

FLOWS IN MICROCHANNELS

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Abstract: The aim of this paper is to present a survey of the results for the flows of simple gases and liquids with substructure through narrow channels, obtained with the Direct Monte Carlo and Molecular Dynamics Simulation methods.

Keywords: microflows, micropolar fluid, Molecular Dynamics Simulation, Direct Monte Carlo Methods, microchannels

1. Introduction

In recent years a very rapid development of microfluidic systems could be noticed. It was enforced by the requirements of the modern industry and it was made possible thanks to quick development of the micromachining technology. Now it is possible to fabricate the micrometer-sized mechanical parts, which may be used to produce a number of microfluidic systems in silicon, glass, quartz, plastics and other materials.

Typical sizes of micromachined elements are of the order of 1 micrometer or less in diameter and 100 micrometers in length [1]. Microchannels belong to the most essential parts of such systems. For instance, fluid flows through channels and valves, driven by pumps, are typical for biomedical analytical systems [2]. Apart from that, microchannels are used in MEMS, in inkjet print heads, computer cooling devices or in heat exchangers. Prediction of flow quantities in microchannels is therefore essential for successful design and future development of micromachines.

Experiments show that when the dimensions of the channels are in the micrometer range, the measured data are different from those predicted by Navier-Stokes Equations [3, 4]. Discrepancies concern flow characteristics, such as: volumetric flow rate, average velocity, pressure drop and Darcy friction factor for incompressible fluids, flowing through microchannels [5, 6]. Moreover, experimental observations have shown that the viscosity of the fluids is altered significantly as compared to the bulk viscosity, measured away from the wall.

Some experiments show, that the data for polar fluid flows in microchannels differ significantly from those obtained for non-polar fluids. One should mention here, for instance, the paper by Pfahler *et al.* [7], who reported data concerning viscosity of such fluids flowing in a microchannel. Also Hasegawa *et al.* (1997) [8] examined pressure drop for flows through micro nozzles. In general it is interesting to note that in micro flows the measured flow properties depend on the fluid used in test whenever a size effect is observed.

Several effects, typically excluded from the description of the macro-scale flows, become increasingly important when considering flows in microscale. Many details of the physical mechanisms of the microscale flows are not known yet. However the surface forces and internal degrees of freedom of the molecules (not considered in classical analyses) seem to be the most important factors, responsible for the behaviour of fluids in very narrow channels.

During the flow the molecules of the liquid are believed to be influenced by surface forces nonuniformly, which results in their non-central collisions, causing rotation of the molecules. This effect is particularly pronounced when polar liquids with substructure (biofluids, liquid crystals) after phase transition [9], are under investigation and when the channel width is sufficiently small. It is worth mentioning here, that molecules with no electric charge may nevertheless have a dipole configuration (*e.g.* water).

Other effects, apart from rotation of the molecules, which are influenced by surface forces are: velocity slip at the walls, temperature jump and capillary effects.

To facilitate the description of the fluids with complex molecules, the micropolar fluid model has been introduced by Eringen in 1966 [10]. It is based on the assumption of continuous medium, however it takes into account microrotation of the molecules and augments the laws of the classical continuum mechanics by incorporating the effects of fluid molecules on the continuum. This becomes increasingly important when considering flows of fluids with substructure (polar fluids, biofluid, *etc.*) in microchannels.

The micropolar model provides a better agreement with the experimental data for microchannel flows than the Navier-Stokes theory [5, 11]. However, the experiments and theoretical estimations indicate, that for real fluid flows the micropolar effects are important if the width of the channel is comparable to the dimensions of the particles of the fluid (width of the channel equal to 10–100 particle diameters). On the other hand, when the dimensions of the container approach the dimensions characteristic for the molecular structure of the medium inside (mean free path, average distance between the neighbouring molecules or the diameter of a molecule – whichever is the largest) the assumption of continuum seems not to be justified. The question arises then, whether the parameter range exists in which the micropolar fluid model is sensible at all. Otherwise the fluid could only be described with some particle based representation method: Direct Monte Carlo Simulation (DMCS) or

Molecular Dynamics (MD) [12, 13]. The results of these two methods will actually be used here as standards to compare with micropolar fluid model, to check the range of its validity.

