Data on the Slip Coefficients

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ABSTRACT

For mathematical modeling of microfluidics it is necessary to calculate a rarefied gas flow through micropumps, microvalves and other elements with a high accuracy. Since the size of microfluidics is close to the molecular mean free path, the gas rarefaction must be taken into account. If the Knudsen number is sufficiently small the gas flow can be calculated applying the Navier-Stokes equation with the slip boundary condition. The slip coefficients depend on the chemical composition of the solid surface and on the species of the gas. They can be calculated applying the Boltzmann kinetic equation with an appropriate gas-surface interaction law. The aim of the present report is to make a critical review of the theoretical and experimental data and to give the recommended data for the slip coefficients.

1 INTRODUCTION

The gas rarefaction is determined by the Knudsen number defined as Kn=λ/a, where λ is the molecular mean free path and a is a characteristics size of a gas flow. If the Knudsen number is sufficiently small a rarefied gas flow can be calculated applying the Navier-Stokes equation with the slip boundary condition, which reads

$$u_t = A_{\mathrm{P}}\frac{\partial u_t}{\partial x_n} + A_{\mathrm{T}}\frac{\partial T}{\partial x_t}, \qquad (1)$$

where x_t is the coordinate tangential to the surface, x_n is the normal coordinate, u_t is the tangential velocity, T is the surface temperature, A_{P} and A_{T} are the slip coefficients. Here, it is more convenient to introduce the dimensionless slip coefficients as

$$\sigma_{\mathrm{P}} = \frac{\sqrt{\pi}}{2\lambda}A_{\mathrm{P}}\,, \qquad \sigma_{\mathrm{T}} = \frac{1}{\lambda}\left(\frac{\pi m T}{2k}\right)^{1/2} A_{\mathrm{T}}\,, \quad (2)$$

where m is the molecular mass of the gas and k is the Boltzmann constant. Nowadays, there is a lot of numerical and experimental data on the slip coefficients σ_{P} and σ_{T}. However, because of many divergences in their definition, in the methods of calculation and in the methods of measurement it is very difficult to get the reliable data that could be applied in the modeling of microsystems.

The aim of the present work is to make a critical review of the theoretical and experimental data and to give the recommended data for the slip coefficients σ_{P} and σ_{T}. Here, all numerical data will be given in accordance with the definitions (1)-(2) independently on the definitions in the original works.

2 VISCOUS SLIP COEFFICIENT

To calculate the viscous slip coefficient σ_{P} one has to consider a stationary rarefied gas flow in the semi - infinite space $x_n \geq 0$ over an infinite plate having a constant temperature T. The behavior of the gas is described by the linearized Boltzmann equation [1], [2]. To simplify the calculations the so-called model kinetic equations are used. The BGK model [3] and the S model [4] are most usable equations. At the surface ($x_n = 0$) the distribution function satisfies the boundary condition derived from the gas-surface interaction law. At infinity ($x_n \rightarrow \infty$) it is assumed that the distribution function coincides with the Chapman-Enskog solution [2] corresponding to the momentum transfer by a constant velocity gradient.

It should be noted that the viscous slip coefficient σ_{P} is not sensitive to the internal structure of gaseous molecules, i.e. the numerical data given below can be successfully used for both monoatomic and polyatomic gases.

2.1 Diffuse scattering

The diffuse reflection is most used boundary condition for calculations of rarefied gas flows. This means that the molecules are reflected with the equilibrium distribution function independently on the distribution of the incident molecules. This gas-surface interaction law is called also the perfect accommodation. Under this condition a numerical solution [5] of the BGK model gave the value $\sigma_{\mathrm{P}} = 1.016$. Resolving the Boltzmann equation with the same boundary condition the value $\sigma_{\mathrm{P}} = 0.985$ was obtained in the works [6] and [7].

So, the value $\sigma_{\mathrm{P}} = 1.0$ can be recommended for any gas in case of perfect accommodation. Since for an imperfect accommodation the slip coefficient σ_{P} is always larger, the value $\sigma_{\mathrm{P}} = 1.0$ can be considered as the smallest one for any gas and any surface.

Table 1: Theoretical data on the viscous slip coefficient σ_P

α	σ_P		
	work [12]	work [13]	Eq.(3)
0.6	2.2554	2.2093	2.2576
0.7	1.8187	1.7766	1.8194
0.8	1.4877	1.4494	1.4877
0.9	1.2272	1.1925	1.2270
1.0	1.0162	0.9849	1.0160

2.2 Diffuse-specular scattering

If the gas-surface interaction is not diffuse, usually the diffuse-specular law is assumed. This means that the α fraction of incident molecules is reflected diffusely and the $(1-\alpha)$ fraction is reflected specularly. The quantity α is called the accommodation coefficient. Because of simplicity of this law it is widely used in practical calculations. However, some theoretical results based on this model contradict experimental data. The matter is that, the gas-surface interaction is very complicated process and for the correct description of the transport process on the gas-surface boundary one has to apply another model obtained from a microscopic analysis of the gas interaction with a solid surface, e.g. the Cercignani - Lampis model [8]. Till now there are no any data on the slip coefficients based on this model. So, the data given here are restricted by the diffuse-specular model only.

