Original Article

EFFECT OF WALL FLEXIBILITY ON THE FLUID – SOLID INTERFACIAL SLIP IN NANOCHANNELS

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Abstract

The speed of fluid transport in nanoscale channels was found to be influenced by the slippage in fluid -solid interface. Manipulating slip length to control nanochannel fluid flow is seen as a viable choice. Using molecular dynamics (MD), the study of the nanochannel is done. The effects like the surface roughness, and channel width are all considered to study the slip length and its influence at fluid – solid interface. In this research, the variation brought about in the interaction potential is used for the slip length manipulation and also and the wall is made elastic by altering the spring constant. The variation in slip length in each scenario is achieved. The slip length increases when the interaction potential is less and vice versa. Similarly, when the wall becomes elastic, the slip length reduces. This manipulation of slip can used in nanofiltration as electro – osmosis velocity will be enhanced with improvement in slip.

Keywords: Slip length, Nanofluidics, Nanoscale, Fluid-Solid Interface, Interaction Potential, Wall Flexibility.

INTRODUCTION

Nanofluidics can be termed as the study and application of fluid flow in and around nanoscale structures [1]. The employment of characterization methods like atomic force microscope (AFM), scanning tunnelling microscope (STM), etc. fabrication methods like an electronic and ion-beam lithography, etc., have led to rapid developments in the field of nanofluidics [1] [2]. These progress have enabled the discovery of novel devices such as lab-on-chip, nanomotors, nano biosensors, etc. Such devices were developed by utilizing the affected behavior of physical systems when confined to nanoscale dimensions [3]. Increased dominance of surface area dependent phenomena, compared to those dependent on volume can be observed when you come to such small dimensions. Hence gravitational and inertia effect becomes negligible compared to phenomenon like surface tension [4].

One such exciting behavior observed in micro nanochannels is the size dependent variations in the fluid–solid interfacial slip. This has immense importance in various applications like water filtration using CNT based membranes, micro heat pipes, chip cooling, etc. Conventionally, we neglect the fluid–solid interfacial slip in channels and use the no–slip boundary conditions.[5] As we are dealing with comparatively smaller spatial and temporal dimensions, continuum based approach may be incompetent for studying the nanoscale systems. When we come to such small systems, the solid–liquid interfacial properties like wettability, surface roughness, etc. become essential. The scientific investigation has to consider these factors in the modeling approach. The wall wettability effect focuses on the hydrophobic and hydrophilic behavior at the interface which has a hand for the slip happening at the interface [6]. Atomistic simulation methods like Molecular dynamics (MD) have arisen as a competent tool to help the numerical investigations of nanoscale systems. Many recent MD studies have shown that tuning the solid – fluid interfacial parameters can help us manipulate the fluid flow rate through nanochannels.

A Study on effect of aerodynamic drag at fluid–solid interfacial slip was carried out by Asef and Babu [7]. It was found that manipulation of slip has a considerable effect on drag. Drag reduction has significant applications in nanomedicine, nanotribology, and electrokinetics [8]. Unconventional reservoirs also have a great value here. Compared to conventional reservoirs the pore size of unconventional reservoirs is in nano, and micro scales, so classical Darcy's law is no longer valid. The nonlinear flow characteristics of low permeability in reservoirs using negative slip length were studied and explained in detail by Song et al. and Anjibabu Merneedi et al. [9][10]. In a study of solid–liquid interfacial region, Kim et al. witnessed that the crystal bonding stiffness, interaction strength, and density are critical parameters for the sudden change in temperature at the interfacial region [11]. Nanofiltration is another application in the tuning of slip length. Electro–osmosis greatly impacts nanofiltration, so an improvement of slip length enhances the electro–osmosis velocity [8]. Channel height does not determine the slip enhancement when in the case of electro-osmosis flow Celebi et al. [12]. This provides a theoretical understanding in membrane fabrication when nanofiltration is electrically assisted. Recent studies of Alizadeh et al. [13] discusses the interaction of electrical double layer where the characteristic length is reduced from micro to nanoscale resulting in improved flow.

