Knudsen effect and a unified formula for mass flow-rate in microchannels

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Abstract. Approximate analytical expressions for mass flow-rate in long isothermal channels are constructed on the basis of quasigasdynamic equations with Maxwell velocity-slip boundary conditions. These expressions correspond to experimental data for Knudsen numbers $Kn < 0.5$ and account for an effect of Knudsen minimum. Special correction are proposed to obtain a unified formula for mass flow-rate, valid up to free-molecular regime.

Keywords: Quasigasdynamic equations, isothermal microchannels, mass flow-rate
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INTRODUCTION

For Knudsen numbers $Kn < 0.1$ Navier-Stokes equation system with Maxwell–type boundary conditions account for velocity slip and temperature jump, are in reasonably agreement with the experimental data. For increasing Kn numbers Navier-Stokes results begin to diverge from the experiments. In particular, calculated values of mass flow-rate in microchannels exceed measured results and don't account for the so-called Knudsen minimum – an effect of minimum of a normalized mass flow-rate for $Kn \sim 1$ (e.g.[1]). Another example of disagreement is the anomalous decreasing of the skin friction drag for a microshpere with increasing Knudsen numbers.

There are two ways to overcome these problems: to improve the governing gasdynamic equations or to modify the boundary conditions. Promising results were obtained by modifying the slip boundary conditions, e.g. [2], [3], [4].

In this work we present the possibilities of quasigasdynamic (QGD) equations with Maxwell boundary conditions for simulation of rarefied gas flows.

QGD EQUATIONS AND POISEUILLE FLOW

In the usual notations the QGD equations have the form (e.g. [5])

$$\frac{\partial \rho}{\partial t} + div\vec{j}_m = 0, \tag{1}$$

$$\frac{\partial(\rho\vec{u})}{\partial t} + div(\vec{j}_m \otimes \vec{u}) + \vec{\nabla} p = div\Pi, \tag{2}$$

$$\frac{\partial}{\partial t}\left[\rho\left(\frac{\vec{u}^2}{2} + \varepsilon\right)\right] + div\left[\vec{j}_m\left(\frac{\vec{u}^2}{2} + \varepsilon + \frac{p}{\rho}\right)\right] + div\vec{q} = div(\Pi \cdot \vec{u}), \tag{3}$$

with a mass flux vector $\vec{j}_m$, a shear-stress tensor Π, and a heat flux vector $\vec{q}$ given by

$$\vec{j}_m = \rho(\vec{u} - \vec{w}), \quad where \quad \vec{w} = \frac{\tau}{\rho}[div(\rho\vec{u}\otimes\vec{u}) + \vec{\nabla} p], \tag{4}$$

$$\Pi = \Pi_{NS} + \tau\vec{u}\otimes\left[\rho(\vec{u}\cdot\vec{\nabla})\vec{u} + \vec{\nabla} p\right] + \tau I\left[(\vec{u}\cdot\vec{\nabla})p + \gamma p div\vec{u}\right], \tag{5}$$

$$\vec{q} = -\kappa\vec{\nabla} T - \tau\rho\vec{u}\left[(\vec{u}\cdot\vec{\nabla})\varepsilon + p(\vec{u}\cdot\vec{\nabla})\left(\frac{1}{\rho}\right)\right]. \tag{6}$$

Here

$$\tau = \eta/(pSc), \tag{7}$$

where Sc is Schmidt's number. System (1) – (6) must be completed by the state equations for the perfect gas

$$p = \rho RT, \qquad \varepsilon = p/(\rho(\gamma-1)),$$

and by the expressions for viscosity η and heat conductivity κ coefficients

$$\eta = \eta_0\Big(\frac{T}{T_0}\Big)^{\omega}, \qquad \kappa = \frac{\gamma R}{(\gamma-1)Pr}\eta.$$

