

Equilibrium Molecular Dynamics Investigation of Fluid Slip in Nanoscale Channels

Mathews Daniel^{1*}, Jeetu S Babu²

¹Department of Mechanical Engineering, Amrita Vishwa Vidyapeetham, Amritapuri, India.

²Department of Mechanical Engineering, Amrita Vishwa Vidyapeetham, Amritapuri, India.

Abstract

Interfacial hydrodynamic slip is an important factor while considering fluid flow through nanochannels. Various studies have been done both in NEMD and EMD to study the fluid slippage over solid surface. Molecular Dynamics Study of Fluid Solid Interfacial Slip and its Effect on Aerodynamic Drag[1] is one such example where dependence of slip and the drag properties are studied. In this paper we try to examine different types of surface roughness affects the fluid slip with MD simulation of poiseuille flow.

1. Introduction

The understanding on the flow of a fluid confined in a nano channel is important for the design of a micro/nano fluidic device[2]. Modern day NEMS, MEMS have small sizes in the order of nano or micrometer compared to contemporary systems. These systems have coexisting domains like fluid, electrical, magnetic etc. In order to model such systems we need to understand the basic physics at nanoscale where continuum concept is not valid. Molecular Dynamics (MD) is a competent tool to model such systems.

In the present study we investigate the fluid-solid interfacial slip in nanoscale channels with the help of MD simulations. Simulations in MD is of two types, Equilibrium Molecular Dynamics(EMD) and Non Equilibrium Molecular Dynamics (NEMD). Conventional method used to find the slip length or other transport phenomena is by NEMD where we assume the initial position and velocity. Main drawback of NEMD simulation is that it gives large error at low pressure gradient.[3]

Another method in MD to calculate slip length is by Equilibrium Molecular Dynamics method, where we first calculate the fluid-solid interfacial friction coefficient using Green Kubo relations and from which we can predict the slip length [4]. Several works exist in the literature which investigates the fluid-solid interfacial phenomena in nanoscale[5]. In the present work we demonstrate a practical approach to manipulate slip length in nanoscale channels by varying the surface roughness of the channel. In the next section we outline the MD methodology to simulate nanoscale nanoscale flows and the following section outline the major results obtained.

2. Methodology

Our present work is done using Molecular dynamics using an open source software called LAMMPS[6] and visualized using OVITO[7]. For the analysis we initially define a region in which atoms are defined. The system is designed for poiseuille flow so that both walls remain stationary during the flow. We assume the system of a boundary and flowing region.

Boundary wall and the flowing region is filled with Platinum and Argon atoms respectively since Argon-platinum system are widely used for the study.

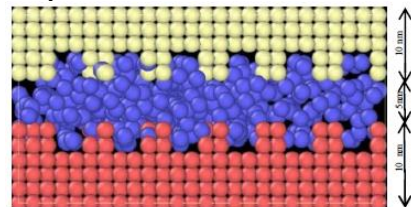


Fig. 1: Schematic diagram of simulation box

Simulation system is defined with a dimension of 50×50×32 Å. In the present study we aim at the dependence of asperities in the slip length for different diameters of flow. The asperities are of square shape of 4 Å and we change the spacing between the asperities and find out the variation of slip length for different diameters also.

Table I: Lennard jones potential used

| Atom type | E(Kcal/mol) | σ(Å) |
|-----------|-------------|--------|
| Ar- Ar | 0.120183 | 2.475 |
| Ar- Pt | 0.238 | 3.04 |
| Pt-Pt | 0.042281 | 2.7575 |

Slip of the fluid flow in the system is calculated using EMD method. Kannam *et. al.* has explained in detail about the the steps for finding the slip length from the transport coefficient[8].

$$\gamma = \int_0^{\infty} \langle A(t)A(0) \rangle dt \quad (1)$$

Taking the autocorrelated and cross correlated function of velocity and force and taking the Laplace of the convolution function we get as

$$CuFx(s) = -\zeta(s)CuU(s) \quad (2)$$

On solving the above equation we get the friction coefficient and dividing over the viscosity we get the slip length.Hence the steps to undergo in the problem is [9]

1. Initially setup the simulation box with given dimension

- with flow and boundary region.
- Find the velocity and Force exerted on atom by the neighbouring atoms for large timestep.
 - Find the autocorrelated and cross correlated function from the velocity and force of atoms.
 - Calculate the Laplace of the correlated function to compute the friction coefficient.
 - Using curve fit we find the interfacial friction coefficient.
 - Dividing the shear force with interfacial friction coefficient we get the slip length
 - Repeat the step 2 to 6 for different initial velocity values

3. Results

In this study we have investigated the effect of varying the fluid-solid interfacial interaction, channel width and the number of surface asperities.

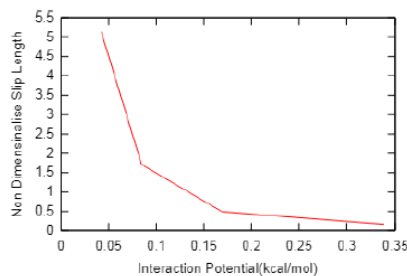


Fig. 2: Variation of slip length with fluid solid interfacial interaction for a 10 Å diameter channel

Figure 2 shows the variation of slip length in a channel of width 1 nm with respect to the Ar-Pt Interaction Potential. We have seen that the slip length decreases with increasing interaction Potential. This is mainly because as the interaction energy increases viscous effects are damped, which will result in improved slip length. Thus we can adjust the slip length by changing the interaction potential. In this study we have also investigated the effect of varying the fluid-solid interfacial interaction, channel width and the surface roughness present in the nanochannel on the slip length. Figure 3 shows the variation of slip length for 10 Å, 15 Å, 20 Å diameter channels with respect to surface roughness.

It can be seen that as the surface roughness is increased slip length is found to increase initially and then decreases. Initially the slip length increases because at higher surface roughness the cavity increases the viscous dissipation reducing the slip length. As the surface roughness is further reduced, presences of sperities are not felt thereby increasing the slip length.

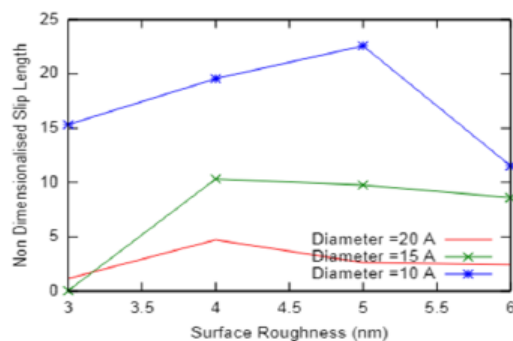


Fig. 3: Variation of slip length for 10 Å, 15 Å and 20 Å diameter channels with respect to surface roughness

As the diameter of the flow domain is increased the slip length is reduced which can be used for the further study.

4. Conclusion

Size of the electronic equipment are getting smaller and smaller by day there by reducing the space constraint. In the present study we have found the slip length variation which is a factor of transport properties varies with the varying diameter. We have also examined the variation of flow properties for various surface roughnesses. Results of the present study can be further expanded for the far reaching results. With the help of MD simulations it is found the dependence of asperities on the slip length for Argon fluid flowing through solid wall of fixed diameter. This system can be extended further for the understating of the behavior of materials at nanoscale.

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