WATER FLOWS IN COPPER AND QUARTZ NANOCHANNELS

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Summary: The molecular dynamics simulations of water flows in rectangular channels, induced by gravitational force field, have been compared with theoretical predictions for micropolar fluid flows. The similarities and differences, particularly in velocity fields and microrotation have been discussed. Two different channel widths and two kinds of wall material have been taken into account. .

INTRODUCTION

Numerous experimental results indicate, that the microscale flows are essentially different from flows in large scale [1], [2]. The continuum Navier-Stokes approach, suitable for large sale flows, is not applicable to small scales. At the same time, however, there exists an extension of the Navier – Stokes approach, also based on the assumption of a continuous medium – the micropolar fluid model – which agrees quite well with some experiments in microscale. The micropolar fluid model – proposed by Eringen in 1966 [3] - takes into account microrotation of the molecules, different from the local vorticity of the flow.
The experiments and theoretical estimations indicate, that for real flows through narrow channels the importance of the micropolar effects grows when the channel width decreases down to the values comparable with the dimensions of the particles of the fluid. However, under such conditions, the assumption of continuous medium, essential for the theory of micropolar fluids, does not seem to be justified. The problem of validity of the micropolar fluid model for the flows through narrow channels is yet to be solved.
Some information on the validity of the micropolar model to description of the flows of Cl_2 or P_5 in narrow channels are given in [4], [5] however these results concern fluids which very rarely flow in microdevices. Moreover, the used molecular model of the channel wall is so simplified, that it cannot simulate any real physical material.
Since water is the fluid, most often flowing through microchannels and the channel walls are most often made of silicon, quartz or copper, we concern ourselves to water flows in copper and quartz channels. We compare the theoretical predictions for flow velocity and microrotation with results of molecular dynamics simulations of flows under gravity field down rectangular channels.

MOLECULAR DYNAMICS SIMULATION

As mentioned before, we calculated the flow of water through narrow slits (plane Poiseuille flow) with walls made of cooper or quartz. Two channel widths, equal to 5 and 10 diameters of the water molecule were considered.
The Lennard-Jones 6–12 potential was assumed for interactions between water molecules and also between water molecules and wall atoms. For water the four site molecular model of Jorgrnsen [6] was employed. The molecular parameters of quartz and copper were taken from [7] and [8].
To minimize the influence of the boundaries of the calculation domain the periodic boundary conditions were used. The number of wall atoms taken for calculation ranged from 236 for copper wall to 250 quartz molecules otherwise. The number of water molecules - from 280 for the flow between quartz walls to 720 for the broader channel between copper walls. Simulations were carried out (in reduced units) with the number density 0.989 for water at T= 3.6. To drive the flow, a constant force F was applied to the centre of mass.of each water molecule. Several values of F, ranging from 0.5 to 5 were used.:The calculation were performed with the MOLDY program [9]. They were carried out over 200000 time steps, equal to t=0.005.

RESULTS

The obtained results show that for channel widths equal to 10 diameters of the molecule the results of the micropolar theory are in a reasonable qualitative agreement with molecular dynamics simulation. In particular, the microrotation velocity (missing in the classical Navier-Stokes theory) and the translational streaming velocity profiles agree well with those from MD simulation.

In all cases under consideration some slip velocity and non-zero microrotation at the walls could be observed. The slip effects are stronger for smaller channel widths and for walls made of copper. They seem to be influenced by interaction of water molecules – which have electric dipole moment - with the charges of the walls. Quartz does have some electric charge, copper does not. For water molecules the quartz wall behaves as an attractive one, whereas the cooper wall (without charge) as a repulsive one.
The obtained results are consistent with earlier research. The effect of attractive and repulsive walls on the slip velocity was observed in Poisseuille flow simulations of dense gas flows in narrow channels [10] [11]. The present results, however, are the first obtained for flows of fluid whose molecules possess electric dipole moment.
The problem of interaction between fluid and solid surfaces has received increased attention over the past ten years as engineering applications reached the micrometer and nanometer scale. For the past century the non-slip boundary condition was considered to be appropriate for macroscopic flows. However, with the decrease of the length scale the non-zero slip velocity should be taken into account. Our results, as well as experimental and simulation results of other authors show that the slip velocity in micro and nanoflow exists and strongly depends on wall – fluid interaction.

CONCLUSIONS

The predictions of the micropolar fluid theory and the results of molecular dynamics simulation of water flows through narrow slits with copper and quartz walls agree reasonably well for channels widths equal to 10 diameters of the water molecule.for more narrow channels the agreement is poor. It can be concluded then, that the micropolar theory may be applied to modelling the fluid flows in channels of width not smaller than 10 fluid molecular diameters. This conclusion is also supported by earlier results of other investigators.
The simulation results show that the velocity slip in micro and nanoflows exists and strongly depends on wall – fluid interaction, particularly on whether the forces between the wall and fluid are attractive or repulsive.

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