Applying different approximate methods to the kinetic equation the following expression for the slip coefficient σ_P was obtained in the works [9]–[11]

$$\sigma_P(\alpha) = \frac{2-\alpha}{\alpha}\left[1.016 - 0.1211(1-\alpha)\right]. \qquad (3)$$

An exact numerical calculation of the slip coefficient σ_P over the whole range of α were carried out by Loyalka *et al.* [12] and by Wakabayashi *et al.* [13]. Their data are compared with Eq.(3) in Table 1. The small disagreement between the works [12] and [13] is explained by the different kinetic equations used by the authors. One can see that Eq.(3) can be successfully used in practical calculations.

2.3 Experimental data

The viscous slip coefficient σ_P can be measured via the mass flow rate in the hydrodynamic regime (Kn$\to$ 0) as was made in the papers [14]–[16]. The slip coefficient is calculated via the difference of the experimental mass flow rate and the theoretical one obtained for the non-slip boundary condition. Since the flow rates are close to each other the relative error of the slip coefficient σ_P measured in the hydrodynamic regime is very large. In Table 2 the experimental data for the gases helium, neon and argon and for a glass surface are given. One can see

Table 2: Experimental data on the viscous slip coefficient σ_P for glass surface

work	σ_P		
	He	Ne	Ar
[14]	1.10	1.11	1.16
[14]	1.32	1.38	1.29
[15]	1.26	1.33	1.20
[16]	1.30	1.34	1.27

that because of large relative error the dispersion of the experimental data for the same gas and the same surface is sufficiently large.

The slip coefficient σ_P can be obtained via the accommodation coefficient α, i.e. if one knows the quantity α one calculates σ_P by (3). The accommodation coefficient α can be measured via the mass flow rate through a long capillary in the free molecular regime, i.e. when Kn$\gg$ 1. In this regime the flow rate $M(\alpha)$ at an arbitrary α is related to that $M(1)$ for the perfect accommodation $\alpha = 1$ as

$$M(\alpha) = \frac{2-\alpha}{\alpha}M(1). \qquad (4)$$

The theoretical value of $M(1)$ for both cylindrical capillary and plane channel can be found in the review [17]. Knowing $M(1)$ and measuring $M(\alpha)$ one can calculate α from Eq.(4).

Some experimental data [14],[18],[19] on the coefficient α measured in the free molecular regime are given in Table 3. In the same table the slip coefficient σ_P calculated by Eq.(3) is given. One can see that two different measurements of α for the glass surface are in good agreement between them. The accommodation on the molybdenum surface is close to the perfect one. At the same time the accommodation on the titanium surface significantly differs from the diffuse one. To my knowledge, the data $\alpha = 0.65$ is the smallest experimental value of the accommodation coefficient α. The corresponding value of the viscous slip coefficient $\sigma_P = 2.02$ can be considered as the largest one. This results was obtained in the titanium surface deposited on a glass capillary in high vacuum, i.e. the surface was very clean. But if the surface is exposed to an open air, it absorbs the oxygen and other gases, then the coefficient α increases. The last row of Table 3 shows the data on the accommodation coefficient α on the same titanium surface but after an exposition to oxygen. One can see that the accommodation becomes almost diffuse.

So in practice, when a capillary or microchannel is staying in open air it is expected that the accommodation coefficient α is not smaller than 0.9 for any gas and any surface. Under this condition the largest value of the slip coefficient is $\sigma_P = 1.23$.

Thus, we conclude that in practice the viscous slip coefficient is restricted by the interval $1.0 < \sigma_P < 1.23$

Table 3: Experimental data on the accommodation coefficient α

		He		Ne		Ar	
work	surface	α	σ_P	α	σ_P	α	σ_P
[14]	glass	0.935	1.15	0.929	1.16	0.975	1.06
[18]	glass	0.932	1.15	0.925	1.17	0.977	1.06
[19]	Mo	0.985	1.04	0.983	1.05	0.993	1.03
[19]	Ti	0.65	2.02	-	-	0.85	1.35
[19]	Ti+O$_2$	0.98	1.05	-	-	0.99	1.04

for any gas and any surface. Its exact value can be calculated via the accommodation coefficient α measured in the free molecular regime of the gas flow.

3 THERMAL SLIP COEFFICIENT

To calculate the thermal slip coefficient σ_T one has to consider a stationary rarefied gas flow in the semi-infinite space $x_n \geq 0$ over an infinite plate having a linear temperature distribution. The same temperature distribution is established in the gas over the whole space occupied by him. The behavior of the gas is described by the linear Boltzmann equation [1], [2]. At the surface $(x_n = 0)$ the distribution function satisfies the boundary condition obtained from the gas-surface interaction law. At infinity $(x_n \to \infty)$ the function tends to the Chapman-Enskog solution [2] corresponding to the heat transfer in the gas by a constant temperature gradient.

