

FLOW AND HEAT TRANSFER RESEARCH IN MICRO- AND NANO- CHANNELS.

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Keywords: flow in micro/ nano-channels, direct simulation method, Molecular Dynamics, heat transfer, cooling systems.

Abstract. In this work the gas flow in micro/nano-channels was investigated. We used the direct simulation method based on the approaches of Molecular Dynamics. The distributions of density, velocity and temperature in the channel were obtained and analyzed with different Knudsen numbers. With an increase Knudsen number velocity distribution differs significantly from the classical Navier-Stokes parabolic profile. Therefore for studying flows in micro- and nano- channels it is necessary to use microscopic approach of the molecular dynamics.

1. The quantity of energy scattered by the cooling systems of electronic components steadily increases¹. Microelectronic components are decreasing in dimension and devices power consumption is increasing, therefore question about their cooling becomes very important.

It is assumed that the cooling systems will consist of the micro- or nano- channels applied on (or penetrate) electronic component. Prototypes of such devices have already appeared in the research institutes of the USA.

In the majority of cases gas and fluid flow is investigated on the basis of macroscopic approach^{2,3}. This description is correct when volume contains sufficient number of molecules and gas can be considered as continuous. However, in such cases as flow in the micro- or nano- channels, the simulation of physical chemistry processes in gas and on surface it is necessary to use the microscopic approach based on the molecular dynamics⁴⁻⁸. In this approach the corpuscular structure of gas is considered. Positions and velocities of molecules at each moment of time are determined. Macroscopic values are computed through the distributions of the corresponding molecular values.

2. Flow in the micro- and nano- channels was investigated in this work. We used the direct simulation method based on the approaches of molecular dynamics: real flow simulation by large quantity of simulating particles⁵. The coordinates, velocities and properties of the molecules are stored in the memory. Their changing is caused by

intermolecular interaction and interaction with the boundaries of physical space. Channel was represented as two plates located at a distance L_y . Gas at the channel inlet had a temperature $T_g = 0.9T_0$, plates had a temperature $T_w = T_0$.

Motion equations were

$$\frac{d\vec{v}_i}{dt} = F_i(\vec{x}_j, \vec{v}_j, t),$$

where \vec{x}_i , $\vec{v}_i = \frac{d\vec{x}_i}{dt}$ - coordinates and velocity of the molecule number i , F is

determined by the selected model of molecular interaction.

Physical space was divided into the cells – small volumes $V_0 = (L_0)^3$ with fixed boundaries. There L_0 is linear cell dimension. Time changing was discrete with step Δt_s .

Molecular motion calculation, checking conditions on boundaries of physical space and redistribution of molecules into new cells was realizing every step.

Molecules were represented as hard elastic spheres (hard sphere model) with diameter $d = 3.78 \cdot 10^{-10}$ m. Velocity of molecules after collision was calculating using energy and impulse conservation law. Initially the particles were distributed evenly in the physical space, their velocities were distributed according with the equilibrium Maxwellian distribution function.

To reduce the computational burden we used probabilistic approach⁵. The simulation of collisions was separately in each cell. The number of collisions N in the unit of volume and time is

$$N = \frac{1}{2}nv = \frac{1}{2}n^2\sigma\overline{c_r},$$

where $\overline{c_r}$ - average relative velocity of two particles, $\sigma = \pi d^2$, d – diameter of molecule, n - concentration, $v = n\sigma\overline{c_r}$ - collision rate of test particle.

Let's note that in this approach disturbances can move with speed $\tilde{a} \cong \frac{L_0}{\Delta t_s}$. Therefore

to prevent this negative effect we provided condition $\tilde{a} \leq a$, where a - sonic speed in current region.

For describing gas-surface interaction diffuse model was used: velocities of molecules after reflection are distributed according to the equilibrium Maxwellian distribution function corresponded with temperature of surface.

3. The plan of simulation region is demonstrated at Figure 1. Flow was supposed symmetrical, therefore we simulated one half of the channel. At the plane of symmetry we used the condition of mirror reflection.

The flow was organized in the region A: gas was cooled to the temperature $T_g = 0.9T_0$ and accelerated to the initial velocity v_0 . The plate had the temperature $T_w = T_g = 0.9T_0$ in this region. The region B was studied: plate had the temperature $T_w = T_0$ here. The endless flow was simulated. After region B the gas came region A and was cooled and accelerated to initial velocity.

Flow was considered as stationary, results were averaged on time to avoid fluctuations.

