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# A molecular dynamics study of fluid flows through slit-like nanochannels using two different driving systems

**Masoud Darbandi**[1]
darbandi@sharif.edu

**Rasool Khaledi-Alidusti**[2]
rasool.khaledi@gmail.com

**Moslem Sabouri**[3]
sabouri.moslem@gmail.com

**Hossein Reza Abbasi**[4]
hosseinreza.abbasi@gmail.com

Center of Excellence in Aerospace Systems
[1, 3, 4] Department of Aerospace Engineering, Sharif University Of Technology
[2] Department of Mechanical Engineering, Sharif University Of Technology
Tehran, P. O. Box 11365-11155, Iran

## ABSTRACT

The Poiseuille flow through slit-like nanochannels is investigated using the nonequilibrium molecular dynamics simulations. To drive a dense flow through the channel, we use two self-adjusting vertical plates strategy. These plates force the liquid to flow through the nanochannel under adjustable inlet and outlet boundary conditions. Comparing with the dual-control-volume grand-canonical molecular dynamics method, the current strategy provides many advantages. The current strategy does not need particle insertion and deletion, therefore, the system dynamics would not be affected at all. Moreover, the number of particles in the simulation system is fixed due to inserting the two self-adjusting vertical plates at the two ends of the nanochannel. The motion of these plates are controlled using a combination of an externally applied force and an internal force produced by the molecules in the system. Using this strategy, we study the transport of liquid argon and oxygen through a few slit-like nanochannels having different sizes. We benefit from the nonequilibrium molecular dynamics (NEMD) strategy in our simulations. To expand our study, we consider different back pressure implementations in the flow through the nanochannel. The current results are eventually compared with those derived by applying a uniform driving force method and their advantages are described.

**Keywords** Molecular dynamics, NEMD, Slit-Like nanochannels, Poiseuille flow

## 1 INTRODUCTION

In recent years, there has been an increasing interest in simulating fluid flow in nanoscale and microscale channels to study the transport of particles in microscopic scales. Since the size of an atom is in the order of $10^{-9}$m, it is comparable to the characteristic length of nanochannels and perhaps the dimensions of nanoflow systems. In such small scales, there is no way except treating the motion of atoms, as discrete collections of atoms rather than a continuous fluid flow stream. Indeed, the Navier-Stokes equations can be used to treat the poiseuille flow in nanochannels having diameters 10 molecular diameters larger than this limit. The molecular dynamics (MD) is a suitable method to simulate fluid flow through nanoscale and microscale channels. The investigation in the behavior of fluids in nanoscale channels, such as nano-slits, has a very important position in both industrial and medical nanoscience applications. Some examples are channels for the transportation of molecules and ions, nano-pumps, sensors, and so on [1].

The behavior of fluids in nanofluidic devices is very different from the corresponding behavior in microscopic and macroscopic channels. A number of studies has investigated various aspects of such behaviors for different types of fluid in various types of nanoscale and microscale channels. There are several important nonequilibrium molecular dynamics (NEMD) techniques to simulate fluid flow in nano and microchannels. These methods have their own advantages and disadvantages. A critical issue in these simulations is to measure the degree to which a nano-pore, is influenced. So, various forms of carbon nano-tubes have been recently collected and reviewed to achieve this goal [2].
A common boundary condition in MD method is the periodic boundary condition. When, we use the periodic boundary condition at both ends of a nanochannel, the downstream and upstream ends are connected directly and it causes some unrealistic interactions between them. In reality, the upstream and downstream ends should not be connected, and the particles inserted in the upstream should not have any


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information from past interactions. Therefore, one task for researchers is to eliminate such deficiencies.