The DMCS method is well suited to gas flows. Its fundamental assumption is, that the density of the medium is low and therefore the particles do not interact with each other, except for elastic collisions. Only binary collisions are taken into account. Between collisions the particles move along straight lines with constant velocities. Partners for collisions are selected with the use of some probabilistic procedure from particles occupying the same cell (the whole flow area is divided into a finite number of cells, whose dimensions are comparable with mean free path of the particles).

In a liquid, the molecules are densely packed and during their motion they interact all the time with their neighbours. There is no free motion of the molecules along straight lines. Since all the neighbours, interacting with a given particle, are known, there is no room for probabilistic selection and the deterministic method, the MD [13] simulation must be used. This method of simulation provides actually the best way of investigation of fluids possessing structured molecules with internal degrees of freedom.

The Molecular Dynamics method is very demanding, as far as the speed of the computer and the memory size are concerned. Only recently, thanks to dramatically increasing computer power there has been greater interest in studying the flows with the use of this method. However, there is still need for simpler and faster methods of calculating real “structured” fluid flows through narrow channels or pores. The model of micropolar fluid may probably be helpful here, however, as it is based on the assumption of continuous medium, all the doubts concerning its applicability to flows in narrow channels remain valid. So our objective is to review current results of molecular simulation of structured fluid flows and their comparison with the results for a micropolar fluid in the hope that the limits of applicability of a micropolar model can be determined this way.

2. Micropolar fluids

As already mentioned in the Introduction, the model of micropolar fluids was introduced in order to facilitate the description of the fluids with complex molecules. The “micropolar fluids” are usually defined as isotropic, polar fluids in which deformation of the particles has been neglected. The theory of micropolar fluids was first formulated by Eringen in 1966 [10]. It defines microrotation velocity $\omega \neq \nabla \times V$ independently of the displacement velocity V , and flow equations are expressed in terms of these two velocity fields.

The micropolar fluid model is the only existing non-Newtonian model which can be used for description of real fluids which possess internal structure. The theory of micropolar fluids is presently being developed very rapidly because of its possible applications in many areas: tribology, biotribology [9], for description of microchannel flows [14], in magnetorheology, *etc.* The number of papers dealing with that subject is quite substantial. The books [15, 16] summarize results achieved in this field.

The equations of motion of the micropolar fluid may be written as follows:

$$\rho \frac{dV}{dt} = \rho f - \nabla p + (\lambda + 2\mu + \kappa) \nabla \nabla V - (2\mu + \kappa) \nabla \times \nabla \times V + \kappa \nabla \times \omega \quad (1)$$

$$\rho \frac{d\omega}{dt} = (\alpha + \beta + \gamma) \nabla \nabla \omega - \gamma \nabla \times \nabla \times \omega + \kappa \nabla \times V - 2\kappa \omega \quad (2)$$

where symbols used in the equations denote: ρ – density of the fluid; p – pressure; λ , μ , κ – the bulk, shear and vortex viscosities; α , γ , β – the respective couple viscosities and f – mass force density.

The Poiseuille flow is one of the very few flow cases in micropolar fluid dynamics for which, under suitable assumptions, a full analytic solution is available [15] and stands:

$$V_x = PE \left[1 - \bar{y}^2 + \frac{2\kappa}{(\mu + \kappa)Kh} \coth(Kh) \left(\frac{\cosh(Kh\bar{y})}{\cosh(Kh)} - 1 \right) \right] \quad (3)$$

$$\omega_z = \frac{PE}{h} \left(\bar{y} - \frac{\sinh(Kh\bar{y})}{\sinh(Kh)} \right) \quad (4)$$

where:

$$K^2 = \frac{4\mu\kappa}{(\mu + \kappa)(\gamma)}$$

$$PE = \frac{h}{2} \frac{dp}{dx}$$

$$\bar{y} = y/h$$

$$V = (V_x, 0, 0)$$

$$\omega = (0, 0, \omega_z)$$

$$h = \text{width of the channel.}$$

3. Surface forces

The unique features of the microchannel flows are perhaps the most intriguing ones in the whole fundamental fluid mechanics. In the following we shall briefly describe the surface forces, which seem to be responsible for the complex phenomena observed in microflows. An excellent review on this subject may be found in the book [17].

The fundamental parameter deciding which forces govern the physical phenomena in the flow is the length scale. In the macroscale certain surface forces may be ignored. In the microscale this may not necessarily be possible. The forces which must be taken into account in the microflows are: van der Waals forces, electrostatic forces and steric forces.

