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MODELING OF THE SLIP BOUNDARY CONDITION IN MICRO-CHANNEL/PIPE FLOW VIA FRACTIONAL DERIVATIVE

Vladan Djordjević

University of Belgrade, Faculty of Mechanical Engineering
Kraljice Marije 16, 11120 Belgrade, Serbia
E-mail: vladj@rcub.bg.ac.yu

Summary. *Rarefied gas flow in micro-channels/pipes which height/radius is measured in micro- or nanometers is treated in the paper. Knudsen number in these geometries may vary from very low values present in the continuum flow to very large values pertinent to the free molecular flow. In order to cover the entire Knudsen number range with a single physical model we model the wall slip boundary condition by means of a fractional derivative, whereby its order conveniently depends on the local value of the Knudsen number in the channel flow, or on an average value of this number in the pipe flow. Excellent agreement with both experiments and the results of numerical simulations is achieved.*

Keywords: *micro-channel/pipe flow, slip boundary condition, fractional derivative*.

1 INTRODUCTION

Due to both their practical importance and theoretical attractiveness several problems of rarefied gas dynamics have drawn much attention in the literature recently. This particularly holds for internal gas flows encountered in low-pressure or vacuum environments as well as in micrometer or sub-micrometer size geometries at standard atmospheric conditions. Applications in the first category include devices used in hypersonic flight, and several types of vacuum instruments, e.g., ionization gauges, partial pressure and residual gas analyzers, while applications in the second category are encountered in micro-electromechanical systems (MEMS), and include small accelerometers, pressure sensors, micro actuators, etc. Several new fabrication techniques have been developed in order to make the application of these devices in our everyday life possible (for a review on the variety of MEMS devices and fabrication techniques, s. [1]).

The flow of a gas in a MEMS device, e.g. in a micro-channel, or in a micro-pipe is characterized by the rarefaction effect, which consists in the fact that the Knudsen number Kn=$\frac{\lambda}{\beta}$, where λ is the mean free path of the molecules and β is some characteristic length scale (the height h of the channel, or the radius a of the tube), is not small enough so that continuum hypothesis does not hold. As a consequence gas slips along the channel walls, and classical no-slip boundary conditions cannot be employed. As a rule of thumb, for $\mathrm{Kn} < 10^{-3}$ the fluid can be considered as a continuum, while for $\mathrm{Kn} > 10$ the fluid flow is considered as a free molecular flow. Between these two extreme regimes of flow further classification is needed, i.e. slip-flow for $10^{-3} < \mathrm{Kn} < 0.1$ and transition flow for $0.1 < \mathrm{Kn} < 10$. Particular attention in the formulation of boundary conditions was paid to slip-flow regime by Beskok et al. [2] for both pressure driven and shear driven flow. Based on an approximate analysis of the motion of a monatomic gas near an isothermal surface they defined a high-order boundary condition, which allows simple analytic solutions for compressible, viscosity dominated flows. Agreement with available experiments and results of numerical simulations was shown to be very good.

In very long micro-channels, or pipes exhausting to a low-pressure environment, with the inlet pressure comparable with atmospheric conditions, gas flow may happen to pass through all regimes mentioned above. In such a case it is highly desirable to have a model for the slip boundary condition, which would cover all regimes of flow, from continuum one, to free molecular flow. The first model of this kind was proposed by Beskok and Karniadakis [3]. The model was introduced on a purely empirical basis in the form of a "rarefaction coefficient", by means of which the expression for the mass flow rate, obtained for relatively small values of the Knudsen number in the slip-flow regime, is "corrected" so as to embody the entire Knudsen number regime. The results obtained for volumetric and mass flow rate as well as for the pressure distribution are fitted well with the results of the direct-simulation Monte Carlo (DSMC) method and the solutions of linearized Boltzmann equation.