A common method to simulate the fluid flow is to employ a constant gravitational force field [1]. Most of researchers use the gravity-fed flow strategy. Another widely method is to use the dual-control-volume grand-canonical molecular dynamics (DCV-GCMD) [3,4]. Comparing with them, the implementation of our method is simpler and it is computationally inexpensive. It is because, we are not to insert extra fluid particles in the system and that we do not need any reservoir. However, the current method is favorable only for the planar shapes or at least physically uniform geometries stretched in the flow direction. This restricts the application of the current method. We have to find the magnitude of the applied force using a trial and error procedure for each specific situation. This force magnitude seriously affects the fluid velocity through the channel. Generally, the periodic boundary condition is applied in flow direction while this type of boundary condition is unrealistic. To resolve this matter, we can use inserting-and-deleting algorithms, e.g., USHER, reflecting particle method (RPM), DCV-GCMD, and so on [5,6]. The DCV-GCMD method uses a chemical potential to drive the particles. This method is a hybrid algorithm consisted of MD and the grand canonical Monte Carlo (GCMC) methods. Two control volumes (CVs) are located at each end of the system and each CV is maintained at a chemical potential using GCMC. The dynamics itself is solved by the MD scheme. After each time step in MD, a certain number of GCMC steps are taken to insert or delete particles in each CV. Consequently, the fluid particles are transported in the channel by the chemical potential gradient. The necessary number of GCMC steps to maintain the constant prescribed chemical potential is determined by some trial runs. This number becomes extremely large in simulating the dense fluid systems because finding a new position for inserting a newly created particle becomes very difficult. If we simulate a system with polyatomic molecule, this matter becomes more severe. In these situations, the computation of the DCV-GCMD becomes very expensive. The disadvantages of DCV-GCMD method make a disruption to the system dynamics that are normally created by inserting or deleting particles from the control volumes. So, the deleting and inserting methods are useful for low density fluids, otherwise they are very expensive. Therefore, we cannot use this method in most simulations.

There are some reports on MD simulations in which the DCV-GCMD method is improved and that the disruptions matter is resolved. One of them uses one molecular reservoir with a constant high pressure at one end instead of inserting two reservoirs at the two ends. This makes a constant pressure gradient along the channel. The pressure in the reservoir is maintained constant by controlling the number of molecules right there. When a molecule enters into the channel, a new molecule is inserted at a special location, where the minimum potential energy fluctuation is generated. If a molecule returns back, another molecule is deleted randomly [5]. So, the pressure in the reservoir remains approximately constant. Therefore, this method is less expensive than the DCV-GCMD method and makes less disruption to the particles in the system. Another choice uses two self-adjusting vertical plates to keep the number of particles participated in the simulation system constant. Two plates are located at the upstream and downstream of the nanochannel and their motions are controlled by a combination of an externally applied force $(P_f, P_b)$ and an internal force, produced by the molecules in the system [5]. Indeed, the constant pressure gradient along the channel is established in this method by correct implementations of these two self-adjusting plates automatically. This method resolves the disruption matter in the system.

From another perspective, the fluidized piston model is a new method, which enables the microfluidics and nanofluidics users to drive a hydrodynamic dense polyatomic fluid using the MD and imposing a pressure gradient. Additionally, the computational cost is relatively low [6]. Using the method of local external field, the fluid in the upstream region acts as a fluidized piston (FP) that continuously presses and supplies the downstream fluid. The fluid in the sampling region is driven by the pressure from the upstream site. In this method, the periodic boundary condition is not used in the flow direction.

The analytic results for (incompressible) Poiseuille flow can be summarized in a few sentences. Assuming the no slip and uniform state variables for density and temperature, the streaming velocity of the flow in the pores can be obtained by solving the Navier–Stokes equations as follows [7]:

$$v_x(y) = -\frac{\rho g}{2\eta}(y^2 - \alpha^2) \qquad (1)$$

where ρ and η are the density and viscosity of the fluid, respectively, and α represents the half-width of the slit-like channel.

## 2 SIMULATION CONDITIONS

We benefit from the molecular dynamics method [7,8] in our simulations. In the molecular dynamics simulation, the dynamics of system are obtained in a deterministic manner by numerically solving the equations of motion for the atoms (or molecules). The forces acting on each molecule are derived from the potential energy function that describes the interaction energy of the atomic system. Molecular dynamics simulation is a powerful tool to be used for solving the classical equation of motion for many-body systems. It has been successfully used to simulate fluid flow in channels.

In this simulations, the oxygen–oxygen intermolecular force is modeled by a harmonic oscillator model. The interactions between other atoms are modeled using the Lennard-Jones (LJ) 12-6 potential as follows:


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$$V_{LJ}(r) = 4\varepsilon[(\sigma/r)^{12} - (\sigma/r)^{6}]. \quad (2)$$

The chosen parameters are listed in Table 1. The cut-off distance for the Lenard-Jones potential is taken to be 2.5 σ.

**Table 1. The chosen Parameters for the Lenard-Jones potential.**

| Pair of atoms | σ($\dot{A}$) | ε(kJ $mol^{-1}$) |
|---|---|---|
| Ar-Ar | 3.350 | 1.197 |
| O-O | 3.110 | 0.4529 |

In this paper, we use uniform driving force method and vertical adjustable plates to simulate flow for liquid argon and oxygen. We compare the results obtained for different sizes of nanoscale and microscopic channels in Table 3.