3.1. Van der Waals forces

The van der Waals forces are short range forces and have an interaction free energy that varies as r^{-6} . If large molecules or surfaces are involved the van der Waals forces can produce an effect at distances longer than $0.1 \mu\text{m}$.

The van der Waals forces consist of three components: orientation force, induction force and dispersion force. The orientation force is the dipole-dipole interaction force between polar molecules. The induction force arises from the interaction between a polar molecule and a nonpolar one. The dispersion forces act on all atoms and molecules even if they are neutral, like those of helium and oxygen.

3.2. Electrostatic forces

The electrostatic forces act between charged molecules. They have an inverse-square dependence on the distance between interacting molecules, r^{-2} so they are of longer range than the van der Waals forces.

The electrostatic forces at the walls of the channel are often difficult to evaluate because of uncontrollable surface charges. In fact, any surface is likely to carry some charge, due to broken bonds and surface charge traps.

3.3. Steric forces

This is a special kind of forces, occurring when chain molecules (*e.g.* polymers) are attached to the surface at one end, with the other end dangling into solution (liquid for most of the cases), where they are mobile. The forces, known as steric forces, arise whenever a free molecule or surface approaches. It is a result of an entropy change caused by the confined molecules. The complex molecules can produce complex interactions, and steric forces can be attractive or repulsive. They are rather long range ($0.1\ \mu\text{m}$) and they are important when a fluid flow has significant amount of long chain molecules.

4. Molecular dynamics simulation

The Molecular Dynamics (MD) method is applicable mainly to simulation of liquids. In a liquid the molecules are densely packed (1 cubic micrometer of liquid contains approximately $3.35 \cdot 10^{10}$ molecules; the average distance between the molecules is equal to about 0.31 nanometer). During their motion the molecules interact all the time with their neighbours. Knowing the positions and velocities of the molecules in certain volume and the interaction potential between them it is possible, at each time instant, to calculate short pieces of their trajectories. The Newton's equations of motion, as well as Lagrange or Hamilton's equations may be used for this purpose.

Since each molecule is constantly influenced by its neighbours, its trajectory, in general, is curved. Therefore to calculate this trajectory and also the trajectories of the neighbours with reasonable accuracy one must use very short time steps.

It is, of course, impossible to consider the motion of the molecules in an infinite area. One must limit himself to a finite volume (MD cell), containing a reasonable number of molecules. To diminish the effect of the walls one simply surrounds the cell with an infinite number of identical cells [13] containing identical distributions of molecules inside.

With the described method it is possible to calculate the bulk parameters of a liquid. It is also possible to simulate the flow in a microchannel assuming that some molecules stay at fixed positions, forming the wall of the microchannel [13]. Since it is difficult to impose a pressure difference to drive the flow, some gravitational – type force field is usually introduced.

In the following chapter we will present some results of the simulation of the flow through capillary channels of different widths.

5. Results

To get a feeling about the possible discrepancies between the classical, continuum solutions for some simple flows and the corresponding results of the molecular simulation for flows in narrow channels we performed the DSMC calculations for plane Couette and Poiseuille flows of a simple, monoatomic gas. The widths of the channel were equal to 10, 5, 3 and 1 mean free paths for the Couette flow and 10, 5 and 3 for the Poiseuille flow.

The length of the channel for Couette flow was equal to 324 mean free paths; to avoid the disturbances due to finite channel length the periodic boundary conditions were applied. The length of the channel for Poiseuille flow was equal to 200 mean free paths. In both cases the hard-sphere molecular model was employed; at the channel walls the diffuse reflection of the molecules was assumed.

In the Couette flow one of the walls of the channel was stationary, the other moved with constant velocity U , equal to 0.1 of the speed of sound. This seemed sufficiently low to have negligible influence of compressibility.

The results of the simulation for the four widths of the channel are shown in Figure 1. In each picture a straight line (marked “CONTINUUM”), corresponding to the continuum solution, is shown too.

