FINITE VOLUME CALCULATIONS OF GASEOUS SLIP FLOW PAST A CONFINED SQUARE IN A TWO-DIMENSIONAL MICROCHANNEL

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ABSTRACT
In this paper we study the movement with constant velocity of a square-shaped particle confined in a microchannel filled with hard-sphere monoatomic gas. The problem is solved using two completely different methods: direct simulation Monte Carlo (DSMC) (molecular approach) and finite volume method (FVM) (continuum approach). Continuum model is described on the basis of the Navier–Stokes equations for a compressible viscous gas with diffusion coefficients determined by the first approximation of the Chapman–Enskog theory for low Knudsen numbers. First order velocity-slip and temperature-jump boundary conditions are used. All presented results are calculated at Knudsen number $\text{Kn} = 0.0498$. The blockage ratio is equal to $B = H_{ch}/a = 10$, where $H_{ch}$ is the channel height, $a$ is the square particle size. 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 gas flow past stationary square confined in a microchannel with moving walls. The calculations are made for subsonic ($M = 0.1$) and supersonic ($M = 2.43$) speeds, leading to different regimes of the gas microflow. The results obtained from DSMC and FVM calculations for the considered speeds at $\text{Kn} = 0.0498$ are in a very good agreement.

1. INTRODUCTION

All devices with character dimensions between 1 $\mu$m and 1 mm are called micro-devices. Micro mechanical devices are rapidly emerging technologies, where new potential applications are continuously being developed. Microchannel fluid flow is currently modeled using either the continuum approach or the non-continuum approach most commonly called molecular approach. The Knudsen number ($\text{Kn}$), a nondimensional parameter, determines the degree of appropriateness of the continuum model. It is defined as the ratio of the mean free path $l_0$ to the macroscopic length scale of a physical system $L$.

$$\text{Kn} = l_0 / L,$$  (1)

The traditional requirement for Navier-Stokes type equations to be valid is that the Knudsen number should be less than 0.1. This can be misleading if $L$ is chosen to be some overall dimension of the flow [1]. Here $L$ is chosen to be equal to the particle size $a$.

In this paper we present numerical results for a gas flow past a confined square in a microchannel at subsonic ($M = 0.1$) and supersonic ($M = 2.43$) speeds for $\text{Kn} = 0.0498$. The problem is solved using two completely different methods: the direct simulation Monte Carlo (DSMC) [1] (molecular approach) and the finite volume method (FVM) [2], [3] (continuum approach). Fluid flow past an object with non-aerodynamic cross-section is often encountered in engineering applications. The problem is investigated

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under conventional flow conditions by many authors, experimentally in [4], [5] and numerically in [6], [7], [8]. Here the Finite Volume Method results are calculated by using first order velocity slip and temperature jump boundary conditions at the solid walls.

2. PROBLEM FORMULATION AND METHODS OF SOLUTION

2.1 Continuum model equations

A two dimensional system of equations describing the unsteady flow of viscous, compressible, heat conductive fluid can be expressed in a general form as follows:

\[
\rho \frac{Du}{Dt} = -A \frac{\partial p}{\partial x} + B \left[ \frac{\partial}{\partial x} \left( \Gamma_1 \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( \Gamma_1 \frac{\partial u}{\partial y} \right) \right] + B \left[ \frac{\partial}{\partial x} \left( \Gamma_2 \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial y} \left( \Gamma_2 \frac{\partial v}{\partial y} \right) - 2 \frac{\partial}{\partial y} \left[ \Gamma_1 \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) \right] \right],
\]

\[
\rho \frac{Dv}{Dt} = -A \frac{\partial p}{\partial y} + B \left[ \frac{\partial}{\partial x} \left( \Gamma_1 \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( \Gamma_1 \frac{\partial u}{\partial y} \right) \right] + B \left[ \frac{\partial}{\partial x} \left( \Gamma_2 \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial y} \left( \Gamma_2 \frac{\partial v}{\partial y} \right) - 2 \frac{\partial}{\partial x} \left[ \Gamma_1 \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) \right] \right],
\]

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho v)}{\partial y} = 0,
\]

\[
p = \rho T,
\]

\[
\rho \frac{DT}{Dt} = C^{T1} \left[ \frac{\partial}{\partial x} \left( \Gamma_1 \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( \Gamma_1 \frac{\partial T}{\partial y} \right) \right] + C^{T2} \Gamma \Phi + C^{T3} \frac{Dp}{Dt},
\]

where:

\[
\Phi = 2 \left[ \left( \frac{\partial u}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial y} \right)^2 \right] + \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right)^2 - 2 \frac{\partial}{\partial y} \left[ \Gamma_1 \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) \right]^2.
\]