For $\tau = 0$ the QGD system coincides with the Navier-Stokes one. For stationary flows, the dissipative terms (terms in τ) in QGD equations have the asymptotic order of $O(\tau^2)$ for $\tau \to 0$. For perfect gas the entropy production for QGD system is the entropy production for Navier-Stokes system completed by the additional terms in τ, that are the squared left-hand sides of of classical stationary Euler equations with positive coefficients:

$$X = \kappa\Big(\frac{\vec{\nabla}T}{T}\Big)^2 + \frac{(\Pi_{NS}:\Pi_{NS})}{2\eta T} + \frac{p\tau}{\rho^2 T}\Big[div(\rho\vec{u})\Big]^2 + \frac{\tau}{\rho T}\Big[\rho(\vec{u}\cdot\vec{\nabla})\vec{u} + \vec{\nabla}p\Big]^2 + \frac{\tau}{\rho\varepsilon T}\Big[\rho(\vec{u}\cdot\vec{\nabla})\varepsilon + pdiv\vec{u}\Big]^2. \tag{8}$$

To construct an analytical expression for the mass flow-rate in a long isothermal channel we will follow the method of [6], where a similar expression was obtained using the quasihydrodynamic (QHD) equations system. For the problem under consideration the QGD and QHD systems coincide. Let us analyze a gas flow in a plane channel of the length L in x–direction and width H in y–direction. The pressures at an entrance and exit of a channel are p_1 and p_2, where $p_1 > p_2$. According to [7] (chap.2, sec.18, problem 6) suppose that a pressure gradient along a channel is small, and along a small distance dx gas density ρ may be regarded as a constant. Let us look for the solution of the system (1)–(6) in the form

$$u_x = u(y), \quad u_y = 0, \quad p = p(x), \quad T = T_0. \tag{9}$$

In this case the Navier-Stokes, QGD, and QHD systems reduce to the same equation

$$\frac{dp(x)}{dx} = \eta_0\frac{d^2u(y)}{dy^2}. \tag{10}$$

Using Maxwell velocity-slip boundary conditions [8]

$$\Big(u - \frac{2-\sigma}{\sigma}\lambda\frac{du}{dy}\Big)\Big|_{y=0} = 0, \quad \Big(u + \frac{2-\sigma}{\sigma}\lambda\frac{du}{dy}\Big)\Big|_{y=H} = 0,$$

one obtains the modified Poiseuille formula (e.g. [1])

$$u_x = -\frac{1}{2\eta_0}\frac{dp(x)}{dx}\Big[y(H-y) + \frac{2-\sigma}{\sigma}\lambda H\Big].$$

Here σ is the coefficient of accommodation for velocity, and λ is the mean free-path

$$\lambda = A\frac{\eta}{p}\sqrt{RT}, \tag{11}$$

where $A = \sqrt{\pi/2}$ for Chapman formula [8], or $A = 2(7-2\omega)(5-2\omega)/(15\sqrt{2\pi})$ for Bird formula [9].

Mass flow-rate calculation

For the Navier-Stokes system the mass flux vector is $j_{mx} = \rho u_x$. According to [7] we replace $\rho = p/RT_0$ and the calculate mass flow-rate through the section of the channel is

$$J_{NS} = \int_0^H j_{mx}dy = \int_0^H \rho u_x dy = -\frac{H^3}{8\eta_0 RT_0}\Big[\frac{2}{3}p\frac{dp}{dx} + 4\frac{2-\sigma}{\sigma}p\frac{dp}{dx}\frac{\lambda}{H}\Big]. \tag{12}$$

For both QGD and QHD models $j_{mx} = \rho(u_x - w_x)$, where

$$w_x = -\frac{\tau}{\rho}\frac{dp}{dx} = -\frac{\eta}{pSc}\frac{1}{\rho}\frac{dp}{dx}.$$

This additional mass flux is connected with the self-diffusion, and is proportional to the pressure gradient. So, the mass flow-rate in a channel section becomes

$$J = \int_0^H \rho(u_x - w_x)dy = \int_0^H \rho u_x dy - \frac{\eta}{Sc}\int_0^H \frac{1}{p}\frac{dp(x)}{dx}dy =$$
$$= -\frac{H^3}{8\eta_0 RT_0}\Big[\frac{2}{3}p\frac{dp}{dx} + 4\frac{2-\sigma}{\sigma}p\frac{dp}{dx}\frac{\lambda}{H} + \frac{8}{A^2Sc}p\frac{dp}{dx}\Big(\frac{\lambda}{H}\Big)^2\Big]. \quad (13)$$

The last term in (13) is obtained by replacing η by λ using (11).

