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SIMULATION OF HEAT TRANSFER IN NANOSCALE FLOW USING MOLECULAR DYNAMICS

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ABSTRACT

We investigate heat transfer between parallel plates separated by liquid argon using two-dimensional molecular dynamics (MD) simulations incorporating with 6-12 Lennard-Jones potential between molecule pairs. In molecular dynamics simulation of nanoscale flows through nanochannels, it is customary to fix the wall molecules. However, this approach cannot suitably model the heat transfer between the fluid molecules and wall molecules. Alternatively, we use thermal walls constructed from the oscillating molecules, which are connected to their original positions using linear spring forces. This approach is much more effective than the one which uses a fixed lattice wall modeling to simulate the heat transfer between wall and fluid. We implement this idea in analyzing the heat transfer in a few cases, including the shear driven and poiseuille flow with specified heat flux boundary conditions. In this method, the work done by the viscous stress (in case of shear driven flow) and the force applied to the fluid molecules (in case of poiseuille flow) produce heat in the fluid, which is dissipated from the nanochannel walls. We present the velocity profiles and temperature distributions for the both chosen test cases. As a result of interaction between the fluid molecules and their adjacent wall molecules, we can clearly observe the velocity slip in the velocity profiles and the temperature jump in the cross-sectional temperature distributions.

Keywords: Molecular dynamics, Nanoscale flow, Thermostat, Liquid-solid interface, Lennard-Jones potential

1 INTRODUCTION

The structure of fluid and solid molecules and their interactions are important issues in nanoscale flow studies. The molecular dynamics method is a powerful approach to investigate the interaction of solid and its neighboring fluid molecules in nanoscale flows [1-3]. Kim, et al. [1, 2] present a summary on recent developments in MD simulation of 2d nanoscale flows. As is known, the investigation on fluid and wall molecules interaction and the key parameters in these interactions are important issues in shear driven flows. Moreover, MD is known as a powerful tool in simulating fluids motion by assuming suitable potentials between the fluid molecules. It has provided capability to simulate flow with various physical conditions.

One main objective in this study is to introduce a new wall modeling, which enhances the capability of MD in simulating the transfer heat between solid and fluid molecules. In most past simulations, it is normal to apply the thermostat model to all fluid molecules in order to maintain the system in a thermal equilibrium. Recently, the thermostat models are applied to the wall molecules in order to maintain the system at thermal equilibrium; however, the constant heat flux condition has not been applied to wall molecules yet.

Advanced MD simulations mostly use wall molecules with a fixed lattice structure instead of diffusive or specular walls. Fixed lattice walls consist of molecules, which are fixed in their original positions and can interact with fluid molecules [4]. Kim, et al. [1, 2] examined the boundary conditions at wall-fluid interface using harmonic springs attached to their original positions. This allowed the wall molecules to vibrate. Their work was used in treating the shear driven flow. Because of imposing a constant shear in shear driven flows and because of imposing a constant body force in poiseuille flow, it is necessary to utilize a thermostat to dissipate the heat induced by these phenomena.

In this study, we use wall molecules with harmonic bonds to simulate the correct nature of thermal transport at the wall-fluid interface. Thermal oscillations of wall molecules cause a momentum and heat transfer to fluid molecules due to intermolecular interactions. We treat the walls as heat reservoirs to maintain the system at thermal equilibrium, so there is no need to apply a thermostat to fluid molecules to maintain the system at constant temperature during our MD simulations. In cases of shear driven flow, poiseuille flow, and constant heat flux flow, the energy conveyed to the fluid molecules is dissipated by the constant temperature walls.

This paper is organized as follows. We first present the interactive thermal wall model and the effect of bond stiffness and wettablity on temperature jump in shear driven flow study. Section 3 presents the interactive thermal wall model used in MD to simulate the poiseuille flow. In Section 4, we apply a constant heat flux to the solid wall. Finally, a summary of our findings and conclusions is presented.