\(u\) and \(v\) are horizontal and vertical components of velocities, respectively, \(\rho\) is density, \(p\) is pressure, \(T\) is temperature of the gas, \(t\) is time, \(x\) and \(y\) are coordinates on \(OX\) and \(OY\) axis, respectively. Parameters \(A\), \(B\), \(C^{T1}\), \(C^{T2}\), \(C^{T3}\) and diffusion coefficients \(\Gamma\) and \(\Gamma^d\) depend of the nondimensionalisation of the system of equations. The system of equations (2) - (6) is solved by using FVM. A first order upwind scheme is used for the approximation of the convective terms, and a second order central difference scheme is employed for the approximation of the diffusion terms. The specific details of the computational method will be presented in a separate paper, which is in process of preparation.

The time evolution of the continuum model is described on the basis of the Navier-Stokes equations for compressible, viscous gas with diffusion coefficients determined by the first approximation of the Chapman-Enskog theory for low Knudsen numbers. For a hard-sphere gas, the viscosity coefficient \(\mu\) and the heat conduction coefficient \(\lambda\) (first approximations are sufficient for our considerations) are given in the following form:

\[
\mu = \mu_h \sqrt{T}, \mu_h = (5/16) \rho_0 V_{th} \sqrt{\pi},
\]

\[
\lambda = \lambda_h \sqrt{T}, \lambda_h = (15/32) c_s \rho_0 V_{th} \sqrt{\pi}.
\]

The Prandtl number is given by \(Pr = 2/3\), \(\gamma = c_p / c_v = 5/3\). The dimensionless system of equations (2) - (6) is scaled by the following reference quantities (see Ref. [9]): for velocity - molecular thermal velocity \(V_0 = V_{th} = \sqrt{2RT_0}\), for length - square size \(a\) (Figure 2), for time - \(t_0 = L/V_0\), reference temperature \((T_0)\) and pressure \((p_0)\) are temperature and pressure in the inflow of the channel, respectively.
reference density \( \rho_0 \) is calculated using equation of state (5). Using (8) and (9) one can obtain the explicit expressions of the parameters and diffusion coefficients used in the equation system (2) – (6):

\[
A = 0.5, \quad B = \frac{5\sqrt{\pi}}{16} Kn, \quad \Gamma = \Gamma^0 = \sqrt{T_\infty}, \quad C^{T_1} = Kn \sqrt{\frac{\pi}{1024}} 225, \quad C^{T_2} = \frac{\sqrt{\pi}}{4} Kn, \quad C^{T_3} = \frac{2}{5}
\] (10)

2.2 First order velocity-slip and temperature jump boundary conditions

Velocity slip condition is given by:

\[
v_s - v_w = \zeta \frac{\partial v}{\partial n}, \quad (11)
\]

where \( v_s \) is gas velocity at the wall surface, \( v_w \) wall velocity, \( \zeta = 1.1466.Kn_{local} = 1.1466.Kn / \rho, \quad Kn_{local} \)

is local Knudsen number, \( \frac{\partial v}{\partial n} \) is velocity derivative for the gas at the wall in normal direction. Equation (11) is approximated with a first order accuracy deference formula. Applied to the vertical wall (Figure 1), velocity \( v_s \) is defined at a boundary point with coordinates \( (x_{i+1,j}, y_{i,j}) \).

![Figure 1: Cell volume of \( v \) and \( T \) to the wall](image)

The numerical implementation of the velocity-slip boundary condition is arranged according to the finite volume method:

\[
v_s = \left( a_{BC}^v.v_{i,j} + v_w \right) / \left( a_{BC}^v + 1 \right), \quad (12)
\]

where \( a_{BC}^v = \zeta / (0.5.\Delta x_i) = 1.1466.Kn / (\rho^v .0.5.\Delta x_i) \), \( \rho^v_{i,j} \) is density at the middle node \( (x^v_{i,j}, y^v_{i,j}) \) and it is calculated using an upwind scheme [10], [11]:

\[
\rho^v_{i,j} = \begin{cases} 
0.5(\rho_{i,j-1} + \rho_{i,j}) & \text{if } v_{i,j} = 0, \\
\rho_{i,j-1} & \text{if } v_{i,j} > 0, \\
\rho_{i,j} & \text{if } v_{i,j} < 0.
\end{cases} \quad (13)
\]

Analogously, the temperature jump boundary condition is given in the form:

\[
T_s - T_w = \tau \frac{\partial T}{\partial n}, \quad (14)
\]

where \( T_s \) is gas temperature at the wall surface, \( T_w \) is wall temperature, \( \tau = 2.1904.Kn_{local} = 2.1904.Kn / \rho, \quad \frac{\partial T}{\partial n} \)

is temperature derivative in the normal direction. Applied to the vertical wall (Figure 1) with temperature \( T_s \) at coordinates \( (x^v_{i+1,j}, y^v_{i,j}) \) it gives:
$$T_s = \left( a_{BC}^T T_{i,j} + T_w \right) / \left( a_{BC}^T + 1 \right),$$  

where $a_{BC}^T = \tau / (0.5.\Delta x) = 2.1904.Kn / (\rho_i.0.5.\Delta x)$.