In this paper we make another attempt to cover the entire Knudsen number range by modeling the slip boundary condition via a fractional derivative. For this purpose we define a version of Caputo derivative [4] whose order α is either a function of the local value of the Knudsen number in the channel, or a function of the appropriately defined average value of the Knudsen number in the pipe. For $\alpha = 0$ boundary conditions are classical, no-slip boundary conditions in the continuum model, while as $\alpha \to 1-$ the Knudsen number approaches infinity and the flow becomes a free molecular flow. According to our knowledge such an application of a fractional derivative is specific, because they are mostly used for modeling the rheological properties of different viscoelastic materials and in modeling various phenomena in many branches of physics by fractional order differential equations. Thus, the analysis presented in this paper adds to the vast variety of applications of fractional derivatives and opens a new ground for describing complex flow phenomena in rarefied gas dynamics.

In what follows we will make a presentation of our own results of investigation of the modeling of slip boundary condition in rarefied gas flow by using fractional-order derivatives in micro-channels and micro-pipes, published previously in [5] and [6].

2 MICRO-FLOW IN A CHANNEL

The problem considered here in is depicted in Fig.1. h and ℓ are the height and the length of the channel respectively, $u(x, y)$ is the velocity component in x - direction, and p_i and p_e are the inlet and the exit pressures, respectively. If we assume that $h << \ell$ and that the reference Mach number is low enough we may use the so-called lubrication approximation to describe the isothermal flow in the channel:

$$\mu \frac{\partial^2 u}{\partial y^2} = \frac{dp}{dx}, \tag{1}$$

where μ is viscosity and $p(x)$ is the pressure. In addition to (1) we will also use the continuity equation for a compressible medium. In this simple case of flow it states that the mass flow rate through the channel $\dot{M}$ is constant, and for simplicity we will not quote it here.

It should be noted at this point that, strictly speaking, Navier-Stokes equations and their approximate forms, like (1), cannot accurately describe the flow of a rarefied gas, except in the limit $Kn \to 0$. There are more advanced equations whose validity covers a wider range of the Knudsen number, like Burnett, quasi-gasdynamic equations, and others. However, they are much more complicated, are higher in order, and thus require the additional boundary conditions which are difficult to define. On the other hand the method of the direct simulation Monte Carlo, based on the molecular description, is computationally much expensive. There has been a tendency in the literature for some time to use the Navier-Stokes equations (in spite of their insufficiency) with modified - slip boundary conditions, in order to cover a wide range of Knudsen number, and possibly to cover the entire range, from zero to infinity, in an empirical way. As mentioned in the Introduction, the papers by Beskok and Karniadakis [3], and Djordjevic [5], [6], belong to this category.

One of the boundary conditions for the solution of Equ. (1) is the symmetry boundary condition:

$$y = \frac{h}{2}: \quad \frac{\partial u}{\partial y} = 0. \tag{2}$$

Since the flow in the channel is rarefied, the other condition is the slip boundary condition:

$$y = 0: \quad u = u_0(x). \tag{3}$$

Many efforts have been made in the literature to model the slip velocity $u_0(x)$. By considering the tangential momentum flux near the wall Beskok et al. [2] proposed the following model for an isothermal wall at rest:

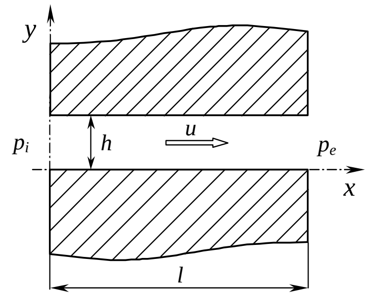

Fig. 1: Flow of the rarefied gas in a micro-channel.

$$u_0 = \frac{2-\sigma}{2} u\Big|_{y=\lambda},$$

where $\lambda(x)$ is the mean free path and $0 < \sigma = \text{const.} < 1$ is the so-called accommodation coefficient. When $u(x,\lambda)$ is expanded into a power series about $y = 0$ we get from above:

$$u_0 = \frac{2-\sigma}{\sigma}\left(\lambda \frac{\partial u}{\partial y}\Big|_{y=0} + \frac{\lambda^2}{2}\frac{\partial^2 u}{\partial y^2}\Big|_{y=0} + \ldots\right) \tag{4}$$

This model gives very good results, which are in agreement with both numerical simulations, and experiments in the slip-flow regime ($10^{-3} < Kn < 0.1$).