The first term in (13) describes the mass flow-rate for non-slip Poiseuille flow, the second one accounts for the flow-rate increasing because of velocity-slip conditions, the third one explains the flow-rate increasing because of self-diffusion. It does not depend from σ. The importance of self-diffusion for rarefied flows is mentioned in, e.g. [1] and [10]. This last term has the order of $O(\tau \cdot \eta)$ or $O(Kn^2)$, where $Kn = \lambda/H$. For stationary flows this fact corresponds with the known difference between QGD and Navier-Stokes models.

The QGD approach allows to obtain the analytical expression of the form (13) for tube, and for tube of annular section channels, and for plane channels with different accommodation coefficients σ for upper and down walls.

According to [1] mass flow-rate in a plane channel for free-molecular flow is

$$J_0^{xy} = \frac{4H^2\sqrt{2}}{3\sqrt{\pi RT_0}}\frac{dp}{dx}. \quad (14)$$

The normalized flow-rate (13) becomes then

$$Q_{xy} = \frac{J}{J_0^{xy}} = \frac{3\sqrt{\pi}A}{8\sqrt{2}}\Big[\frac{Kn^{-1}}{6} + \frac{2-\sigma}{\sigma} + \frac{2}{A^2\,Sc}Kn\Big]. \quad (15)$$

The minimum of Q_{xy} takes place for

$$Kn_m = \frac{A}{2}\sqrt{\frac{Sc}{3}}.$$

This value does not depend from σ. For $Sc = 1$, $A = \sqrt{\pi/2}$, $Kn_m = 0.36$.

Basing on the BGK model for hard-sphere molecules ($\omega = 0.5$) the mass flow-rate in plane, tube, and tube of annular section channels have been calculated in [10], [11], [12] [13], [14]. These results have been presented in form of tables and figures. For small Knudsen numbers ($Kn \to 0$) the corresponding approximative formula for a plane channel is presented in [10] by

$$Q_{cer} = \frac{Kn^{-1}}{6} + \sigma + (2\sigma^2 - 1)Kn. \quad (16)$$

Other data mass-flow rate data been collected in [15]. For $\sigma = 1$ equations (15) and (16) differ only by the numerical factor $2/(A^2Sc) \sim 1$. Note also, that in (15) the last term does'not depend from σ. As will be shown below, expressions (13) and (15) correspond to kinetic results up to $Kn \sim 0.5$.

Corrections to account for mass flow-rate in rarefied flows

Additional terms in the QGD system, which are proportional to a small parameter τ, are related with the additional smoothing, or averaging in time in the definition of the gasdynamic parameters [5, 6]. A value of τ with the accuracy of the coefficient ~ 1 is equal to the collisional mean free-path time. For increasing Kn, τ also increases. For rarefied flows with $\lambda \geq H$, or $Kn = \lambda/H \geq 1$, it is reasonable to limit the averaging time and to connect it additionally with the characteristic dimentions of the problem under consideration. To realize it we introduce a correction for τ-value (7) in the form

$$\tau = \frac{\eta}{pSc(1+Kn)}. \quad (17)$$

For $Kn \to 0$ relation (17) reduces to (7) and does not disturb the previous results. Using λ as (11) one get for $Kn >> 1$

$$\tau = \frac{\eta}{pSc(1+Kn)} \sim \frac{\eta}{pScKn} = \frac{H}{ScA\sqrt{RT}}. \tag{18}$$

So, for a rarefied flow, $\tau \sim H/\sqrt{RT}$ has the order of a mean free-path time between collisions with the boundaries of the volume under consideration.