The presentation of the velocity-slip and temperature-jump slip boundary conditions in forms (12) and (15) is important. In this way the numerical algorithm satisfies the sufficient condition for convergence of the iterative scheme applied at each time step.

The problem is considered in a local Cartesian coordinate system, which is moving with the particle (Figure 2). Thus, for an observer moving along with the particle, the problem is transformed to consideration of a gas flow past a stationary square confined in a microchannel with moving walls. Flow geometry is defined by channel length $L_{ch}$, the length between channel inflow and square is $L_a$ and the blockage ratio is $B = H_{ch} / a = 10$. A long enough microchannel is chosen so that the influence of channel inflow and outflow boundaries can be neglected. To make sure that this influence can be neglected a number of test calculations have been run for different channel lengths and for both subsonic and supersonic regimes of gas flow. Corresponding boundary conditions (BC) at channel inlet (BC$_{in}$) and outlet (BC$_{out}$) are defined in each of cases. Velocity-slip (11) and temperature-jump (14) boundary conditions are applied at the square and channel walls. The channel and square have a constant wall temperature equal to 1.0. Both subsonic and supersonic cases are calculated at Knudsen number $Kn=0.0498$.

![Figure 2](image.png)

*Figure 2*: Flow geometry: a square-shaped particle with size $a$ is fixed in the middle of a microchannel with length $L_{ch}$ and height $H_{ch}$.

The DSMC algorithm follows the basic steps of the “No Time Counter” scheme proposed by Bird [1] and it is described in detail in [12]. It uses a hard sphere model of a monoatomic gas. A boundary condition of diffusive reflection is used at the microchannel and square walls.

3. COMPUTATIONAL RESULTS

3.1 Subsonic flow

The subsonic fluid flow past a square cylinder in a microchannel is calculated at $M=0.1$. Geometry is defined by: $L_{ch}=40$, $L_a=15.5$. We use a two-dimensional uniform mesh with steps $\Delta x = \Delta y = \Delta = 0.025$ (mesh 1600x400, in OX and OY directions, respectively). In the considered coordinate system attached to the moving particle the relative velocity of the channel walls is $u = 0.09129$ (according to $M = 0.1$). The inlet boundary conditions at $x=0$ are:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho v)}{\partial y} = 0, \frac{\partial v}{\partial x} = 0, p = p_{in}, T = T_{in},$$  

The outlet boundary conditions at $x=L_{ch}$ are:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho v)}{\partial y} = 0, \frac{\partial v}{\partial x} = 0, \frac{\partial p}{\partial x} = 0, \frac{\partial T}{\partial x} = 0.$$  

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Horizontal velocity \( u \) at the channel inlet and outlet is found by integrating the continuity equation over the first and last control volumes, respectively. The difference between fluxes at inlet and outlet is found to be \( \left| \left( F_{\text{out}} - F_{\text{in}} \right) / F_{\text{in}} \right| \approx 8.5 \times 10^{-10} \). The drag coefficient calculated by using the FVM method is equal to \( C_{D}^{FVM} = 7.493 \), and it is in an excellent agreement with the drag coefficient \( C_{D}^{DSMC} = 7.488 \) calculated by using the DSMC method. DSMC calculations are performed by using a computational grid with 1600x400 cells and a total number of \( 16.6 \times 10^6 \) particles. The drag coefficient is defined as \( C_{D} = D / (0.5 \rho u^2 S) \), where \( D \) is drag force, \( U \) is square velocity and \( S \) is the projected area.

\[ F_{\text{in}} = \int_{V_{1}} \rho u \, dV, \quad F_{\text{out}} = \int_{V_{2}} \rho u \, dV \]

\[ C_{D}^{FVM} = \frac{\left| F_{\text{in}} - F_{\text{out}} \right|}{F_{\text{in}}} \]

\[ C_{D}^{DSMC} = \frac{D}{0.5 \rho U^2 S} \]

**Figure 3:** Comparison of FVM (solid line) and DSMC (circles) data for: (a) horizontal velocity along the channel at \( H_{ch}/2 \) and (b) vertical velocity along the channel at \( H_{ch}/4 \)

**Figure 4:** Comparison of FVM (solid line) and DSMC (circles) in sections normal to the channel axis in front of the square (\( x = 14.025 \)), in the middle (\( x = 15.5 \)) and past the square (\( x = 18.775 \)) for: (a) the horizontal component of velocity and (b) the vertical component of velocity

As seen in figures 3 and 4, the agreement between continuum and molecular approaches for the subsonic flow regime is very good. The comparison of the results for pressure and temperature (not given here) exhibits a larger dispersion of the DSMC data.