As stated in the Introduction, in this paper we wish to extend the validity of the solution of Equ. (1) far above the slip-flow regime. For this purpose we will define a version of Caputo derivative in the following way (cf. [4]):

$${}_yC_\lambda^{(\alpha)}(u) = \int_y^{\lambda(x)} \frac{\partial u}{\partial y}\Big|_{y=\eta} (\eta - y)^{-\alpha(x)} d\eta, \tag{5}$$

with $0 \le y \le \lambda$ and $0 \le \alpha < 1$, , and we will assume the slip velocity (3) as:

$$u_0 = \frac{2-\sigma}{\sigma} h^\alpha {}_0C_\lambda^{(\alpha)}(u). \tag{6}$$

Note that the order of the derivative α is a function of x. Actually we wish to make a direct relation of α with the Knudsen number $Kn = \lambda(x)/h$: $\alpha = \alpha(Kn)$ in such a way that $\alpha(0) = 0$ so that (6) reduces to no-slip boundary condition associated with continuum flow, and that $\alpha \to 1-$ as $Kn \to \infty$ - the situation pertinent to the free molecular flow. Thus, in order to cover the entire range of the Knudsen number variations by the slip condition (6) we adjust the order of the fractional derivative (5) to the local value of the Knudsen number in every cross section of the channel. The coefficient in front of the fractional derivative (6) is added due to dimensional purposes and in order to make our results coincide with the results obtained in [2] in the slip-flow regime. At that our expectations are based upon the known property of fractional derivatives that they reflect a property of a function over a finite interval ($0 \le y \le \lambda(x)$ in this case), contrary to integer order derivatives, applied for modeling the slip velocity in (4), which represent some local properties of a function.

3 RESULTS AND DISCUSION FOR MICRO-CHANNELS

Mathematical problem defined by Equ. (1) and boundary conditions (2) and (6) is well posed and simple. We can straightforwardly obtain the following results, in order as they appear in the solution procedure:

- slip velocity:

$$u_0 = \frac{2-\sigma}{\sigma}\frac{-h^2}{2\mu}\frac{dp}{dx}K \tag{7}$$

- velocity profile:

$$u = \frac{-h^2}{2\mu}\frac{dp}{dx}\left(\frac{y}{h} - \frac{y^2}{h^2} + \frac{2-\sigma}{\sigma}K\right) \tag{8}$$

- volume flow rate:

$$\dot{Q} = 2\int_0^{h/2} u\,dy = \frac{-h^3}{12\mu}\frac{dp}{dx}\left(1 + 6\frac{2-\sigma}{\sigma}K\right) \tag{9}$$

- mass flow rate:

$$\dot{M} = \rho\dot{Q} = \frac{p}{RT}\dot{Q} = \frac{-h^3}{12\mu RT}p\frac{dp}{dx}\left(1 + 6\frac{2-\sigma}{\sigma}K\right) \tag{10}$$

where: K = $Kn^{(1-\alpha)}/(1-\alpha) - 2Kn^{(2-\alpha)}/(2-\alpha)$, R is gas constant, T is gas temperature, supposedly constant, and where the equation of state for an ideal gas in the form: $p = \rho RT$ is used. As well known [7], Knudsen number is inversely proportional to the pressure for an isothermal flow. Thus, $Kn = Ke/P$, where Ke is the reference Knudsen number taken at the exit cross section of the channel, and $P = p/p_e$.

Our next step is to choose $\alpha(Kn)$ so as to achieve the best fit with available experiments and numerical simulations. For $Kn << 1$ we assume that $\alpha(Kn)$ allows the following expansion:

$$\alpha = aKn^2\left(1 + a_1 Kn + O(Kn^2)\right) \tag{11}$$

The corresponding (first order) expansion for K can be readily obtained to be:

$$K = Kn - Kn^2 + aKn^3\left(1 - \ln Kn\right) + O(Kn^4 \ln Kn). \tag{12}$$

As noticed in the Introduction the mass flow rate (10) is constant according to continuity equation. If (12) is inserted into (10) and the resulting differential equation for the pressure is integrated between the inlet cross section ($x = 0$) where