2 SIMULATION OF SHEAR DRIVEN FLOW WITH CONSTANT TEMPERATURE WALLS

We simulate two-dimensional shear driven flow through a 7 *nm* width channel using MD. For the initial conditions, we assume the Maxwell-Boltzmann distribution for velocities to achieve the target temperature. Then the thermostat is applied to the wall molecules to transfer the heat from the walls. For interatomic interactions, we use the well-known, Lennard-Jones 12-6 interaction potential. The Lennard-Jones 12-6 potential is given by

$$V(r_{ij}) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right] \qquad (1)$$

where ε is the binding energy, r_{ij} is the distance between a pair of *i* and *j* molecules, and σ is the molecular diameter. The first term, which is positive, is the repulsive term. It causes repulsion to the molecules. The second term is the absorptive term, which causes an attraction between the molecules. The interaction force between a pair of molecules is given by

$$F_{ij} = -\frac{\partial V(r_{ij})}{\partial r_{ij}} \qquad (2)$$

The temperature of walls is set at 120 K and the number density ($\rho = \frac{NA}{\sigma^2}$) of the argon to $\rho = 0.8$ and that of the wall to 1. The temperature, in a 2d with N particle systems, can be defined through the average kinetic energy as follows:

$$T = \frac{m_f}{k_B N}\sum_{n=1}^{N}\frac{1}{2}\sum_{i=1}^{2}\frac{1}{2}\Big(v_{n,i} - \frac{1}{N}\sum_{m=1}^{N} v_{m,i}\Big)^2 \qquad (3)$$

where N is the number of fluid particles in the bin, k_B is the Boltzmann constant, and $v_{n,i}$ is the velocity of molecule n in the i(=x, y) direction [5]. The steady-state temperature profiles are time-averaged data sampled during the production run. For argon molecule, the molecular mass is m=40 *gr/mole*, the molecular diameter is $\sigma = 0.34\,nm$, and the binding energy is 10^4 *J/mole*. Intermolecular interaction forces are zero at a cut-off distance of $3\sigma = 1nm$. The top and bottom surfaces are moved in opposite directions with an overall speed of 100 m/s. The computational domain is shown in Fig. 1. The characteristic time is 2 *fs*. The periodic boundary condition is implemented at inflow and outflow sections as is described in Ref. [6]. The number of molecules for simulation is 835. Figure 1 also shows that three wall layers are considered at each wall.

Previous nanoscale MD simulations specify the velocity slip and temperature jump in nanoscale fluid as a function of the wall/fluid interaction strength, the density of fluid, and the shear rate. In our interactive thermal wall model, we have thermal oscillations on the wall molecules because of stiffness bonds and that it exchanges momentum and energy between the fluid and the wall.

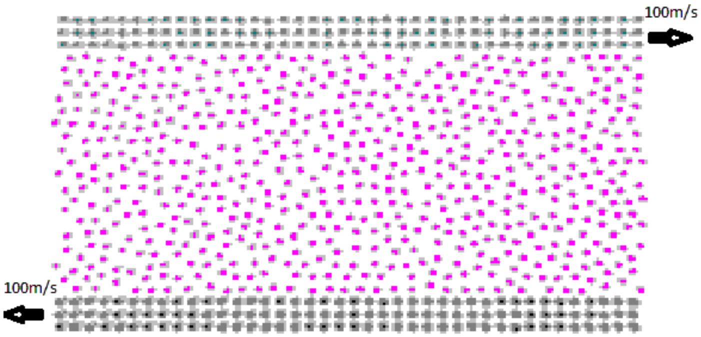


Figure 1. The simulation domain.

We use the velocity Verlet algorithm for the time integration as was used by Allen and Tildesley [7]. For finding the position and velocity of themolecules, we first calculate the intermolecular forces in each step. Then, by suitable integration, we obtain the position and velocity of each molecule. Each molecule can interact with other fluid molecules within the cutoff distance. The total forces used for a fluid molecule are obtained from

$$F_{fluid}(r_i) = \sum_{j=1}^{Nt}\frac{\partial V(r_{ij})}{\partial r_{ij}} \qquad (4)$$

