Two-dimensional Slip-Velocity Gaseous Flow past a Confined Square in a Microchannel

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Abstract. In the present paper we investigate the drag coefficient of a moving square-shaped particle confined in a two-dimensional microchannel by using both compressible and incompressible slip-velocity models for small Knudsen and small Reynolds numbers approaching in this way the incompressible limit. A convergence to a limit value of the drag coefficient is shown for small velocity of the square particle.

Keywords: incompressible limit, compressible and incompressible slip-velocity model, finite volume method.
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INTRODUCTION

The gaseous flow in a microchannels is one of the simplest basic problems of the young but rapidly growing field of microfluidics. For low Knudsen (Kn) and Mach (Ma) numbers the problem was investigated intensively by many authors within the last decade (see Karnadiakis *et. al.* [1]) by using various mathematical descriptions on the base of continuum or molecular flow models, including DSMC method. It was found out from numerical calculations and experiments [2] that isothermal continuum slip-velocity models could be applied successfully for calculation of gaseous flows through microchannels with constant width for $Kn < 0.1$ and $Ma << 1.0$. Moreover, the obtained flow rates for $Ma \to 0$ show that the compressible viscous model solution converges to the corresponding incompressible limit. If one wants to consider a more complicated problem of a gaseous flow through a microchannel with some internal obstacles or channel-size variations the situation becomes rather unclear and the applicability of any continuum model must be investigated. The aim of this paper is to clarify some computational problems regarded to the right choice of fluid model for numerical study of microflows with a more complex geometry. For example, the analysis of the drag coefficient in incompressible limit $Kn \ll 0.1$, $Ma \to 0$ and Reynolds number $Re < 1.0$ is particularly interesting due to existence of an uncertainty $0/0$ in the limit value. Thus the drag coefficient is very sensitive and might behave in a different way for both compressible and incompressible continuum models when approaching the incompressible limit.

In the present paper we report on numerical results obtained for the two-dimensional slip-velocity gaseous flow past a confined square in a microchannel by using both compressible and incompressible slip-velocity continuum models for a set of the governing parameters $Kn < 1$, $Ma < 1$ and $Re < 1$. The Reynolds number, defined by the relation

$$Re = \frac{16}{5\pi}\sqrt{\frac{\gamma\pi}{2}}\frac{Ma}{Kn} \approx \sqrt{\frac{\gamma\pi}{2}}\frac{Ma}{Kn}, \tag{1}$$

is valid for the compressible viscous model (see [3]) . Its choice is consistent with the corresponding Re determined for the incompressible model. A gas flow past a square-shaped particle moving with constant velocity in a two-dimensional microchannel filled out with a gas is considered. It is shown that for this flow the problem formulation is the same for both compressible and incompressible slip-velocity models. The drag coefficient of the confined particle is investigated numerically in the range of small $Kn < 1$, $Ma < 1$ and $Re < 1$ approaching in this way the incompressible limit values. The results obtained from both models are compared for Knudsen numbers in the range $10^{-3} < Kn < 10^{-1}$.

PROBLEM FORMULATION

We study the movement with constant velocity of a square-shaped particle confined in a long microchannel filled out with hard-sphere monatomic gas. We consider isothermal low speed flow in the whole computational domain. The flow geometry is shown in Fig. 1. The problem is considered in a local Cartesian coordinate system which is moving with the particle. Thus for an observer moving along with the particle the problem is transformed to a consideration of a gas flow past stationary square confined in a microchannel with moving walls. The flow geometry is defined by the channel aspect ratio $A = L/H$ and the blockage ratio $B = H/a$. The square particle is positioned in the middle of the computational domain. The aspect ratio is fixed to $A = 160$ which is well in the range where the influence of the channel length can be neglected. The blockage ratio is fixed to $B = 10$. The computational domain is covered with a non-uniform grid compressed in vicinity of the square with a compression factor equal to 5. For a smooth variation of the step-size in x- and y-directions we use a cubic polynomial. The boundary conditions BC_0 and BC_1 for pressure p, velocity in x- and y-directions u and v at inlet $x = -L/2$ and outlet $x = L/2$ are given as follows:

$$p = p_0, \quad \partial u/\partial x = 0, \quad \partial v/\partial y = 0; \tag{2}$$