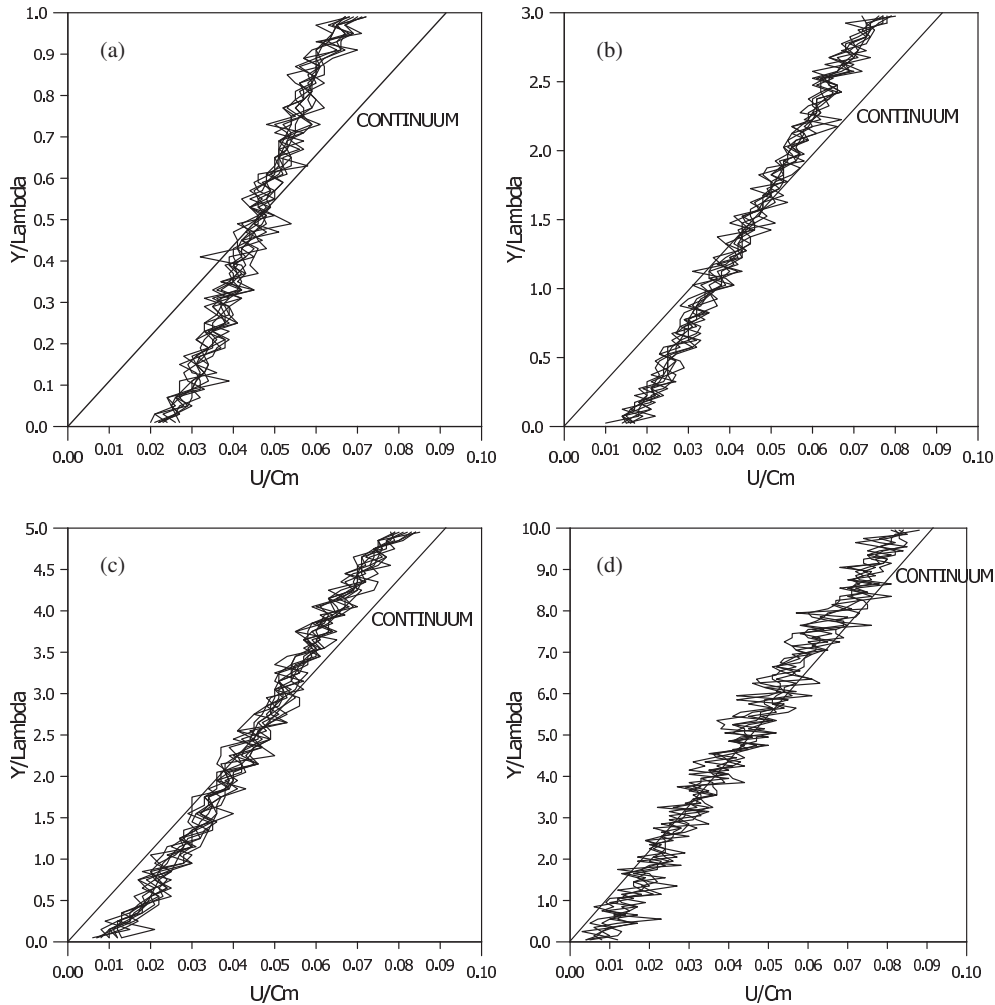


Figure 1. Velocity distributions for a plane Couette flow (Cm – most probable velocity of the molecules): (a) channel width equal to 1 mean free path; (b) channel width equal to 3 mean free paths; (c) channel width equal to 5 mean free paths; (d) channel width equal to 10 mean free paths

The DSMC results for all cases are close to straight lines, which is characteristic for the Couette flow. However, because of the velocity slip, the value of the velocity gradient is different from that of the continuum solution. The difference is more pronounced for narrower channels. The solution for the channel 10 mean free paths wide is so close to the continuum solution, that this value can probably be considered as the limit of applicability of the continuum theory for the present configuration.

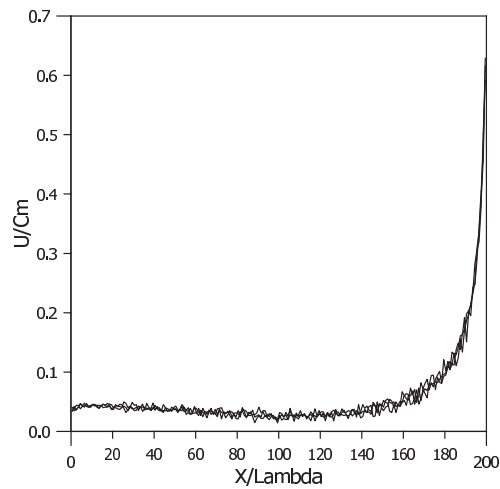


Figure 2. Velocity distribution along the centerline of the channel for a plane Poiseuille flow (C_m – most probable velocity of the molecules); channel width equal to 3 mean free paths

The Poiseuille flow was driven by a stream of gas with density equal to the initial gas density in the channel, flowing into the calculation domain with the speed equal to about 0.11 of the speed of sound. The rear end of the channel was open to vacuum.

