Physica A 515 (2019) 13–30

Contents lists available at ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

Modeling different structures in perturbed Poiseuille flow in a nanochannel by using of molecular dynamics simulation: Study the equilibrium

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HIGHLIGHTS

- Modeling different structures in perturbed Poiseuille flow.
- Study the equilibrium.
- Using of molecular dynamics simulation.

ARTICLE INFO

Article history:
Received 3 July 2018
Received in revised form 5 September 2018
Available online xxxx

Keywords:
Nanochannel
Equilibrium
Molecular dynamics simulation
Poiseuille flow

ABSTRACT

In this study modeling different structures in perturbed Poiseuille flow in a nanochannel by using of molecular dynamics simulation was performed. Nanochannel limited by parallel Platinum plates containing an Argon fluid. We found that the wall roughness increases the velocity in the nanochannel by shrinking the cross-section. Also, the rectangular roughness and hemispherical roughness have the maximum and minimum effects on the flow properties, respectively. The other result is that the nanochannel roughness reduces the range of fluctuations near the walls. This is due to the fact that less fluid particles reside in the vicinity of the rough nanochannel walls compared the ideal nanochannel. Finally, changing the configuration of the nanochannel roughness from ellipsoid to hemi-spherical increases the number of Pt atoms in the structure and the simulated system; therefore, the total energy is also expected to increase.

1. Introduction

Molecular simulation is a branch of computational physics. In this method, relying on accurate solutions to the problems of statistical mechanics, the interactions between atoms and molecules are simulated in a certain time interval based on the laws of physics, providing an outlook on molecular motions. Since molecular systems often include several particles, it is not possible to obtain the properties of complex systems by analytical means. Molecular simulation overcomes this obstacle by employing computational methods. This method relates experiment to theory and can be regarded as a virtual laboratory. The studied systems are often characterized by evaluating the intermolecular forces and energies that are mostly described by theoretical models. Such simulations have been embedded in numerous studies of nanochannel flows over the last years.

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https://doi.org/10.1016/j.physa.2018.09.177
0378-4371/

Ziarani and Mohamad [1] studied perturbed Poiseuille flow in a nanochannel. They found that in the vicinity of the boundaries, a jump in temperature profile has been observed. Yang [2] studied the effects of surface roughness and interface wettability on nanoscale flow in a nanochannel. The dependence between fluid slip and flow rate showed that the slip length increases approximately linearly with the flow rate for both the hydrophobic and hydrophilic surface nanochannels. Liu et al. [3] used MDS for to study electroosmotic flow in nanochannels with regular or random roughness on the walls. They found that roughness reduces the electroosmotic flow rate dramatically even though the roughness is very small compared to the channel width. Sun and Li [4] obtained accommodation coefficients in nanochannels with various wall configurations by using of molecular dynamics simulation. They found that when the Kn increases, the accommodation coefficients decrease due to the less gas–gas interactions near the wall. Chen and Zhang [5] investigated the role of surface roughness on thermal conductance at liquid–solid interfaces. They concluded that the presence of surface roughness diminishes the motion capability of liquid atoms in the wall neighboring region and these atoms could maintain contact with the solid surface for a long time. Noorian et al. [6] studied the effects of surface roughness geometry of flow undergoing Poiseuille flow by molecular dynamics simulation. Their results show that the effect of triangle roughness surface on the flow behavior is more than the cylindrical ones. Yen [7] studied fluid containing gas in hydrophilic rough wall nanochannels. They found that the morphology and behavior of interfacial gas bubbles are influenced by the parameters of wall–fluid interaction as well as the atomic arrangement of the substrate. Zhang [8] studied the effect of wall surface roughness on mass transfer in a nano channel. They found that the effect of the wall surface dent is negligible in spite of the fluid–wall interaction. Jeong et al. [9] investigated the effects of surface wettability, roughness and moving wall velocity on the Couette flow in nano-channel. They found that when the channel height is large enough, the no-slip condition assumption at macroscale is available. Tohidi and Toghraie [10] studied the effect of geometrical parameters, roughness and the number of nanoparticles on the self-diffusion coefficient in Couette flow in a nanochannel. Their results show that by increasing the roughness height, the particles are entrapped within the roughness and hence reduce the local self-diffusion coefficient in the vicinity of the upper wall.

In this study modeling different structures in perturbed Poiseuille flow in a nanochannel by using of molecular dynamics simulation was performed. Nanochannel limited by parallel Platinum plates containing an Argon fluid. The shelving process was used to obtain the temperature, velocity and density profiles in the simulated nanochannels to evaluate the behavior of the particles in the nanochannel at the different sections of the nanochannel.

2. Methodology and simulation model

2.1. Equations of motion

Molecular simulation is a branch of computational physics. In this method, relying on accurate solutions to the problems of statistical mechanics, the interactions between atoms and molecules are simulated in a certain time interval based on the laws of physics, providing an outlook on molecular motions. Since molecular systems often include several particles, it is not possible to obtain the properties of complex systems by analytical means. Molecular simulation overcomes this obstacle by employing computational methods. This method relates experiment to theory and can be regarded as a virtual laboratory. The studied systems are often characterized by evaluating the intermolecular forces and energies that are mostly described by theoretical models. A macroscopic property is the average of an ensemble and a mean representing a system of molecules (in equilibrium or not). A statistical "ensemble" is a large (sometimes infinite) hypothetical set of identical physical systems. These systems are copies of each other, each assuming one of all possible states. An ensemble is, in fact, a probability distribution for the possible physical conditions of the system. The main goal in molecular dynamics simulation is to obtain the phase space. For N particles, there will be $6N$ ordinary differential equations. The analytical solution of this system of equations is very difficult when N is greater than 2, but it may be easily solved using numerical methods. The differential equations are discretized to obtain the locations and velocities of all particles with the help of a proper time step. All equilibrium and non-equilibrium properties of the system may be obtained by knowing the location and velocity of the particles in each step. From the perspective of theorists, the importance of molecular dynamics is that it provides accurate semi-experimental results for a fully-specified model [11]. In general, there are four common, constant statistical ensembles, namely the canonical ensemble (NVT), the microcanonical ensemble (NVE), the isothermal, isobaric ensemble (NpT), and the grand canonical ensemble (μVT). The aforesaid thermodynamic variables are constant for each ensemble and the other variables must be calculated by averaging. The simulation raises a few questions, including:

(a) How long should the simulation take? Considering that the simulation cannot continue indefinitely, it will suffice to consider a simulation time a few times larger than what it takes for the slowest phenomenon in the system to reach equilibrium.
(b) How to make sure that the considered region in the phase space is in equilibrium? By applying different initial conditions to the system or disrupting it, one can make sure that the system will definitely remain in the phase space if nothing changes.
(c) Has the system reached equilibrium? If the fluid is exposed to an external field, the simulation is of the non-equilibrium type. External fields push the system out of equilibrium and, if such conditions persist long enough, a permanent non-equilibrium state will develop. To simulate this system, in addition to inter-particle forces, external forces resulting from the external fields (pressure gradients and gravitational forces) shall be also taken into account in the equations of motion. The best way to start a simulation is to use the ultimate configuration (the ultimate state