In nanochannels, the heat removal rate does not subject to the flow rate, here interaction energy is dominant over the flow rate.[14] So while considering nanochannels in the case of heat transfer applications, the slip length effect on interfacial thermal resistance (ITR) needs to be considered. Mohammed et al. has studied the effect of ITR and found that ITR is proportional to the slip length [15][16]. Based on the form or shape of nanoparticles, the convective heat transfer is affected. Motlagh et al. [17] explained that it is affected due to the difference in structure and velocity of nanofluid atoms.

Experimental studies of fluid flow via nanochannels are difficult due to its extremely small length and time scales. Its been long known that, the atomistic modelling approach like Molecular dynamics (MD) can overcome these drawbacks and be utilized for studying the behavior of nanoscale confined fluids.[18] In the present study, we use MD investigations to study the effect of wall flexibility on the fluid–solid interfacial slip in nanochannels. The MD methodology used in the present study is discussed in the section hereafter , following a discussion on particular results.

METHODOLOGY

In this work, behavior of atoms and molecules were analyzed using MD. MD is a time integrated algorithm that helps us follow the motions of interacting atoms and molecules. It follows classical laws of mechanics, i.e. Newton's Law:

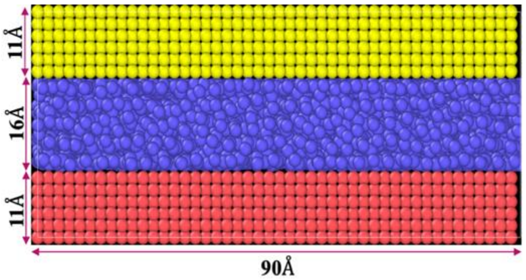
$$F = m_i a_i \tag{1}$$

Of which **F** the force acting on the atom, **m** the mass of the atom, and **a** acceleration of the atom due to force. MD is executed using an open source library package LAMMPS [19] and for visualizing OVITO [20] is used. An integration algorithm is used in MD for determining the trajectory of atoms, concerning the initial position and estimating the velocity with respect to time.

Simulation Model

A simulation block of size 90 x 42 x 90 Å with a channel diameter of 20 Å is used, as shown in Figure 1. We have considered Argon (Ar) as the fluid and Platinum (Pt) as the wall.

FIGURE 1. Simulated Ar – Pt Nanochannel



Lenard Jones potential (Equation 2) is considered for every interaction in this paper.

$$\phi(r_i) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right] \tag{2}$$

Where r_{ij} is the intermolecular distance from molecule i to j. Also, ε is the energy parameter, and σ is the length parameter, i.e. distance at which the particle–particle potential energy is 0. ε and σ values at the interfacial region were calculated using Lorentz–Berthelot rule as in Table 1.

TABLE 1 ε and σ values

	ε (kcal/mol)	**σ (Å)**
Pt – Pt	0.120183	2.475
Pt – Ar	0.169125	2.7575
Ar – Ar	0.238	3.04

In this paper, we have manipulated the Ar–Pt energy parameter, ε to investigate its effect on the slip length. We have considered ε values 0.25, 0.5, 1.25, and 1.5 times the ε of Ar–Pt obtained from the mixing rule by Lorentz Berthelot. To study the effect of wall flexibility on the slip behavior, the wall atoms were modeled as atoms bonded to their equilibrium positions using elastic springs, and the spring constants were varied.

EMD Simulation

EMD method is considered for finding the slip length of the system. Using MD, the shearing force, F between wall–fluid in the x–direction and the fluid's velocity, u are found. The correlation to get slip length was proposed by Kannam et al. [21]. We consider the velocity autocorrelation function Equation 3 and velocity force cross correlation function Equation 4.

$$C_{uu}(t) = \langle u_{slab}(0)u_{slab}(t)\rangle \tag{3}$$

$$C_{uF'_x}(t) = \langle u_{slab}(0)F'_x(t)\rangle \tag{4}$$

Laplace transform of the above correlation function is calculated as in Equation 5 and then followed by Maxwellian fitting between the two Laplace transformed functions and a memory function, ζ_0, also known as zero frequency coefficient.

$$\tilde{C}_{uF'_x}(s) = -\tilde{\zeta}(s)\tilde{C}_{uu}(s) \tag{5}$$

$$\zeta = \frac{B_i}{\lambda_i} \tag{6}$$

So we could fit $\tilde{C}_{uF'_x}$ using B_i and λ_i Ref. Equation 6 as fitting parameter.