It took quite an appreciable amount of computing time for the flow to stabilize. The diagram of the flow velocity along the centerline of the channel, obtained for the channel 3 mean free paths wide after long time of computation, is shown in Figure 2. After entering the channel the flow slows down, then the velocity stays approximately constant and, finally, the flow accelerates to about the speed of sound. The character of the flow in the other two channels is similar.

Figures 3a, 3b and 3c show the velocity distributions in the perpendicular cross-sections of the three channels, in the area where the velocity at the centerline of the channel is approximately constant. In all three cases the velocity slip at the walls is visible, however its relative value is appreciable only for narrower channels. For the channel 10 mean free paths wide the velocity distribution is close to the parabolic continuum solution. Probably this value can also be considered to be the limit of applicability of the continuum theory for the Poiseuille flow.

One thing should be mentioned at this point – the presented DSMC results fluctuate considerably. The momentary distributions of velocity may actually be quite far from anything expected. Only the distributions averaged over sufficiently long time may be comparable and may agree with continuum solutions.

There are only two papers [18, 19] in which results of molecular dynamics simulations of structured fluids in microchannel flows are reported and compared with the analytical solutions, Equations (1) and (2). Both papers concern plane Poiseuille flow, however they employ different MD methodologies and consider different fluids. Numerical results in both cases show that short linear molecules exhibit rotational motion.

In the first of the papers Travis and Todd [18] present some results obtained with nonequilibrium molecular dynamics (NEMD) simulations for a fluid, consisting of non-spherical, uniaxial (diatomic) molecules in a plane Poiseuille flow. The uniaxial molecule