$P = P_i = p_i / p_e$ and the exit cross section ($x = \ell$) where $P = 1$, we get as the first order solution:

$$\frac{\dot{M}}{\dot{M}_0} - 1 = \frac{2-\sigma}{\sigma}\frac{12Ke}{P_i^2 - 1}\left[P_i - 1 - Ke\ln P_i + 2aKe^2\left(1 - \frac{1}{P_i}\right) - aKe^2\left(\ln Ke + \frac{1}{P_i}\ln\frac{P_i}{Ke}\right)\right], \quad (13)$$

where $\dot{M}_0 = h^3 p_e^2 (P_i^2 - 1) / 24\mu RT\ell$ represents the mass flow rate through the channel with neglected rarefaction effects. Thus, the expression (13) is actually a relative increase of the mass flow rate due to the slip of flow on the channel walls. This increase is plotted in Fig. 2 against the overall pressure ratio P_i for two values of Ke, $\sigma = 1$ (relatively rough surface!) and the fitted value for the coefficient $a = 4.6$. While our theory overpredicts the theory presented in [2] only slightly for relatively small value of $Ke = 0.075$, the overprediction for a large value of $Ke = 0.165$ is much more pronounced, and is in a much better agreement with experiments conducted by Arkilic et al. [8].

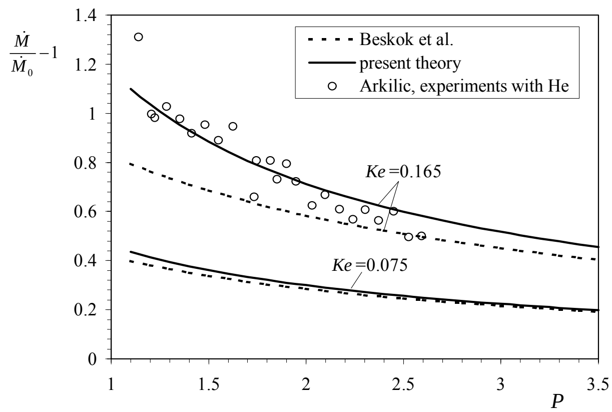

Figure 2. Comparison of the results for the relative increase of the mass flow rate through the channel with the results by Beskok et al. [9], and with experiments.

For $Kn >> 1$ we assume that $\alpha(Kn)$ allows the following asymptotic expansion:

$$1 - \alpha = \frac{b}{aKn}\left(1 + \frac{b_1}{Kn} + O(Kn^{-2})\right). \quad (14)$$

Then the corresponding first order expansion for K reads:

$$K = (\frac{a}{b} - 2)Kn + (1 - 2\frac{b}{a})\ln Kn + O(1). \quad (15)$$

Inserting this expression into (9) we get the volume flow rate through the channel:

$$\dot{Q} = \frac{-h^3}{2\mu}\frac{dp}{dx}\frac{2-\sigma}{\sigma}\left[(\frac{a}{b} - 2)Kn + (1 - 2\frac{b}{a})\ln Kn + O(1)\right]. \quad (16)$$

In Fig.3 we compare this volume flow rate with the results of DSMC calculations for $\sigma = 1$ and the fitted value of $b = 1.08$. The agreement for $Kn > 10$ is excellent. In the same figure we plot our first order solution for $Kn << 1$ ((12) inserted into (9)) and also get an excellent agreement with DSMC calculation. We conclude also that our first order solution (16) offers an excellent approximation for the volume flow rate in the whole interval $0 \le Kn \le 0.2$, while the high order solution given in [2] fails to provide satisfactory results for $Kn > 0.1$.

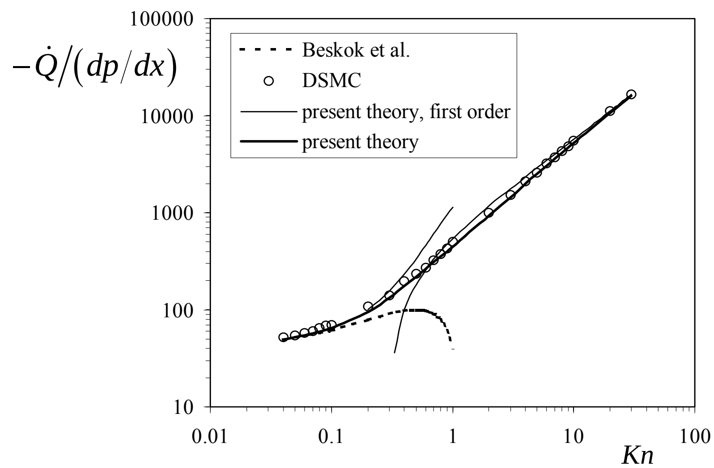

Figure 3. Comparison of the results for the volume flow rate with the results by Beskok et al. [2] and with DSMC simulations, in the entire Knudsen number range.