It should be noted that the data given below were calculated for a monoatomic gas. Since the thermal slip coefficient σ_T is very sensitive to the internal molecular structure, these data cannot be used for polyatomic gases, but they must be recalculated applying an appropriate kinetic equation and gas-surface interaction law.

3.1 Diffuse scattering

An accurate numerical calculation based on the BGK model with the diffuse scattering on the surface was performed by Sone [20], Onishi [21] and Loyalka [12], [22]. All of them obtained the same result, namely $\sigma_T = 1.149$. The variational method applied to the S model [4] gave the value $\sigma_T = 1.125$ [11]. The direct numerical solution of the Boltzmann equation for rigid spheres obtained by Loyalka [23] and by Ohwada et al. [7] gave the values $\sigma_T = 1.01$.

From these data one can see that the thermal slip coefficient σ_T is sensitive to the kinetic equation applied in the calculation. Moreover, it is sensitive to the model of the intermolecular interaction. Since the exact Boltzmann equation was solved for the hard sphere molecules we cannot say that the value $\sigma_T = 1.01$ is more reliable than that obtained from the approximate model equation. The reliable result could be obtained from the

Table 4: Theoretical data on the thermal slip coefficient σ_T

	σ_T		
α	work [12]	work [13]	Eq.(5)
0.0	0.7500	0.7755	0.7500
0.2	0.8344	0.8286	0.8250
0.4	0.9165	0.8789	0.9000
0.6	0.9963	0.9266	0.9750
0.8	1.0739	0.9720	1.0500
1.0	1.1495	1.0152	1.1250

exact Boltzmann equation for the Lennard-Jones intermolecular potential, which is more physical than the hard sphere model.

The non-diffuse gas-surface interaction gives a smaller value of the slip coefficient σ_T. So, the largest theoretical value obtained for the perfect accommodation, i.e. $\sigma_T = 1.15$ can be assumed as the largest value of σ_T for any monoatomic gas and any surface.

3.2 Diffuse-specular scattering

Applying the method of elementary solutions to the BGK equation [3] with the diffuse-specular scattering Loyalka and Cipolla [22] obtained the following expression

$$\sigma_T = 0.75 + 0.3993\alpha .$$

The variational method applied to the BGK [3] and to the S-models [4] in the works [15], [22], respectively, gives the following expression

$$\sigma_T = 0.75 + 0.375\alpha . \qquad (5)$$

Loyalka et al. [12] solved the BGK model by the integro-moment method. Wakabayashi et al. [13] solved the Boltzmann equation by the discrete velocity method. In Table 4 the numerical results of the works [12], [13] are presented and compared with the expression (5). It can be seen that the expression (5) describes finely the exact numerical results based on the BGK model.

3.3 Experimental results

The thermal slip coefficient σ_T can be measured via the mass flow rate caused by a temperature gradient in the hydrodynamic regime (Kn$\to$ 0). Since the mass flow

Table 5: Experimental data on the thermal slip coefficient σ_T for glass surface

gas	He	Ne	Ar
σ_T	1.004	0.988	1.030
α	0.68	0.63	0.75

is very small its measurements must be carried out using a high precision equipment.

Some experimental data on the thermal slip coefficient σ_T for monoatomic gases on the glass surface [24] are presented in Table 5. In the third row the accommodation coefficient α calculated using Eq.(5) is given. Comparing these data on α with those given in Table 3 one can see that there is a large disagreement between them. This shows that the diffuse-specular model of the gas-surface interaction cannot provide reliable data. The model should contain at least two parameters: the accommodation coefficient of the tangential momentum α_t and the accommodation coefficient of the molecular kinetic energy α_e. Most probable, the viscous slip coefficient σ_P is determined by α_t only, while the thermal slip coefficient σ_T is determined by α_e. Since the diffuse-specular model has the only parameter α we do not know how to interpret this parameter calculated via the thermal slip coefficient σ_T. To understand the dependence of σ_T on the gas-surface interaction law this coefficient should be calculated from the exact Boltzmann equation with the Lennard Jones intermolecular potential assuming the Cercignani - Lampis [8] model of the gas-surface interaction.

Since we do not know the variation of the energy accommodation coefficient α_e the conclusion on the variation of the quantity σ_T can be deduced from Eq.(5). Assuming the smallest value of α as 0 we obtain the smallest value of the slip coefficient $\sigma_T = 0.75$. Its largest value has been already deduced, it is $\sigma_T = 1.15$. Thus, the thermal slip coefficient for any monoatomic gas and arbitrary surface is restricted by the interval $0.75 < \sigma_T < 1.15$. To reduce this interval and to give the recommended data for polyatomic gases some additional calculations must be carried out.

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