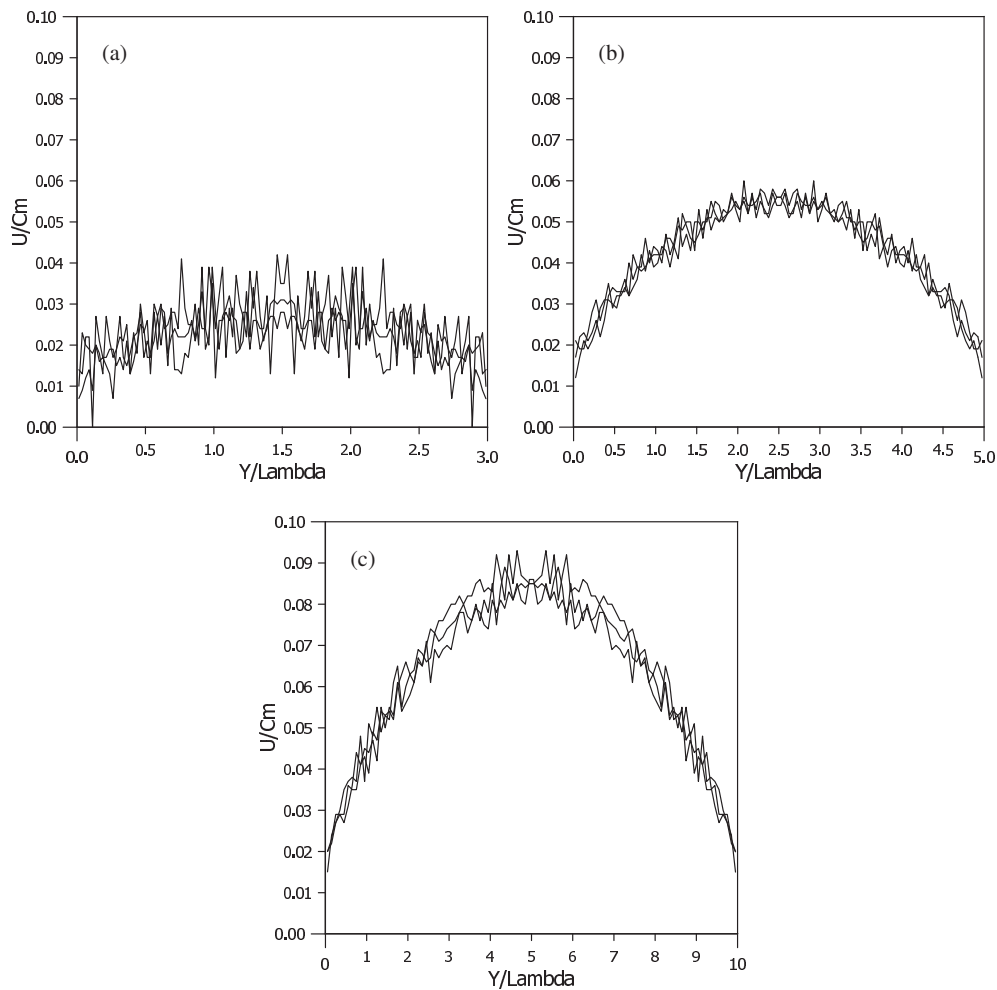


Figure 3. Velocity distributions in the cross-section of the channel for a plane Poiseuille flow (Cm – most probable velocity of the molecules): (a) channel width equal to 3 mean free paths; (b) channel width equal to 5 mean free paths; (c) channel width equal to 10 mean free paths

consists of two hard – sphere molecules. The slit pore width is equal to $W = 5.1$ maximum uniaxial molecular diameters (it means $W = 10.2$ molecular diameters). The fluid flows down a rectangular channel undergoing gravity. The system consists of 360 uniaxial molecules.

The comparison of the results of simulation with theoretical predictions of micropolar fluid theory is presented in Figure 4 and Figure 5. They indicate that the shape of the velocity profile is almost the same as that obtained with the use of the micropolar fluid theory. The microrotation profile gives a reasonable qualitative agreement with the theoretically predicted one.

The simulation of the channel flows of various fluids consisting of short linear chain molecules were presented in the second of the above mentioned papers [19]. In this simulation each molecule consisted of four soft spheres, which could be connected in several different ways to produce either fully flexible chains, stiff chains with restricted internal degrees of freedom and rigid, rod-like molecules. The molecules were forced to flow

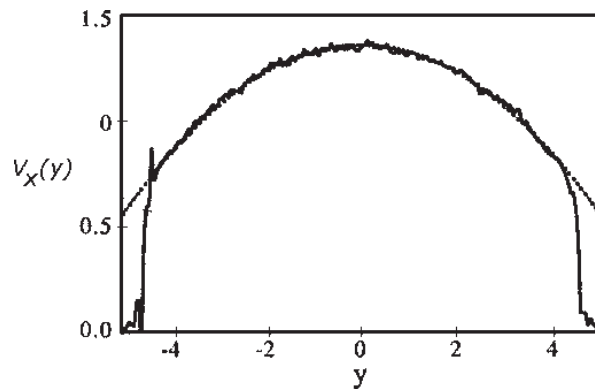


Figure 4. Velocity distributions in the cross-section of the channel for a plane Poiseuille flow. Channel width h equal to 5.1 diatomic molecules diameters, (after [18])

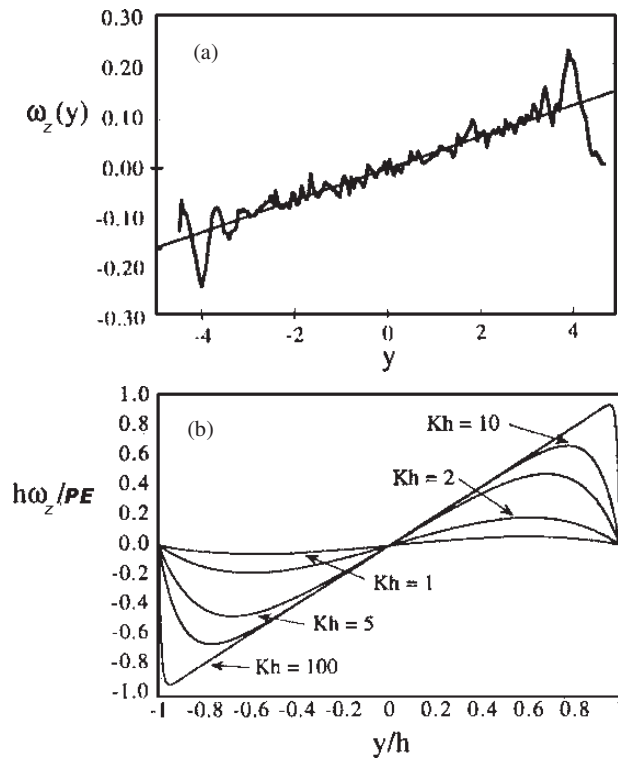


Figure 5. Microrotation distributions in the cross-section of the channel for a plane Poiseuille flow: (a) channel width h equal to 5.1 diatomic molecules diameters, (after [18]); (b) theoretical, Equation (4), for various values Kh