The aspect ratio $A = 160$ is large enough to ensure a flat velocity profile at both channel ends. A Maxwell slip-velocity boundary condition BC is imposed at the channel and particle walls

$$u - u_w = F.Kn \left.\frac{\partial u}{\partial \mathrm{n}}\right|_s, \tag{3}$$

where u is velocity of the gas adjacent to the wall, u_w – wall velocity, $F = (2-\sigma)/\sigma$, $\mathbf{n}$ – unity vector normal to the wall surface. The constant σ is the tangential momentum accommodation coefficient (TMAC) which can vary from zero (specular reflection) to one (diffuse reflection). In our consideration σ is fixed $\sigma = 1.0$.

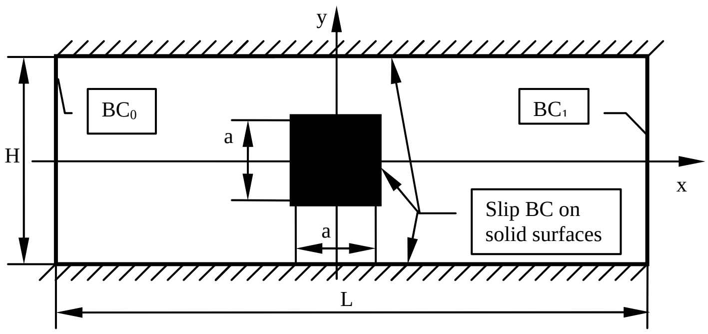


FIGURE 1. Flow geometry: a square-shaped particle with size a is fixed in the middle of a microchannel with length L and height H.

UNIFIED EQUATION SYSTEM

In our considerations of both compressible and incompressible models we have transformed the corresponding system of equation to a unified form in order to be solved numerically by using a unified algorithm of the finite volume method.

Compressible Navier-Stokes-type systems

The dimensionless form of the momentum, continuity equations and equation of state for the compressible viscous model are written as follows:

$$\frac{\partial \bar{u}}{\partial \bar{t}} + \bar{u}\frac{\partial \bar{u}}{\partial \bar{x}} + \bar{v}\frac{\partial \bar{u}}{\partial \bar{y}} = -A_c \frac{\partial \bar{p}}{\partial \bar{x}} + B_c\left(\frac{\partial^2 \bar{u}}{\partial \bar{x}^2} + \frac{\partial^2 \bar{u}}{\partial \bar{y}^2} + \frac{1}{3}\left(\frac{\partial^2 \bar{u}}{\partial \bar{x}^2} + \frac{\partial^2 \bar{v}}{\partial \bar{x}\partial \bar{y}}\right)\right) \tag{4}$$

$$\frac{\partial \bar{v}}{\partial \bar{t}} + \bar{u}\frac{\partial \bar{v}}{\partial \bar{x}} + \bar{v}\frac{\partial \bar{v}}{\partial \bar{y}} = -A_c \frac{\partial \bar{p}}{\partial \bar{y}} + B_c\left(\frac{\partial^2 \bar{v}}{\partial \bar{x}^2} + \frac{\partial^2 \bar{v}}{\partial \bar{y}^2} + \frac{1}{3}\left(\frac{\partial^2 \bar{v}}{\partial \bar{x}^2} + \frac{\partial^2 \bar{u}}{\partial \bar{x}\partial \bar{y}}\right)\right) \tag{5}$$

$$\frac{\partial \bar{\rho}}{\partial \bar{t}} + \frac{\partial(\bar{\rho}\bar{u})}{\partial \bar{x}} + \frac{\partial(\bar{\rho}\bar{v})}{\partial \bar{y}} = 0 \tag{6}$$

$$\bar{p} = \bar{\rho} \tag{7}$$

The dimensionless system of equations (4) – (7) is scaled by the following reference quantities: for velocity - molecular thermal velocity $V_{th} = \sqrt{2RT_0}$, for length - square size a , for time - $t_0 = a/V_{th}$, the reference pressure is given as $p_0 = \rho_0 RT_0$. Thus the non-dimensional variables are given with the formulas:

$t = t_0\bar{t}$, $x = a\bar{x}$, $y = a\bar{y}$, $u = V_{th}\bar{u}$, $v = V_{th}\bar{v}$, $p = p_0\bar{p}$, $\rho = \rho_0\bar{\rho}$, $T = T_0\bar{T} = const = 1$ (isothermal flow).