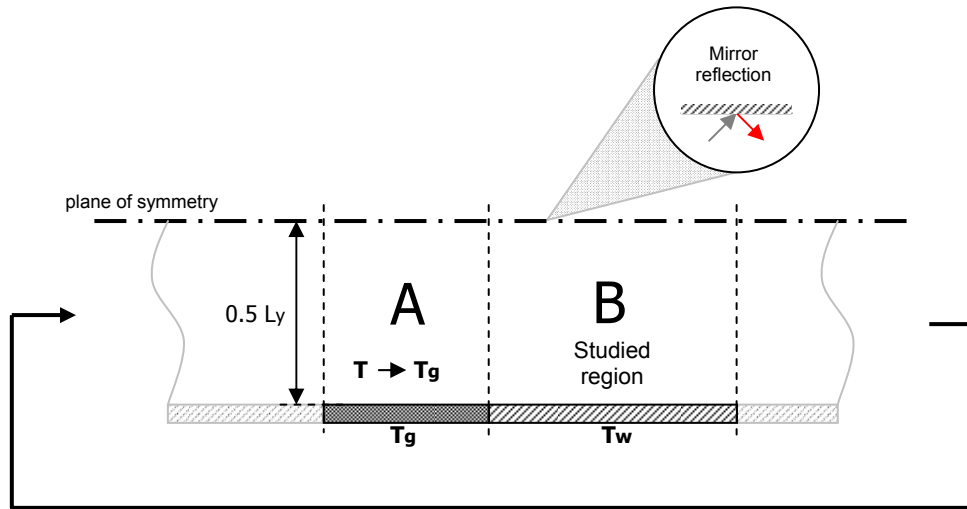


Figure 1. The plan of simulation region

We investigated the nitrogen flow ($m = 28 \text{ g} \cdot \text{mol}^{-1}$). The free path length λ and the molecular diameter d had the same order of magnitude. The stagnation temperature $T_0 = 77 \text{ K}$.

The dimensionless velocity $\frac{v}{v_a}$ distribution is presented at the Figure 2 (v_a - section average velocity). Different lines correspond with different Knudsen numbers $Kn = \lambda/L_y$. With small Knudsen numbers the parabolic velocity profile is obtained and calculations coincided with the solution of Navier-Stokes equations. With an increase Kn the velocity profile is equalized practically.