Encouraged by that we are now able to propose a rational function as an approximation for $\alpha(Kn)$, which allows both expansion (11) and expansion (14). It reads:

$$\alpha = \frac{aKn^2}{1 + bKn + aKn^2} \tag{17}$$

with $a = 4.6$ and $b = 1.08$, and covers the entire range of variations of the Knudsen number. Calculations by using (17) are plotted in Fig.3 and checked against DSMC results. The agreement in the entire range of the Knudsen number is obvious.

4 MICRO-FLOW IN A PIPE

Under the same physical conditions as in the case of channel flow (s. Sec. 2) the governing equation for the pipe flow, with the same notations, reads:

$$\mu \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) = \frac{dp}{dx}, \tag{18}$$

where r is the radial coordinate. The boundary conditions that correspond to (2) and (3) for the channel flow are, respectively:

$$r = 0 : \frac{\partial u}{\partial r} = 0, \quad r = a : u = u_0(x).$$

The solution of (18) for any value of the slip velocity $u_0(x)$ reads:

$$u = u_0(x) - \frac{1}{4\mu}\frac{dp}{dx} y(2a - y), \tag{19}$$

where y=a-r is the distance from the wall. We now model the slip velocity as in the case of channel flow (6):

$$u_0 = \frac{2-\sigma}{\sigma} a^{\alpha} \; {}_0C_{\lambda}^{(\alpha)}(u), \tag{20}$$

where ${}_oC_{\lambda}^{(\alpha)}(u)$ is defined exactly as in (5).

In the case of channel flow the order of the derivative α was a function of x via the local value of the Knudsen number in the channel. However, there is a lack of precise experimental data in the case of micro-pipe flow. As a rule, all characteristic quantities in this case are given in terms of the average value of this number – the value computed at the average pressure in the pipe. This also holds for the data obtained by numerical simulations, and for the results obtained from the linearized Boltzmann equation. That is why we will now assume that α is a function of the average Knudsen number in the pipe, which will be denoted by $\widetilde{Kn}$, and thus is a constant for any particular case of flow.

5 RESULTS AND DISCUSSION FOR MICRO-PIPES

The problem posed by (19) and (20) can be easily solved. At that the following results are straightforwardly obtained for:

- slip velocity:

$$u_0 = -\frac{2-\sigma}{\sigma}\frac{a^2}{2\mu}\frac{dp}{dx}\widetilde{K},$$

- velocity profile:

$$u = -\frac{a^2}{4\mu}\frac{dp}{dx}\left[\frac{y}{a}\left(2 - \frac{y}{a}\right) + 2\frac{2-\sigma}{\sigma}\widetilde{K}\right],$$

- volume flow rate:

$$\dot{Q} = \int_0^a 2r\pi u dr = -\frac{\pi a^4}{8\mu}\frac{dp}{dx}\left(1 + 4\frac{2-\sigma}{\sigma}\widetilde{K}\right),$$

- average velocity:

$$U=\frac{\dot{Q}}{\pi a^2}=-\frac{a^2}{8\mu}\frac{dp}{dx}\left(1+4\frac{2-\sigma}{\sigma}\widetilde{K}\right),$$

