

Analysis of wall effect on the process of diffusion of nanoparticles in a microchannel

K. Zembrzycki, T. A. Kowalewski.
Institute of Fundamental Technological Research,
Department of Mechanics and Physics of Fluids.

Recently, the classical nonslip hypothesis for the tangential velocity of liquid adjacent to the solid surface became questioned for the flow in micro- and nanofluidic devices. The topic is of fundamental interest and has potential practical consequences in many areas of applied sciences. Hence, several experimental and numerical studies were performed to elucidate presence of the molecular-scale slip for the flow of Newtonian liquids in microchannels. It came out that in the most investigated configurations the slip velocity (or so called *slip length*) exists and can be measured. However, values obtained for the slip length strongly vary from the experiment to experiment, covering range of several nanometers to several microns. It is partly due to the experimental difficulties in performing accurate velocity measurements of flow at molecular distances from the wall. To avoid problems appearing in reconstructing flow velocity profile in nanometric layers, we propose to evaluate how the slip/non-slip boundary conditions affect behaviour of a Brownian particle performing its chaotic motion close to the wall. According to the theoretical model by E. Lauga and T. Squires [1] the diffusion coefficient of a single colloidal nanoparticle is directly related to the distance from the wall, and the slip velocity. In this work we apply this outcome to determine the slip length from measured and calculated variations of the diffusion coefficient of particles as a function of distance from the wall. For this purpose the effect of the wall on the Brownian motion of nanoparticles suspended in water is examined both in the numerical simulations using molecular dynamics and in the experimental study.

The Brownian diffusion of 24 nm nanoparticle suspended in water in an infinite channel formed between two quartz walls is simulated by the molecular dynamics code LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator). The computations were performed for the square domain of 310.5 nm size and periodic boundary conditions for the two side walls. All interactions between particles were described by the granular potential, which is a modification of the Lennard-Jones potential. Several simulations were performed to evaluate Brownian motion of colloidal particles placed at different distances from the wall. The outcome of the numerical analysis is still not quite clear, our preliminary results suggest absence of the slip velocity. However, due to the well known constraints of the numerical model (short physical simulation time, two-dimensional domain) it may be an artefact. The work is still in progress.

In the experimental study we analysed Brownian motion of fluorescent particles with a diameter of 300nm located between two walls of the microchannel. To obtain precise measurements very close to the wall evanescent wave was generated by total internal reflection of the illuminating laser beam. Fine adjustment of the laser illumination angle allowed us for a precise control of the penetration depth of the evanescent wave. The measurements were performed for particle located in the plane 107 nm from the wall and in the middle plane of the channel. The temporary position of the particles was evaluated from the long sequences of acquired microscopic images by means of especially developed filtration and image analysis codes written in the MATLAB environment. The preliminary experiments resulted in the measured slip length of nearly 0.7 μ m. The work is continued using smaller particles (24 nm) and taking into account modification of the wall properties (hydrophobic/hydrophilic).

References:

[1] E. Lauga, T. M. Squires. Brownian motion near a partial-slip boundary: A local probe of the no-slip condition. *Physics of Fluids* 17, 103102 (2005).