### 3.2 Supersonic flow

The supersonic gas flow past a square in a microchannel is calculated at \( M = 2.43 \). Geometry is defined by: \( L_{ch} = 50 \), \( L_{a} = 5.5 \). The spatial steps along both axes are equal to \( \Delta x = \Delta y = \Delta = 0.00625 \) (mesh 8000x1600, in OX and OY directions, respectively). The channel wall velocity is equal to \( u = 2.215 \) (according to \( M = 2.43 \)). The inlet boundary conditions at \( x=0 \) are:

\[ u = 2.215, \quad v = 0, \quad p = p_w, \quad T = T_w, \]

The outlet boundary conditions at \( x=L_{ch} \) are:

\[ \frac{\partial u}{\partial x} = 0, \quad \frac{\partial v}{\partial x} = 0, \quad \frac{\partial p}{\partial x} = 0, \quad \frac{\partial T}{\partial x} = 0 \]
The computed difference between inlet and outlet fluxes is \( \left| \frac{F_{\text{out}} - F_{\text{in}}}{F_{\text{in}}} \right| \approx 1.1 \times 10^{-8} \). Drag coefficients are found to be \( C_D^{\text{FVM}} = 1.8480 \) calculated by using FVM method and \( C_D^{\text{DSMC}} = 1.8597 \) calculated by using the DSMC. The DSMC calculations are performed over a grid with 4000x800 cells and for a total particle number 96.1 \times 10^6.

In the following figures we present comparison of FVM and DSMC data along the channel for \( u \) at \( y = H_{ch}/2 \) (Figure 5), \( v \) at \( y = H_{ch}/4 \) (Figure 6), pressure at \( y = H_{ch}/2 \) (Figure 7) and temperature at \( y = H_{ch}/2 \) (Figure 8). Profiles of \( u, v, \) pressure and temperature in front of, in the middle of and behind the square, being normal to the channel axis, are shown in Figure 9. The comparison shows differences between DSMC and FVM data in the shock wave areas, where gradients are significant. Comparing pressure and temperature, one can see the shock wave displacement in front of the square. The difference between the molecular and continuum approach are pointed out in the works of other authors (for example, see [1]). The difference between the results of both approaches is more tangible after the shock wave reflection from the channel walls. This is seen within the areas of shock interefation past the square.

Figures from 10 to 13 present the corresponding macroscopic fields calculated by using the FVM and DSMC methods.

![Figure 5](image1.png): Horizontal velocity profiles calculated by using FVM (solid line) and DSMC (circles) in the midplane along the microchannel in front of (a) and behind (b) the square

![Figure 6](image2.png): Vertical velocity profiles calculated by using FVM (solid line) and DSMC (circles) at \( y = H_{ch}/4 \)
Figure 7: Pressure profiles calculated by using FVM (solid line) and DSMC (circles) in the midplane along the microchannel in front of (a) and behind (b) the square.

Figure 8: Temperature profiles calculated by using FVM (solid line) and DSMC (circles) in the midplane along the microchannel in front of (a) and behind (b) the square.
Figure 9: Comparison of FVM (solid line) and DSMC (circles) data in sections normal to the channel axis in front the square ($x=4.5$), in the middle of the square ($x=5.5$) and behind the square ($x=19.375$) for: (a) horizontal component of velocity, (b) vertical component of velocity, (c) pressure and (d) temperature.

Figure 10: Horizontal velocity field calculated by FVM (upper part) and DSMC (lower part).
4. CONCLUSIONS

The problem of a square-shaped particle moving with constant velocity in a microchannel is calculated by using two completely different approaches: molecular approach (DSMC) and continuum approach (FVM). The problem is solved for subsonic ($M=0.1$) and supersonic ($M=2.43$) speeds at $Kn=0.0498$. The comparison of the drag coefficients of square, velocity, pressure and temperature fields shows a very good agreement between both solutions for subsonic speed. For supersonic speed, both solutions are very close to each other except for the area of the shock waves where more tangible differences are exhibited. The analysis of the results found for $Kn=0.0498$ shows that the use of both approaches - molecular (DSMC) and
continuum (FVM) ones, is justified for a large range of subsonic and supersonic speeds at small Knudsen number, $Kn<0.1$.

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REFERENCES AND CITATIONS