For each molecule on the wall, a stiff Hookean spring connects it to the lattice position using a potential of

$$\emptyset_{spring} = \frac{1}{2}K_w R^2 \quad (3)$$

where $K_w$ is the stiffness of spring and R is the distance of the wall atoms from their lattice sites. To keep the displacement of wall atoms at low level, we choose a large constant stiffness.

The intermolecular interaction in an oxygen molecule is defined by a harmonic vibration model. The equilibrium diatomic bond length is taken as 1.208 $\dot{A}$, and the force constant is selected to be 1178 (J $m^{-2}$) [6].

**Table 2. The details of employed boundary conditions.**

| Case | B. C. type | Force Magnitude ($\times 10^{17}$ $N/mol$) | External force($P_f, P_b$) ($\times 10^{17}$ $N/mol$) |
|---|---|---|---|
| a | Uniform driving force | $1.0\times10^{-6}$ | --- |
| b | Vertical adjusted plate | --- | ($6.0\times10^{-4}$,- $3.0\times10^{-4}$) |

**Table 3. The chosen test cases.**

| Case | Fluid | B. C. detail | Channel dimension($\dot{A}$) | fluid particles (#) | wall atoms (#) |
|---|---|---|---|---|---|
| 1 | Ar | a | 131×26.2 | 198 | 790 |
| 2 | $O_2$ | a | 131×26.2 | 180 | 790 |
| 3 | Ar | a | 186×37.45 | 414 | 1122 |
| 4 | $O_2$ | a | 186×37.45 | 336 | 1122 |
| 5 | Ar | b | 131×26.2 | 1190 | 940 |
| 6 | $O_2$ | b | 131×26.2 | 1347 | 940 |

The equation of motion is solved using a time step of 0.1 fs. The calculation is stopped after 30,000,000 steps, and the data is sampled after 1,000,000 steps. Only the temperature of channel walls is controlled with scaling thermostat imposing a target temperature of 77 K to prevent any phase change chance in the fluid.

Figure 1, shows the snapshot of channel in case 4. The flow is in the x direction. The Channel walls are constructed from 3 layers, having properties similar to the fluid.

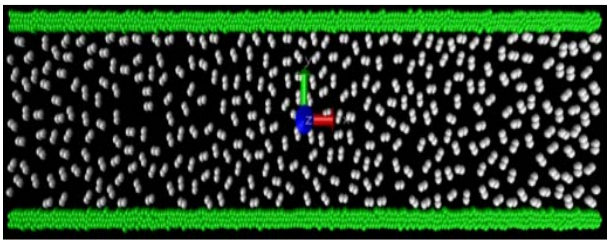

**Figure 1. A snapshot of channel, case 4.**

## 3 RESULTS AND DISCUSSION

We study the transport of liquid argon and liquid oxygen separately inside a few nanochannels having various sizes. The


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atomic construction for argon and oxygen is different. Oxygen consists of two simple atoms connected by a bond, however argon is a monatomic molecule. Of course, the atomic properties for the wall atoms are considered to be the same as those of the fluid, but considering a large number density to prevent fluid particles to penetrate out.

The atomic mass of oxygen is larger than that of argon. In this study, we considered the force that is necessary to accelerate the oxygen particles faster than the argon particles. However, these conditions do not lead to the same average streaming velocity because the friction drag created by the interactions between the particles, is not unique for different fluid choices.

Figurs 2 to 4 show that the velocity for argon flow is larger than that of oxygen. Therefore, the friction drag for argon particles is less than that of the oxygen particles. The average velocity for the argon flow is 99.5 m/s for Case 1 and that of the oxygen is 33.5 m/s for Case 2.

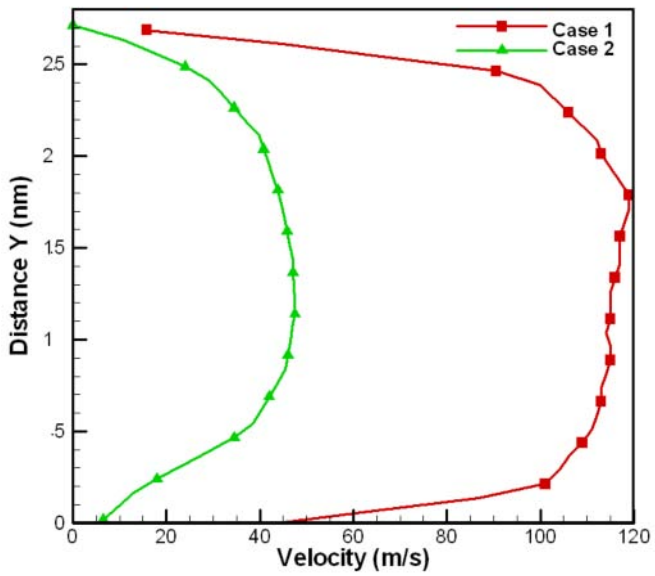


**Figure 2. Comparison of the bulk axial velocity at the mid-channel section, cases 1, 2.**

Figure 3 shows that the velocity increases as the channel height increases. The average velocity for argon is 110 m/s in Case 3 and the average velocity for oxygen is 72 m/s in Case 4. It means that increasing the channel height, the difference between the mean velocity for the two argon and oxygen flows decreases.