Two variants of parameter definition for A_c and B_c are possible: the first is based on the classical formulation of a non-dimensional equation system of the isothermal compressible flow by using non-dimensional Reynolds and Mach numbers Re and Ma . In the unified equation system we use the non-dimensional velocity of the square particle $\bar{u}_s = u_s/V_{th}$ instead the Mach number $Ma = u_s/\sqrt{\gamma RT_0}$ in order to be closer to the incompressible model description. In the second definition the transport coefficients (only viscosity in the isothermal case) is defined from the first order approximation of the Chapman-Enskog expansion of the kinetic Boltzmann equation solution.

Thus in the first variant we have two governing parameters Re and $\bar{u}_s$ in the equations. The Reynolds number is based on velocity of square:

$$Re = \frac{u_s.\rho_0.a}{\mu} \tag{8}$$

From the first definition we bring out the following non-dimensional A_{c1} and B_{c1} :

$$A_{c1} = 0.5, \qquad B_{c1} = \frac{\bar{u}_s}{Re} \tag{9}$$

The second variant of parameter definition of A_{c2} and B_{c2} in the dimensionless equations is based on the kinetic theory [4], [5]. Here we use the following expressions for the Knudsen number and viscosity:

$$\mathrm{Kn} = \ell_0 / \mathrm{a}, \quad \mu = \frac{5}{16}\rho_0 \ell_0 V_{th}\sqrt{\pi}\ , \tag{10}$$

where ℓ_0 is mean free path of gas molecules. Finally, the parameters A_{c2} and B_{c2} take the form

$$A_{c2} = 0.5, \qquad B_{c2} = \frac{5\sqrt{\pi}}{16}Kn \quad . \tag{11}$$

The two variants are equivalent if

$$B_{c1} = B_{c2}\,. \tag{12}$$

The relation (12) leads to the following definition of the Reynolds number

$$Re = \frac{u_s \rho_0 a}{\mu} = \frac{16}{5\sqrt{\pi}}\frac{\bar{u}_s}{Kn}\,. \tag{13}$$

Let us consider the boundary conditions. On both ends of the channel the boundary conditions in both variants are equivalent. We need to make equivalent the boundary conditions on the walls of channel and square. This is fulfilled automatically for no-slip boundary conditions. For slip-boundary conditions both variants of problem definition are consistent when we use the relation (13) in the boundary condition (3) i.e.:

$$\bar{u}-\bar{u}_w = F.\frac{16}{5\sqrt{\pi}}\frac{\bar{u}_s}{\mathrm{Re}}\frac{\partial \bar{u}}{\partial \mathrm{n}}\bigg|_s \,. \tag{14}$$

Incompressible Navier-Stokes-type system

To obtain the non-dimensional form of the equations of the incompressible fluid model we apply the same approach as this is done for the compressible model.

In result the unified dimensionless form of the incompressible equation system is given in the form:

$$\frac{\partial \bar{u}}{\partial \bar{t}}+\bar{u}\frac{\partial \bar{u}}{\partial \bar{x}}+\bar{v}\frac{\partial \bar{u}}{\partial \bar{y}} = -A_i\frac{\partial \bar{p}}{\partial \bar{x}}+B_i\left(\frac{\partial^2 \bar{u}}{\partial \bar{x}^2}+\frac{\partial^2 \bar{u}}{\partial \bar{y}^2}\right) \tag{15}$$

$$\frac{\partial \bar{v}}{\partial \bar{t}}+\bar{u}\frac{\partial \bar{v}}{\partial \bar{x}}+\bar{v}\frac{\partial \bar{v}}{\partial \bar{y}} = -A_i\frac{\partial \bar{p}}{\partial \bar{y}}+B_i\left(\frac{\partial^2 \bar{v}}{\partial \bar{x}^2}+\frac{\partial^2 \bar{v}}{\partial \bar{y}^2}\right) \tag{16}$$

$$\frac{\partial \bar{u}}{\partial \bar{x}}+\frac{\partial \bar{v}}{\partial \bar{y}} = 0 \tag{17}$$

To be consistent with the compressible model definitions in both variants we must impose the following relations between parameters:

$$A_{i1}=A_{i2}=A_{c1}=A_{c2}=0.5, \quad B_{i1}=B_{c1}, \quad B_{i2}=B_{c2} \quad . \tag{18}$$

In the case $B_{i2}=B_{c2}$ the Knudsen number Kn enters in the equations of the incompressible model through viscosity definition (10) in a similar way as shown in [5].