In order to employ the corrected τ formula, it is useful to introduce in (17) a numerical factor $\alpha \sim 1$, rewriting τ

$$\tau = \eta/(pSc(1+\alpha Kn)),$$

the mass flow-rate (13) taking the form

$$J = -\frac{H^3}{8\eta_0 RT_0}\left[\frac{2}{3}p\frac{dp}{dx} + 4\frac{2-\sigma}{\sigma}p\frac{dp}{dx}\frac{\lambda}{H} + \frac{8}{A^2Sc}p\frac{dp}{dx}\left(\frac{\lambda}{H}\right)^2\frac{1}{(1+\alpha\lambda/H)}\right]. \tag{19}$$

The normalized flow-rate (analog to (15)) becomes then:

$$Q_{xy} = \frac{J}{J_0^{xy}} = \frac{3\sqrt{\pi}}{8}\frac{A}{\sqrt{2}}\left[\frac{Kn^{-1}}{6} + \frac{2-\sigma}{\sigma} + \frac{2}{A^2\,Sc}\frac{Kn}{(1+\alpha Kn)}\right]. \tag{20}$$

From this relation a minimum of the mass flow rate is reached for

$$Kn_m = \frac{A}{2}\sqrt{\frac{Sc}{3}}\left(1-\alpha\frac{A}{2}\sqrt{\frac{Sc}{3}}\right)^{-1}.$$

For $\alpha = 1$, $Sc = 1$, $A = \sqrt{\pi/2}$ (Chapman formula), and $Kn_m = 0.56$.

The condition of existence of Knudsen minimum $Kn_m > 0$ imposes the limit for coefficient α:

$$\alpha < \frac{A\sqrt{Sc}}{2\sqrt{3}} \sim 3.$$

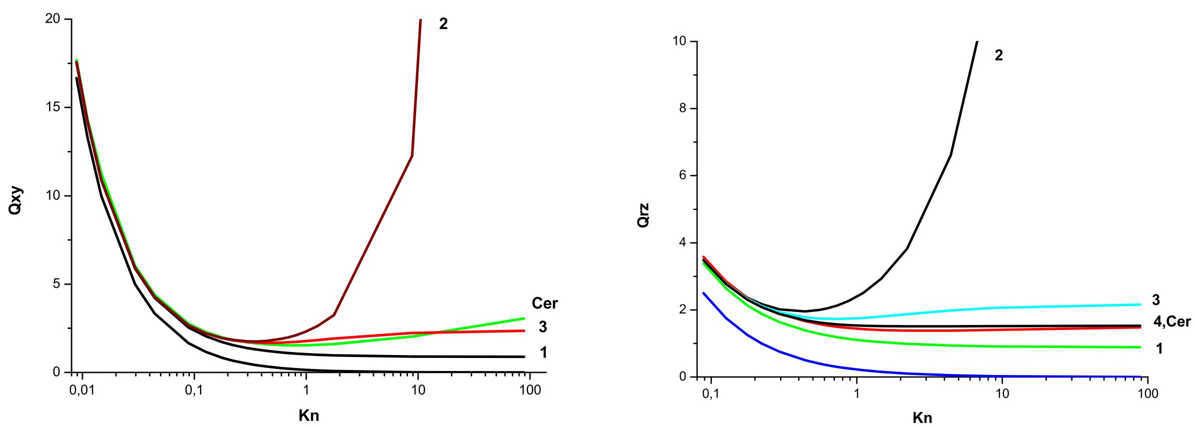

FIGURE 1. Q_{xy} (left) and Q_{rz} (right) for $\sigma = 1$, $A = \sqrt{\pi/2}$, $Sc = 1$. Comparison with BGK results from [10]. Line "Cer" stands for BGK results. Line 1 stands for Navier-Stokes solution with velocity slip condition, line 2 — QGD model without correction ($\alpha = 0$), line 3 – QGD for $\alpha = 1$. Line 4 (right) QGD for $\alpha = 2$.