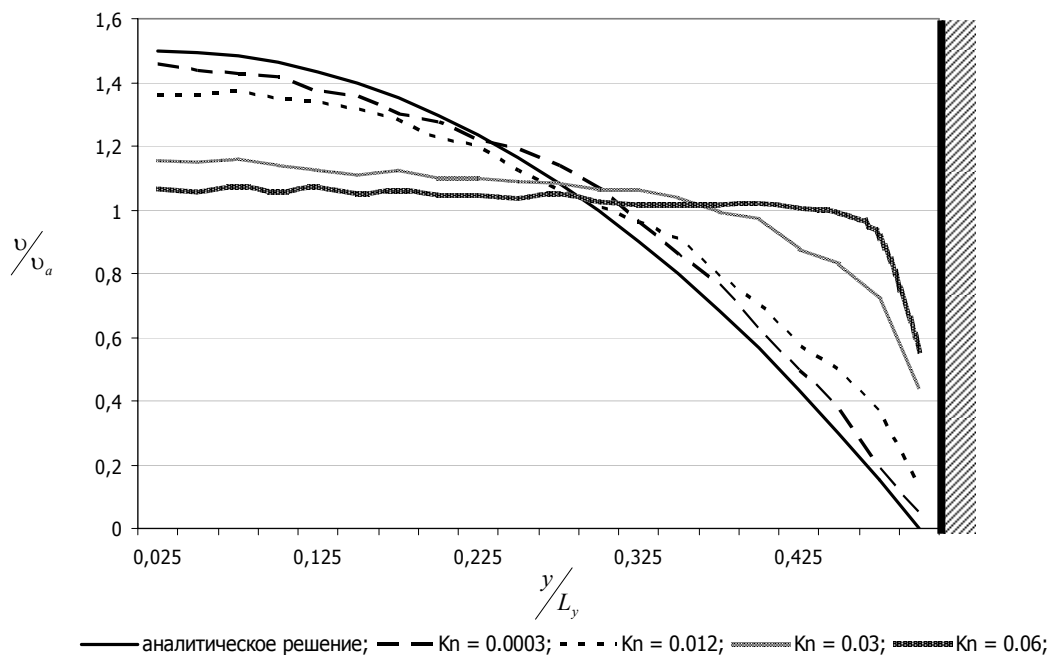


Figure 2. The dimensionless velocity distribution

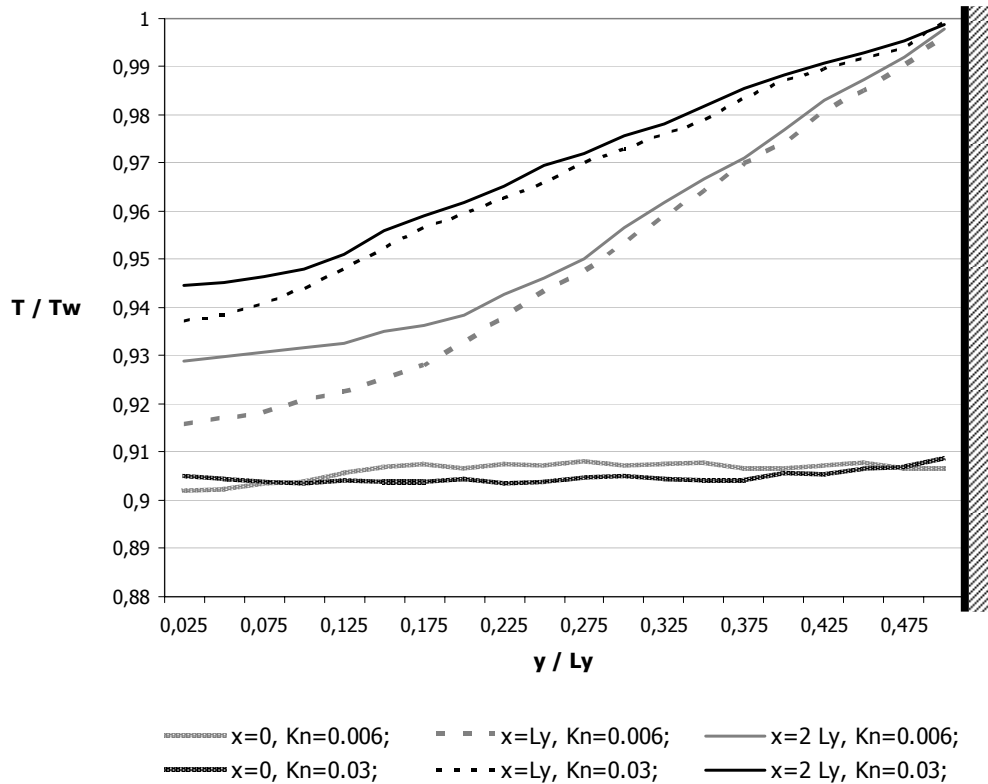


Figure 3. The dimensionless temperature distribution

The dimensionless temperature $\frac{T}{T_w}$ distribution in several sectors is presented at the Figure 3. This distribution was obtained with $T_w = T_0, T_g = 0.9T_0, Kn = 0.006$ and $Kn = 0.03$. The dimensionless temperature gradient is 0.222 and 0.133 for $Kn = 0.006$ и $Kn = 0.03$ respectively. But in dimensions coordinates the temperature gradient for $Kn = 0.03$ is three times as much than for $Kn = 0.006$. The typical distribution of density, velocity and temperature for $Kn = 0.006$ are presented at the Figure 4.

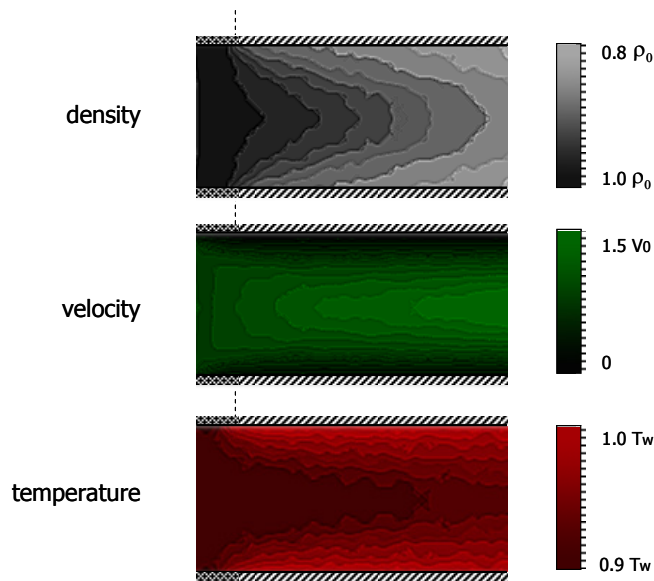


Figure 4. The typical distribution of density, velocity and temperature

With an increase the Kn the distribution of main parameters differs significantly from the results of continuum mechanics, therefore for studying flows in micro- and nano-channels it is necessary to use microscopic approach of the molecular dynamics.

Work was supported by Russian Foundation for Basic Research Grant No.05-01-00843

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