Simulations of micro- and nano -channel flows by a Dissipative Particle Dynamics Method

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The numerical modeling of micro- and nano- flows is very important for understanding micro-fluidics phenomena in industrial applications. However the methods, which are widely used, have various limitations. The continuum models cannot provide correct description of near wall behavior of fluids (no–slip boundary conditions is enforced). Molecular Dynamics approach is very expensive computationally. Therefore the industrial application is limited.

In this paper we propose to model nano- and micro-flows by Dissipative Particle Dynamics. The method is particle based simulation techniques. The method can be derived from Molecular Dynamics by means of coarse graining. Dissipative Particle consists of many molecular particles. Therefore the simulations by DPD are much less computationally expensive than MD and easier to apply for industrial flows modeling.

The dissipative particle can be defined in two ways. Soft fluid particle model assumes that particles are spherical and interparticle interaction is restricted to specified region. The Voronoi particle model [5,6,7,8] describe particles as Voronoi cells and interacting with adjusted neighbors. The Voronoi approach helped to solve many problems such as treatment of boundary conditions, fluctuation in the volume and inaccuracies in equilibrium fluid properties. Here, we will present results of 2-D computations of some flow configurations (micro-channel) applying Voronoi approach of Dissipative Particle Dynamics. This is a new and promising approach to compute micro and nano- fluidics phenomena.

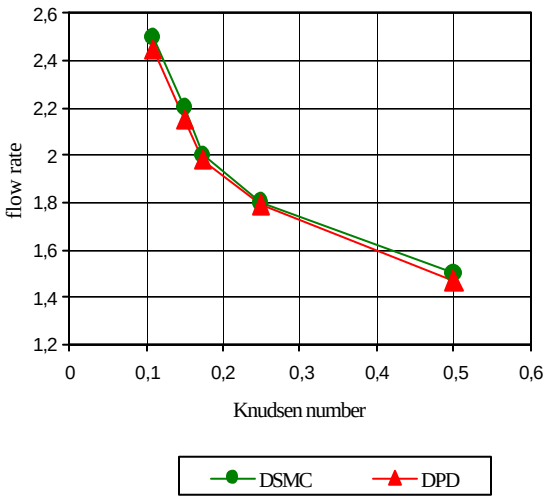

Figure 1.: Flow in the micro-channel simulated by Dissipative Particle Dynamics (DPD) and Direct Simulation Monte Carlo (DSMC). Figure presents the flow rate – Knudsen number relation.

References

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