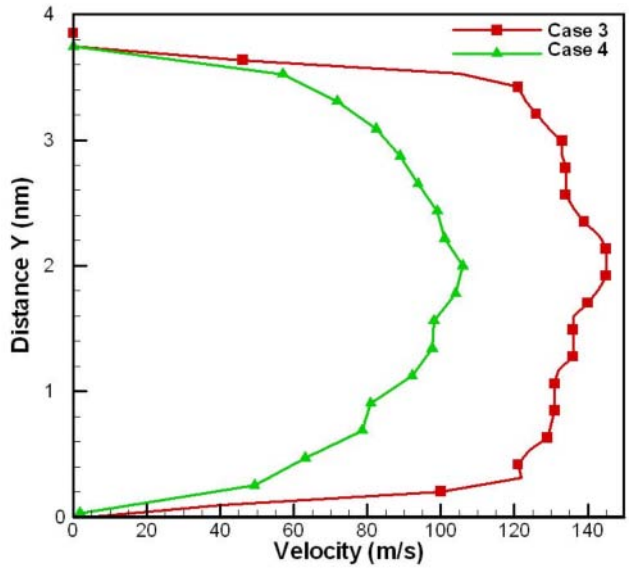


**Figure. 3. Comparison of the bulk axial velocity at the mid-channel section, cases 3, 4.**

Figure 4 shows the results for the fluid driven by vertical adjustable plates modeling. The results show that the choice of correct external force implementations, results in similar conditions for the two methods are almost unique.

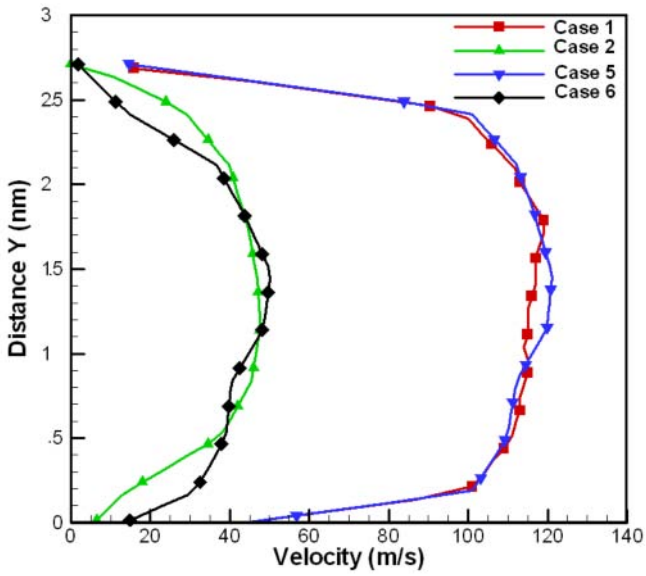


**Figure 4. Comparison of the bulk axial velocity at the mid-channel section, cases 1, 2, 5, 6.**

As a result, the velocity in a complex molecule such as liquid oxygen molecule is less than that of a monatomic molecule, such as argon. It is because the friction drag for monatomic molecules is less than that of the polyatomic molecules. This means that the interaction between molecules for the monatomic molecules is less than that of polyatomic


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molecules. Moreover, the decrease in interaction between the polyatomic molecules is more than that between the monatomic molecules in case of increasing the channel height.

## 4 CONCLUSIONS

We studied the transport of argon and oxygen liquid molecules through different nanoscale slit-like channels imposing both uniform driving force and vertical adjustable plates methods. The advantages of uniform driving force method relative to the vertical adjustable plates method can be counted as a simpler method with less computation. However, its results are not totally realistic because the two downstream and upstream ends are connected directly. This causes imposing unrealistic conditions at the two ends. The velocity distribution for the cases with imposing the vertical adjustable plates method depends on the front and back force magnitudes. Eventually, it is more realistic to drive the nano flow through the nano-slits using vertical adjustable plates method althought the uniform driving force is computationally less expensive than that of another methods.

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