- and the mass flow rate approximately evaluated with the average density $\widetilde{\rho}$ in the pipe:

$$\dot{M}\approx\widetilde{\rho}\dot{Q}=\frac{\widetilde{p}}{RT}\dot{Q}=-\frac{\pi a^4}{8\mu RT}\widetilde{p}\frac{dp}{dx}\left(1+4\frac{2-\sigma}{\sigma}\widetilde{K}\right),\qquad(21)$$

where: $\widetilde{K}=\widetilde{K}n^{(1-\alpha)}/(1-\alpha)-\widetilde{K}n^{(2-\alpha)}/(2-\alpha)$, $\widetilde{p}=(p_i+p_e)/2$ is the average pressure in the pipe (p_i- inlet pressure, p_e- exit pressure), and where the equation of state for an ideal gas in the form: $\widetilde{p}=\widetilde{\rho}RT$ is used. As well known [7], the following relation for the average Knudsen number holds:

$$\widetilde{K}n=\frac{\mu}{a\widetilde{p}}\sqrt{\frac{\pi RT}{2}},$$

which means that it is simply inversely proportional to the average pressure for an isothermal flow.

According to the continuity equation the mass flow rate is constant, and we can easily integrate the expression (21) between $x=0$ and $x=l$, and get:

$$\dot{M}=\frac{\pi a^4(p_i-p_e)\widetilde{p}}{8\mu RTl}\left(1+4\frac{2-\sigma}{\sigma}\widetilde{K}\right).$$

We can further write this expression in nondimensional form by employing two well-established formulas for the mass flow rate $\dot{M}_C$ in the continuum flow ($\widetilde{K}n=0$), and $\dot{M}_{FM}$ in the free molecular flow ($\widetilde{K}n\to\infty$):

$$\dot{M}_C=\frac{\pi a^4}{16\mu RTl}(p_i^2-p_e^2),\ \dot{M}_{FM}=\frac{4a^3(p_i-p_e)}{3l}\sqrt{\frac{2\pi}{RT}},\qquad(22)$$

and get:

$$\frac{\dot{M}}{\dot{M}_C}=1+4\frac{2-\sigma}{\sigma}\widetilde{K},\quad\frac{\dot{M}}{\dot{M}_{FM}}=\frac{3\pi}{64\widetilde{K}n}\left(1+4\frac{2-\sigma}{\sigma}\widetilde{K}\right).$$

Our next step is to choose $\alpha(\widetilde{K}n)$ so as to achieve the best fit with available results in the literature. More precisely, we wish to fit our results with the solutions of linearized Boltzmann equation obtained by Loyalka and Hamoodi [9]. For $\widetilde{K}n>>1$ we assume that $\alpha(\widetilde{K}n)$ allows the following asymptotic expansion:

$$\alpha=1-\frac{A}{\widetilde{K}n}+h.o.t.\qquad(23)$$

where A is an arbitrary constant. Then it can be routinely shown that the corresponding expansion for $\widetilde{K}$ is:

$$\widetilde{K} = \frac{1-A}{A}\widetilde{K}n + (1-A)\ln\widetilde{K}n + A + h.o.t.$$

If this is now inserted into the second of Equ. (22) for $\sigma = 1$, and the condition: as $\widetilde{K}n \to \infty, \dot{M} \to \dot{M}_{FM}$ applied, the following value for the constant A is obtained: $A = (3\pi + 16)/3\pi \approx 0.3707.$ A more precise analysis shows that the form of the first two terms in (23) is the only one, which leads to a finite value for the mass flow rate when $\widetilde{K}n \to \infty.$

For $\widetilde{K}n << 1$ we assume the following expansion for $\alpha(\widetilde{K}n)$:

$$\alpha = B\widetilde{K}n^{n} + h.o.t. \tag{24}$$

with $n > 1.$ Then the expansion for $\widetilde{K}$ is:

$$\widetilde{K} = \widetilde{K}n - \frac{1}{2}\widetilde{K}n^{2} + B\widetilde{K}n^{n+1}\left(1 - \ln\widetilde{K}n\right) + h.o.t.$$

When only the first two terms in this expansion are included into the calculations, one may easily verify that the obtained results coincide exactly with the ones obtained in the slip-flow regime by using the boundary condition (4). The sense of introducing the coefficient $(2-\sigma)/\sigma$ in our boundary condition (20) is just the need for the two solutions to coincide in this flow regime. However, while the series (4) truncates at the second term in this case of flow, because the velocity profile is parabolic, we have more terms of higher order in our expansion for $\widetilde{K}$. These terms may serve as a correction when one wishes to extend the validity of the theory to higher values of $\widetilde{K}n$. If this is done by using the first three terms, then the fitting with the results of Loyalka and Hamoodi [9] stated in [7] (s. Fig. 5.11), in the interval $0 \le \widetilde{K}n \le 0.3$ gives the following values for B and n: $B = 1.9, n = 1.8.$

