b

δ	Q_T			
	$a/b = 1$	$a/b = 0.1$	$a/b = 0.05$	$a/b = 0$
0	0.4193	0.9955	1.186	∞
0.001	0.4181	0.9839	1.162	1.855
0.01	0.4110	0.9165	1.044	1.246
0.02	0.4037	0.8658	0.9662	1.078
0.05	0.3857	0.7695	0.8291	0.8719
0.1	0.3637	0.6763	0.7089	0.7320
0.2	0.3390	0.5814	0.5968	0.6105
0.5	0.2953	0.4490	0.4553	0.4620
1.	0.2545	0.3553	0.3593	0.3633
2.	0.2070	0.2667	0.2693	0.2719
5.	0.1366	0.1598	0.1609	0.1621
10.	0.0868	0.0956	0.0961	0.0966
20.	0.0495	0.0522	0.0524	0.0526
40.	0.0263	0.0269	0.0270	0.0270

a polyatomic gas flow one has to introduce additional variables of the distribution function and to apply an appropriate kinetic equation.

For further derivations it is convenient to introduce the following dimensionless quantities

$$\mathbf{r} = \frac{\mathbf{r}'}{a}, \quad \mathbf{c} = \beta \mathbf{v}, \quad u = \beta u'_x, \quad q = \frac{\beta}{P} q'_x,$$

where $\beta = \sqrt{m/2kT}$. Here, we assume the bulk velocity and the heat flow vector to have the x -component only, that is why the subscript x is omitted in the dimensionless notations u and q .

To linearize the S model (8) the distribution function is presented as

$$f(\mathbf{r}, \mathbf{c}) = f^0 \left[1 + h(y, z, \mathbf{c}) + vx + \left(c^2 - \frac{5}{2} \right) \tau x \right], \quad (9)$$

where f^0 is the absolute Maxwellian. Substituting (9) into (8) we obtain the linearized S model.

Because of the smallness of the gradients v and τ the solution of the linearized S model can be split in two parts

$$h = h_P v + h_T \tau. \quad (10)$$

The distribution function moments can be also split as

$$u = u_P v + u_T \tau, \quad q = q_P v + q_T \tau.$$

Then, the coefficients Q_P and Q_T are expressed as

$$Q_P = -2 \frac{a}{b} \int_{-b/2a}^{b/2a} \int_{-1/2}^{1/2} u_P(y, z) dy dz, \quad (11)$$

$$Q_T = 2 \frac{a}{b} \int_{-b/2a}^{b/2a} \int_{-1/2}^{1/2} u_T(y, z) dy dz. \quad (12)$$

Thus, the linearized S model is decomposed on the two independent equations. The solution of the first of them h_P provides the coefficient Q_P and the solution of the second one h_T gives the coefficient Q_T . However, the Onsager relation [7] allows us to substitute u_T by q_P in (12). So, to calculate both coefficients Q_P and Q_T it is enough to solve only the first equation.

The S model equation with the diffuse boundary condition has been solved by the optimized discrete velocity method [15].

NUMERICAL RESULTS

The numerical calculations have been performed for three values of the ratio $a/b=1; 0.1; 0.05$. The numerical values of the coefficients Q_P and Q_T are given in Tables 1 and 2, respectively.

It should be noted that according to the analysis made in the review [5] the influence of the internal molecular structure on the coefficient Q_P is very weak, while the coefficient Q_T essentially depends on the molecular structure. So, the data given in Table 1 are applicable to any polyatomic gas, but the coefficient Q_T must be recalculated for every specific polyatomic gas.

Some words should be said about the lateral wall influence on the coefficients Q_P and Q_T . For the small values of the rarefaction parameter δ this influence continue to be large even if the ratio a/b is small. From Table 1 one can see that for $\delta = 0.001$ the difference of the Poiseuille flow Q_P at $a/b = 0.05$ and at $a/b = 0$ is about 80% instead of the expected value 5%. The same can be said on the thermal creep Q_T . For the large values of δ the lateral wall influence becomes small even for rather large values of the ratio a/b . One can see that for $\delta = 40$ the difference of the coefficient Q_T at

Table 3: Reduced flow rate G vs δ_1 and a/b at $P_2/P_1=1$

δ_1	G		
	$a/b = 1$	$a/b = 0.1$	$a/b = 0.05$
0.001	0.4087	0.9702	1.1563
0.01	0.4033	0.9187	1.0618
0.1	0.3694	0.7262	0.7805
1.	0.2718	0.4090	0.4158
10.	0.1151	0.1354	0.1364
100.	0.0187	0.0190	0.0191

$a/b = 0.1$ and at $a/b = 0$ is less than 1% instead of the expected difference 10%. So, the lateral wall influence on the Poiseuille flow Q_P and on the thermal creep Q_T essentially depends on the rarefaction parameter δ .

With help of (4)-(7) we obtain the differential equation analogous that derived in the work [16] for the circular capillary

$$\frac{1}{P_1} \frac{dP}{dx} = \frac{1}{Q_P} \left[Q_T \frac{P}{P_1 T} \frac{dT}{dx} - \frac{a}{\ell} \left(\frac{T}{T_1} \right)^{1/2} G \right]. \quad (13)$$

The unknown function of the equation is the pressure $P = P(x)$, which must satisfy the boundary condition $P(-\ell/2a) = P_1$. The quantity G is a parameter of the equation and we must fit G so the pressure $P(x)$ would be equal to P_2 at $x = \ell/2a$.

The differential equation (13) was solved by the finite difference method. The only value of the temperature ratio has been considered, $T_2/T_1 = 3.8$, which corresponds to the situation when one reservoir is placed in liquid nitrogen ($T_1 = 77.2$ K) and the other one is maintained at the room temperature ($T_2 = 293$ K).

Two values have been taken for the pressure ratio: $P_2/P_1=1$ and $P_2/P_1=100$. The first value of the pressure ratio corresponds to the situation when there is no the pressure difference between the reservoirs and the gas flow is caused only by the temperature difference. The numerical results of this flow are given in Table 3. One can see that: (i) the reduced mass flow G is positive, i.e. the gas flows from the left ("cold") reservoirs to the right ("hot") one; (ii) the mass flow rate G decreases with the increasing rarefaction parameter δ_1 .

The second value of the pressure ratio $P_2/P_1 = 100$ corresponds to the situation of large pressure difference. The behavior of the reduced flow rate G completely differs from that obtained for $P_2/P_1 = 1$: (i) it is negative, i.e. the gas flows from the right reservoirs to the left one; (ii) the quantity G increases with the increasing rarefaction parameter δ_1 .

Since Eq.(13) contains the coefficient Q_T strongly depending on the internal molecular structure, the data given in Tables 3 and 4 are valid only for monoatomic gases.

Table 4: Reduced flow rate G vs δ_1 and a/b at $P_2/P_1=100$

δ_1	$-G$		
	$a/b = 1$	$a/b = 0.1$	$a/b = 0.05$
0.001	41.88	96.37	111.9
0.01	40.97	87.14	95.45
0.1	46.16	89.16	92.66
1.	125.2	259.1	268.3
10.	939.6	2070.	2138.
100.	9094.	20190.	20860.

ACKNOWLEDGEMENT

The author gratefully acknowledges the support by the Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq).

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