XX Fluid Mechanics Conference KKMP2012,
Gliwice, 17-20 September 2012

PROBLEMS WITH THE MODELING OF WATER FLOW IN NANOCHANNELS

Janusz Bytnar[1], Anna Kucaba-Piętal[2]
1Institute of Technical Engineering PWSTE, Jaroslaw, Poland;
2 Rzeszow University of Technology, The Department of Fluid Mechanics and Aerodynamic, Rzeszow, Poland
E-mail: janusz.bytnar@pwste.edu.pl

Key words:nanoflows, Molecular Dynamics, computer simulations

Dynamic behavior of water in nano-channels is crucial for the design of molecular sensors, devices, and machines and for many biological applications.

The understanding of the water transport inside graphene flat nanochannels is highly desired in practice. The study of diffusion of water molecules through nanochannels can help to explain the operating mechanisms of water channels, which are responsible for many important biological processes in the cell [1].

When characteristic dimensions of the flow is less than approximately ten molecules, the continuum hypothesis breaks down and Molecular Dynamics method should be employed to simulate the atomistic behavior of such system. To simulate nanoflow by use MD, the atomistic description is necessary for liquids contained in nanochannels and material from which channel is made, moreover the computer simulations need specific input parameters characterizing systems in question, which either come from theoretical considerations or are provided by experiment.

The anomalies that exist in the bulk properties of water caused that a large number of atomistic models for water have been developed. It seems to be very important to properly understand the effect of various atomistic water models on MD results before they can be used for nanotechnology design.

Aim of the paper is to examine the effect of various molecular models on MD simulation of water nanoflows. A Poiseuille flow with constant force on each fluid molecule was used as prototypical problem.

The simulations of water nanoflows in coopper channels for three molecular models: TIP4P, PPC, TIP5P were performed. MD simulation input parameters characterizing the systems were identical.

The nanochannel walls were built from copper atoms and its width was equal to 5 diameters of the water molecule. The physical properties of materials and their electrostatic interactions were taken into account. The Lennard-Jones potential was assumed for interactions between water molecules and also between water molecules and wall (copper) atoms. All Lennard-Jones parameters (δ, ε) were taken from [2]. The program MOLDY [3], suitably modified, was used for this purpose. The Gaussian thermostat was applied to controlling the temperature of water molecules during the whole simulation. On the beginning this temperature was fixed as 300 K.

To drive the flow, a constant nondimensional force Fx was applied to the centre of mass of each water molecule. A time step of 0.5 fs was used and the total simulation time was about a few nanoseconds.

Figure 1 shows the velocity profile obtained from MD simulation of Pouisseuille flow in an 5-fluid diameter cooper channel. We observe that the velocity obtained from MD simulation by use TIP5P model is much less than by use PPC and TIP4P models.

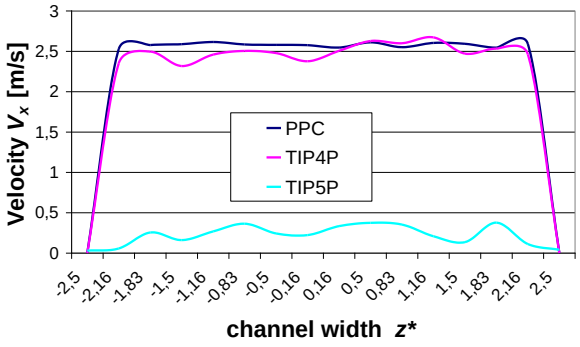

Fig. 1. Velocity distributions for flow of water in nanochannel, (Fx=2.5)

Corresponding Radial Distribution Functions (RDF) were presented in Figure 2. The radial distribution function (RDF) is a basic measure of the structure of matter, its shape is different for different states of matter, gaseous, liquid and solid. The RDF shape for TIP5P is typical for solid state, RDF shape for PPC and TIP4P is typical for fluid state.

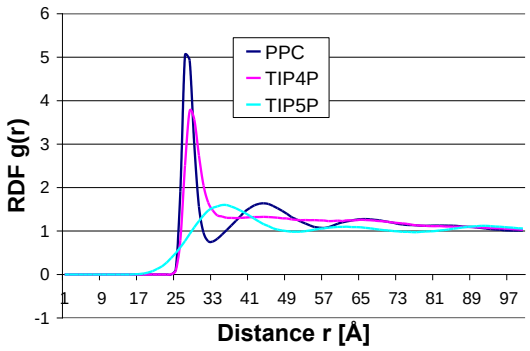

Fig. 2. Radial distribution function for simulated nanoflows

So we can conclude that during the nanoflows simulation by use TIP5P model, the water change state from liquid to solid (ice).
Question is: can we choose the MD simulation input parameters for TIP5P model to receive nanoflow of water in liquid state or TIP5P model is is inappropriate for the dynamic simulation of water?

Acknowledgement

The simulations were performed on computers in Department of Mechanics and Physics of Fluids, Institute of Fundamental Technological Research PAS (IPPT PAN), and for this possibility the authors would like to thank.

References

[1] Karniadakis G., Beskok A., Aluru N. (2005): *Microflows and Nanoflows – Fundamentals and Simulation*, Interdisciplinary Applied Mathematics, Springer
[2] Allen, M.P., Tildesley D. J. (1987): *Computer simulations of Liquids*, Oxford University Press
[3] Refson K.: *Moldy User's Manual*. Chapter II, ftp://ftp.earth.ox.ac.uk/pub