The Friction coefficient, ξ_0 is found by dividing ζ_0 by the surface area of flow, i.e. Argon in our system. Finally the Navier slip length, L_s is calculated by dividing shear viscosity, η_0 to the friction coefficient, ξ_0 as shown in Equation 7.

$$L_s = \frac{\eta_0}{\xi_0} \tag{7}$$

RESULTS AND DISCUSSION

In our study, we have discussed the variation of slip length for change in interaction potential, ε values and the spring constant k. Considering a constant nanochannel width of 20Å, we have changed the interaction potential ε. The results show that as interaction potential is manipulated, we get a considerable variation in slip length, as shown in Figure 2. The graph trend was similar to the result obtained for Mohammed and Babu [15]. The fluid becomes more phobic when interaction energy is reduced, resulting in an increase in flow rate. We could see that as interaction potential, ε increases the slip length decreases. This decrease in slip length happens due to the increase in viscous effect at the interface, i.e. increase in interaction potential at the wall–fluid interface leads to the domination of wall–fluid interaction over fluid–fluid interaction in nanochannels.

FIGURE 2. Slip length variation to Interaction potential.

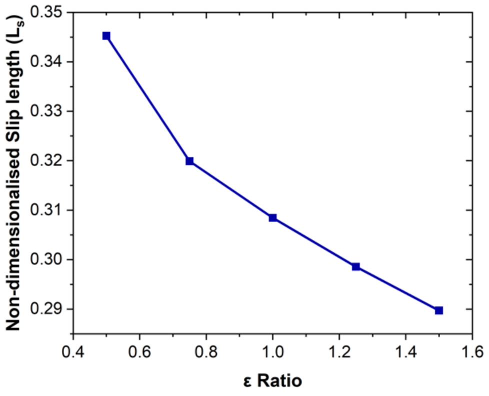
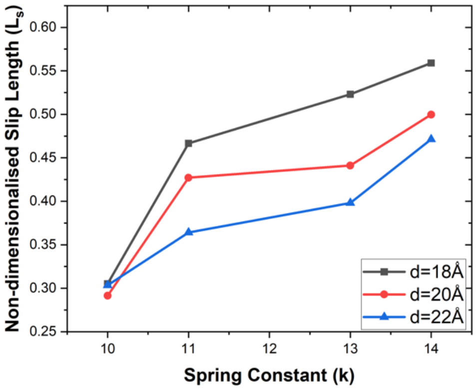


FIGURE 3. Variation in slip length when wall is made elastic.



Slip length variation is depicted in Figure 3 for various spring constant, k. Here in nanochannel, we apply the spring constant to the wall of the nanochannel. Depending on the value of the spring constant, the wall's rigidity changes, i.e. when there is a decrease in the spring constant, the wall's rigidity reduces and energy transfer increases. Figure 3 represents this variation, and it is found that slip length decreases as the value of spring constant, k decreases. So we could say that when the rigidity of the wall reduces, i.e. when the wall becomes flexible, the slip length increases.

In a further study, we know that when k is greater, the wall becomes stiffer. The atom's oscillation will be less, but when k is small, the atoms oscillate more, and fluid atoms have more possibility to approach the wall closely, which leads to the reduction in slip.

CONCLUSION

Molecular dynamics (MD) simulations of Ar–Pt nanochannel system were studied by varying interaction potential at fluid–solid interfacial region and the spring constant i.e. making the wall elastic. The variation in slip length in each scenario is achieved. The slip length increases when the interaction potential is less and vice versa. Similarly, when the wall becomes elastic, the slip length reduces. The results highlights the importance for both interaction potential and wall elasticity in nanoscale fluid flow. This manipulation of slip can get used in nanofiltration as electro–osmosis velocity can be enhanced with improvement in slip.

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