RESULTS AND DISCUSSION

We use the finite volume method [6], [7] to solve numerically the unified systems of equations of both incompressible and compressible models. We are interested in the established flow which is obtained after passing the transition period. The flow is investigated for the two variants of the parameter definition considered in the previous section. The compressible flow streamlines past the square are shown in Fig. 2. as an typical illustration of the established flow for $Re=0.5$, $\bar{u}_s=0.25$ and $Kn=0.01$ in a part of the computational domain near to the square. As one can see the flow is fully laminar with almost flat velocity profile at the both ends of the shown area.

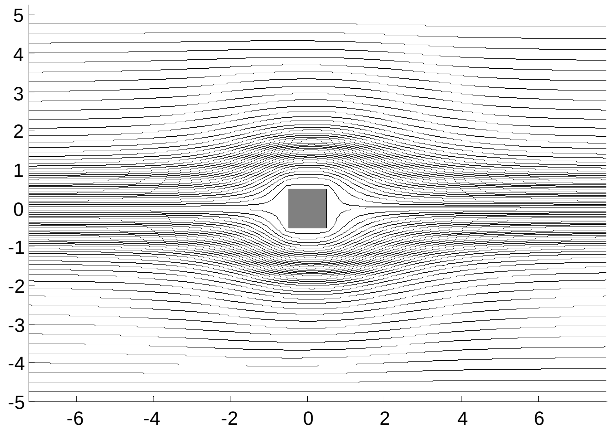


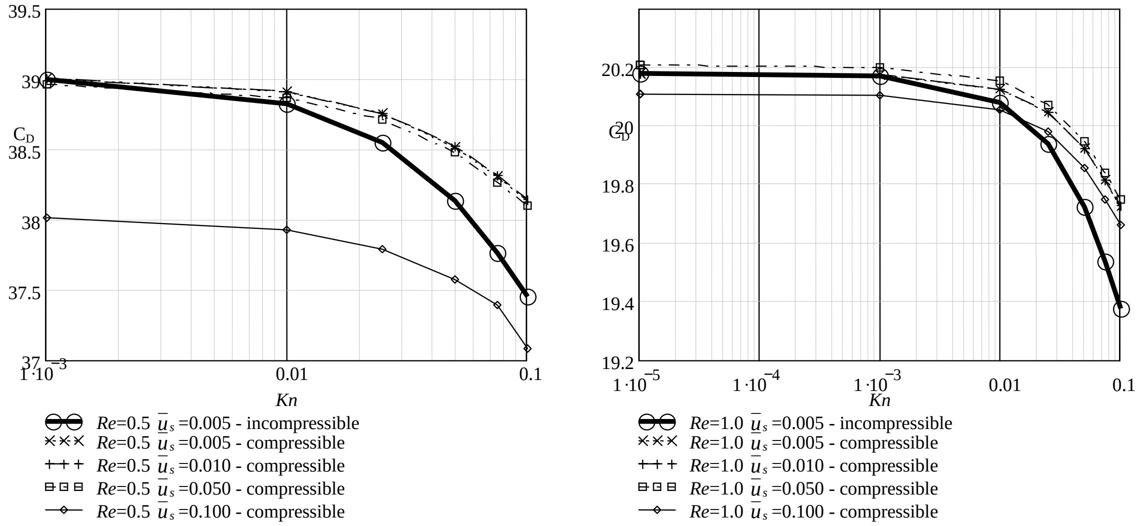
FIGURE 2. Streamlines for compressible flow at $Re=0.5$, $\bar{u}_s=0.25$ and $Kn=0.01$.

Now we are ready to proceed to the results obtained for the drag coefficient of the square-shaped particle. The particle drag coefficient C_D is written as follows

$$C_D = \frac{F_x}{0.5\rho_0 \overline{u}_s^2 S}, \tag{19}$$

where F_x is the total force exerted by the particle in x-direction. In our consideration $S = a$.