through a channel by uniform gravitational field with gravitational acceleration g oriented in the y direction. The (two-dimensional) channel had two infinite walls perpendicular to the x direction. The initial molecular array consisted of 45 molecules in both x and y directions; in the z directions the array was three molecules deep. The periodic boundary conditions were employed. The width of the channel h is equal 16.5 dimension of linear chain molecules.

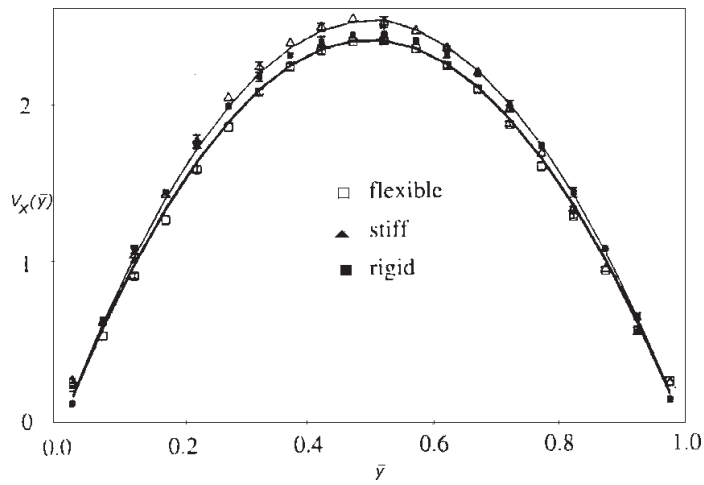


Figure 6. Velocity distributions in the cross-section of the channel for a plane Poiseuille flow, for flexible, stiff and rigid chain molecules. The width of the channel h is equal 16.5 dimension of linear chain molecule, after [19]

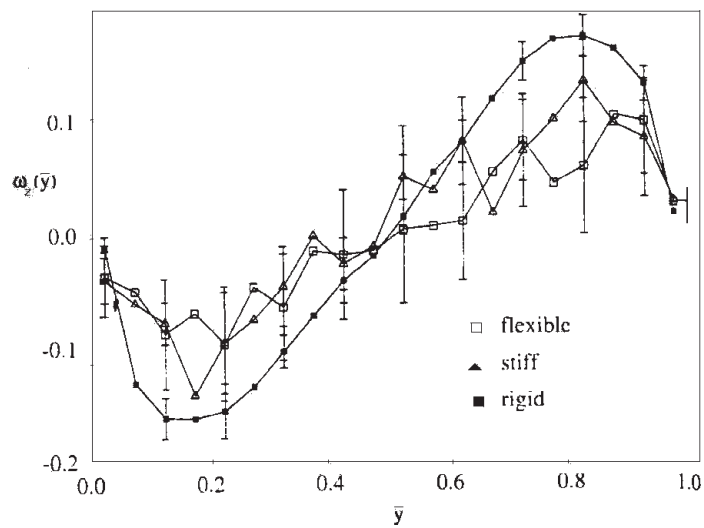


Figure 7. Microrotation distributions in the cross-section of the channel for a plane Poiseuille flow, for flexible, stiff and rigid chain molecules. The width of the channel h is equal 16.5 dimension of linear chain molecule, after [19]

The corresponding results for microrotation and velocities (Figure 6 and Figure 7) show general agreement with the profile predicted with the micropolar fluid theory. The profile of microrotation for rigid molecules agrees nearly perfectly with the theoretical one for $Kh = 4.7$.

6. Conclusions

We present the results of the numerical simulation of the flows of simple gases and “real” liquids through capillary pores. The flow is considered as a motion of separate

molecules, interacting among themselves and with the walls. The model of interactions in a liquid takes into account rotation of the molecules. Large number of the performed numerical simulations makes it possible to obtain the average distribution of velocity. This average distribution is compared with analytical solution of the Eringen equations for the Poiseuille flow.

The presented results provide quantitative tests of the applicability of micropolar fluid theory to modeling relatively complex fluid flows in very narrow channels.

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