For $Kn >> 1$ the mass flow-rate is equal to the flow-rate in free molecular flow, obtained by a simple kinetical model in, e.g. [1], and (20) looks as

$$Q_{xy} = \frac{J}{J_0^{xy}} = \frac{3\sqrt{\pi}}{8}\frac{A}{\sqrt{2}}\left[\frac{2-\sigma}{\sigma} + \frac{2}{\alpha A^2\,Sc}\right] = 1. \tag{21}$$

From this relation one can determine α. For $\sigma = 1$

$$\alpha = \frac{6\sqrt{\pi}}{ASc(8\sqrt{2} - 3A\sqrt{\pi})}.$$

For $A = \sqrt{\pi/2}$, $Sc = 1$, one gets $\alpha = 1.82$. The BGK solution from [10] gives $Q_{xy} \sim \ln Kn$ for $Kn \to \infty$.

In a similar way we obtained the normalized mass flow-rate for tube flow of radius H

$$Q_{rz} = \frac{J}{J_0^{rz}} = \frac{3\sqrt{\pi}}{8}\frac{A}{\sqrt{2}}\Big[\frac{Kn^{-1}}{4} + \frac{2-\sigma}{\sigma} + \frac{2}{A^2\,Sc}\frac{Kn}{(1+\alpha Kn)}\Big], \tag{22}$$

where mass flow-rate for free molecular flow [1] is

$$J_0^{rz} = \frac{4H^3}{3}\sqrt{\frac{2\pi}{RT_0}}\frac{dp}{dz}.$$

For the tube flow the exact BGK solution from [10] in the limit $Kn \to \infty$ gives also the constant asymptotic solution $Q_{xy} \sim const$.

The normalized flow-rate has a minimum for Knudsen number

$$Kn_m = \frac{A}{2}\sqrt{\frac{Sc}{2}}\Big(1 - \alpha\frac{A}{2}\sqrt{\frac{Sc}{2}}\Big)^{-1}.$$

In the figures 1 the calculated mass flow-rate for a plane and tube channels in forms (20) and (22) are shown in comparison with BGK calculations [10] as a function of Kn. In our calculations $\sigma = 1$, $A = \sqrt{\pi/2}$, $Sc = 1$. On both figures line 1 corresponds to Navier-Stokes calculations with Maxwell velocity-slip boundary conditions; line without markers - for Navier-Stokes non-slip calculations.

From both pictures it is clear, that up to $Kn \sim 0.1$ Navier-Stokes solution with velocity-slip condition corresponds well with BGK results. Up to $Kn \sim 0.5$ the QGD solution accounts well for BGK data, and then rapidly tends to infinity. The QGD formula with correction corresponds rather well with the BGK solution for Knudsen numbers up to $Kn \sim 100$ for a plane channel, and up to free-molecular regime for a tube channel. Here for a plane channel $\alpha = 1$, for a tube channel $\alpha = 2$.

Comparison with the experiment

In figures 2 mass flow-rate J_{xy} for the plane channel is comapared with the experimental data from [16], where data are presented in nondimentional form, normalized for Poiseuille flow-rate

$$J_P = H^3 p/(12\eta_0 RT_0)dp/dx$$

and presented as

$$S_T = 1 + 6\frac{2-\sigma}{\sigma}Kn + 12A_2Kn^2. \tag{23}$$

In [16] λ is calculated for hard sphere molecules. Coefficient A_2 is supposed to be a function from σ and Kn, $A_2 = A_2(\sigma, Kn)$. The mass flow-rate (19) normalized for Poiseuille flow J_P has the form

$$S = \frac{J_{xy}}{J_P} = 1 + 6\frac{2-\sigma}{\sigma}Kn + \frac{12}{A^2\,Sc(1+\alpha Kn)}Kn^2, \tag{24}$$

which differs from (23) in the form of coefficient A_2.