We first present the variation of the drag coefficient for the case $A_{i1} = A_{c1} = 0.5,\quad B_{i1} = B_{c1}$ and for Knudsen numbers in the range $10^{-3} < Kn < 10^{-1}$; The Reynolds number is small $Re = 0.5, 1.0.$ In this case for both compressible and incompressible models the Knudsen number enters only in boundary conditions BC (3) imposed on the channel and square walls. We vary Kn independently on Re and $\overline{u}_s$. The results for the drag coefficient C_D versus Knudsen number Kn are shown in Fig. 3 a) and b) for $Re = 0.5$ and $Re = 1.0$, respectively, and different velocities of the particle $\overline{u}_s = 0.005, 0.01, 0.05, 0.1$.



a) b)

FIGURE 3. Drag coefficient versus Knudsen number for a) Re=0.5, b) Re=1.0.

The results of the incompressible model do not depend on the velocity variation. Approaching the incompressible limit the drag coefficient calculated from the compressible slip-model converges to the incompressible result for small particle velocity $\overline{u}_s < 0.05$ and diverges for $\overline{u}_s = 0.1$. For small particle velocities the drag coefficient calculated from the compressible model overpredicts the incompressible result in the whole Knudsen number range. An interesting result is that for larger particle velocities the drag coefficient computed from the compressible model underpredicts the corresponding incompressible value.

The drag coefficient variation in the second case of parameter definition $A_{i2} = A_{c2} = 0.5,\ B_{i2} = B_{c2}$ is illustrated in Fig. 4. In this case we use the boundary condition (14) . The dependence of the drag coefficient on the non-dimensional particle velocity is presented in Fig. 4 for Reynolds numbers a) $Re = 0.5$ and b) $Re = 1.0$. As one can see the drag coefficient calculated from both compressible and incompressible models converges to a limit value with the decrease of the particle velocity. For larger particle velocity the drag coefficient value decreases for both models but in a different way. The drag coefficient functional dependence on the governing parameters in the second case is more complicated and needs a more detailed investigation. Such an study is in progress and will be presented in a separate paper.

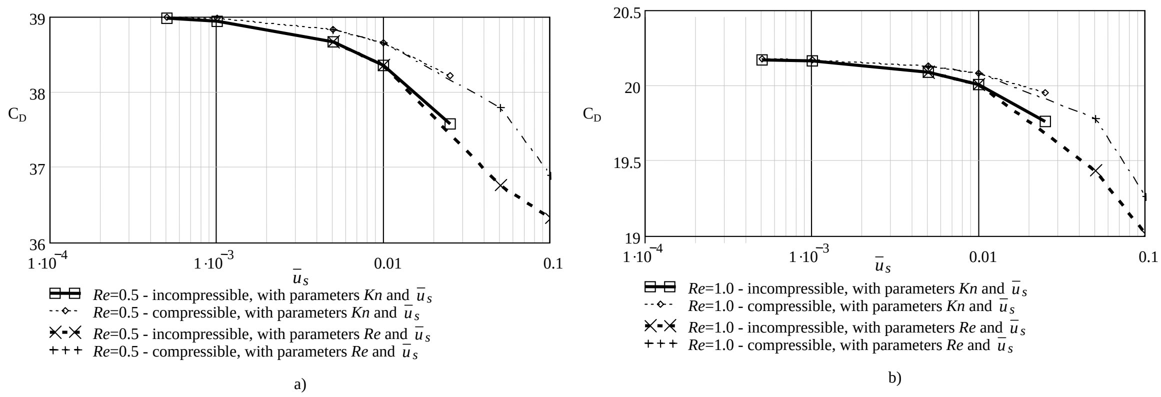


FIGURE 4. Drag coefficients in function of $\overline{u}_{sq}$ for a) Re=0.5, b) Re=1.0.

CONCLUSIONS

In the present paper we investigate the drag coefficient of a confined square-shaped particle by using both compressible and incompressible slip-velocity models. The governing parameters vary in ranges that ensure the approach to the incompressible limit. A unified equation system is used that allows both models to be investigated numerically by using a unified algorithm of the finite volume method. Two variants of the parameter definition are considered. In both cases a convergence to a limit value of the drag coefficient is shown for small velocity of the square particle. In a future investigation on the same subject we will present a comparison of the drag coefficient computed from continuum slip-velocity model with the result obtained from hard sphere particle model simulated using the DSMC method.

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