Encouraged by that we are now able to propose the dependence $\alpha(\widetilde{K}n)$, which would cover the entire Knudsen number range:

$$\alpha = \frac{B\widetilde{K}n^{n}}{1 + AB\widetilde{K}n^{n-1} + B\widetilde{K}n^{n}}, \tag{25}$$

with numerical values for the constants A, B and n as above. One may easily verify that (25) allows both expansions (23) and (24). By using this dependence we now plot $\dot{M}/\dot{M}_{FM}$ versus $\widetilde{K}n$ in Fig. 4, and compare our results with the solutions obtained in [9]. The agreement is very good, because the deviations do not exceed 5%. The so-called Knudsen minimum is not pronounced in this case of flow as it is in micro-channel flow case [5], but it is still clearly evidenced, and takes place approximately at $\widetilde{K}n \approx 4.$.

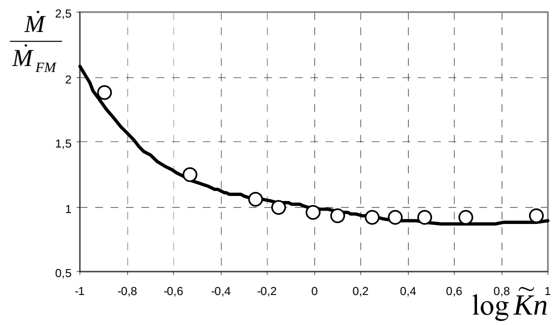

Figure 4. Mass flow rate made nondimensional by its free molecular value versus the average Knudsen number in the pipe, and its comparison with the solution of linearized Boltzmann equation [9] ($A = 0.3707, B = 1.9, n = 1.8)$.

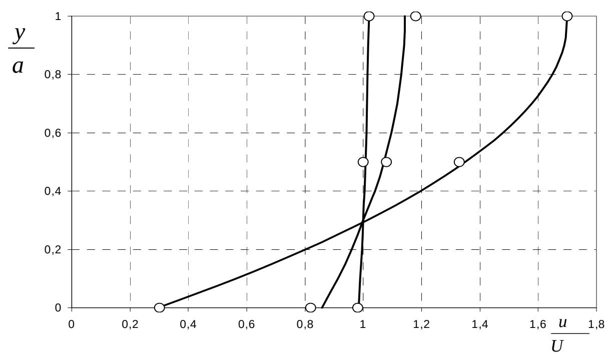

Figure 5. Velocity profiles in the pipe made nondimensional by the average velocity for different values of the average Knudsen number, and their comparison with the solution of linearized Boltzmann equation [9].

Finally, in Fig. 5 we plot velocity profiles in the pipe made nondimensional by means of the average velocity U , for different values of the average Knudsen number.

We note an extensive increase of the slip velocity with the increase of the Knudsen number, and simultaneous decrease of the maximum velocity at the axis, so that approximately for $\widetilde{Kn} > 10$ the profile is almost uniform. The agreement with the results by Loyalka and Hamudi [9] obtained from the linearized Boltzmann equation is very good in this case also.

5 CONCLUSIONS

We have demonstrated in this paper that fractional derivatives can be successfully utilized for modeling the slip velocity in rarefied gas flow in channels and pipes at micro and nano scales. By defining a version of Caputo derivative and by adjusting its order to the local value of the Knudsen number in the channel, or with its average value in the pipe, we are able to cover the entire range of the Knudsen number, from the continuum flow to the free molecular flow, by employing a single, wall slip boundary condition. The procedure carried out in this paper points out to the possibility that fractional derivatives can be in the same manner used for the solution of some other, more complex problems of rarefied gas dynamics. In addition, employment of fractional derivatives conducted in this paper is specific in that fractional derivative is neither used for modeling rheological properties of viscoelastic materials, nor it is used for modification of various differential equations that appear in the mathematical physics. Thus, such employment enriches the list of applications of this noticeable mathematical apparatus in physics

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