In figures 2 the calculated mass flow-rates for a plane channel (24) are shown in comparison with experimental results [16]. On both figures line 1 corresponds to Navier-Stokes calculations with Maxwell velocity-slip boundary conditions. In our calculations $\sigma = 1$, $A = 16/5\sqrt{2\pi}$. On the left figure QGD results without correction are presented for $Sc = 0.75$ and $Sc = 0.88$. Up to $Kn \sim 0.5$ the numerical results correspond to the experimental ones for the right Sc number. On the left figure numerical results with correction are presented for $Sc = 0.75$. It is seen, that adjusting α it is possible to fit experimental and numerical results properly.

In [4], a special velocity-slip boundary condition, non-linear in Kn, was used to obtain a mass flow-rate. The resulting expressions are very similar to the ones obtained here with the τ-correction. The good agreement of results [4] with the experiment indirectly confirm the validity of expressions (19), (20), (22) and (24).

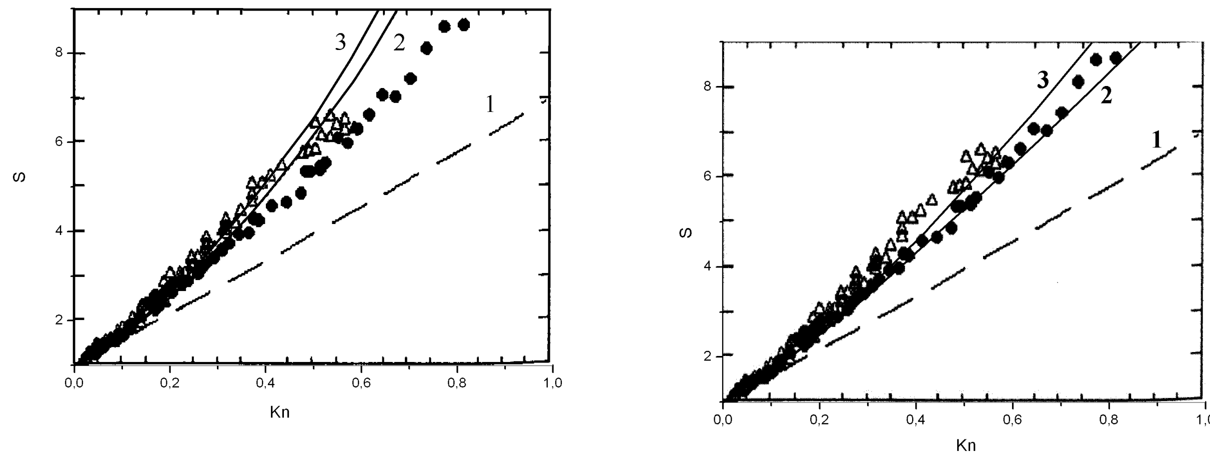

FIGURE 2. Comparison of normalized mass-flux S with the experimental data for nitrogen (triangles) and helium (points) from [16]. Line 1 corresponds to Navier-Stokes calculations with Maxwell velocity-slip boundary conditions. Left — QGD calculations without correction ($\alpha = 0$). Line 2 stands for $Sc = 0.88$, line 3 – for $Sc = 0.75$. Right — QGD with correction, $Sc = 0.75$. Line 2 stands for $\alpha = 2$, line 3 – for $\alpha = 1$.

CONCLUSIONS

The results obtained for isothermal microchannel flow demonstrate that the Navier-Stokes model with Maxwell velocity-slip conditions is valid up to $Kn \sim 0.1$.

The QGD equations allow to construct approximate analytical expressions for the mass flow-rate in long isothermal microchannels, which correspond to experimental data up to $Kn \sim 0.5$, and predicts the existence of Knudsen minimum.

The correction of a relaxation time $\tau \to \tau/(1+\alpha Kn)$, where α is a numerical factor of order unity, leads to the unified approximate mass flow-rate formula for long isothermal channels, valid up to near free-molecular regime.

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