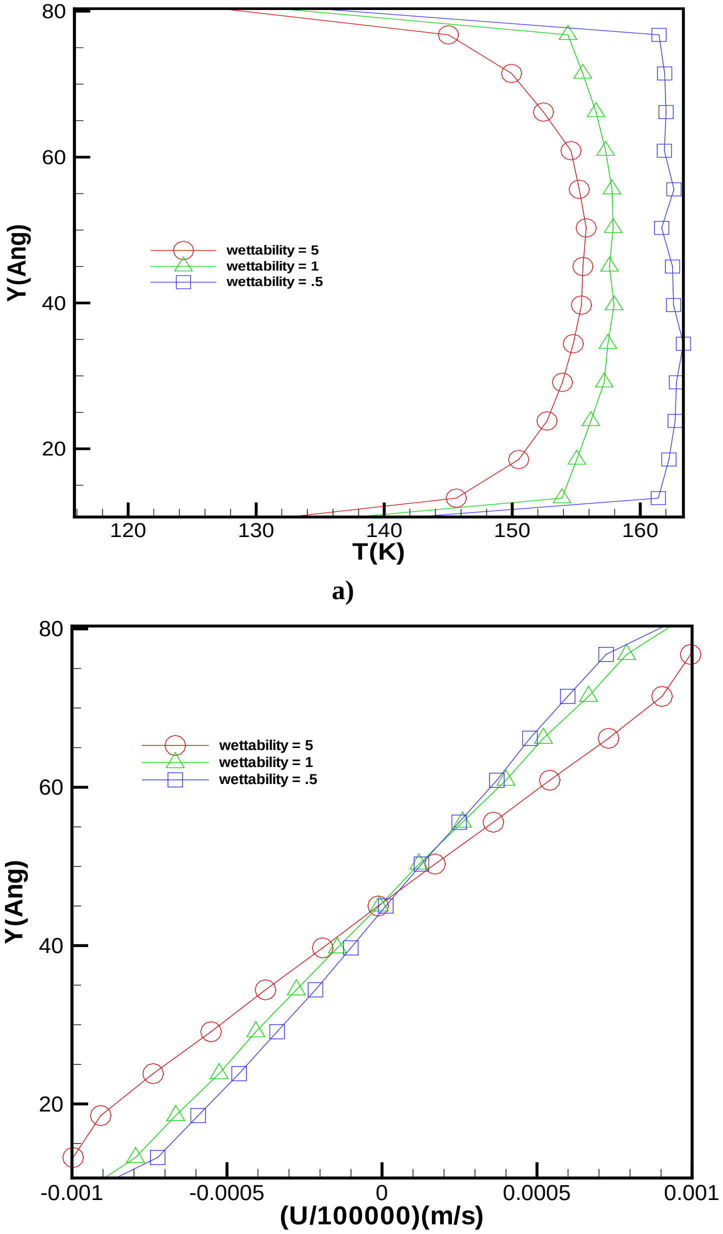
$$F_{solid}(r_i) = \sum_{j=1}^{Nt}\frac{\partial V(r_{ij})}{\partial r_{ij}} + K(|r_0 - r_i|) \qquad (5)$$

where K is the wall bonding stiffness and $|r_0 - r_i|$ is the distance between the original position and the current position of the wall molecule. Equation (4) is the force exerted on a fluid molecule by other fluid molecules and wall molecules, However, Eq. (5) is the force exerted on a wall molecule by other molecules and the connected springs. The ideal approach for thermal wall modeling is to construct a wall with infinite number of molecules, which is impossible due to its heavy computational cost. However, we want to simulate the thermal interaction of fluid molecules with wall molecules in a manner to benefit from the restrictive wall molecules for our modeling. For the interactive thermal wall model, we apply the scaling thermostat to each wall layer separately. At each time step, the scaling parameter modifies the thermal velocity, so we can obtain the target temperature in each layer. In our simulations, we impose three layers of wall molecules for wall modeling and set their temperature at 120 K. Because of the wall motion, heat is produced and the viscous heat is dissipated through the walls.

In the current shear driven nanoflow simulation, we use bonding stiffness of K=0.01$(gr/mole\,(fs)^2)$. The velocity profile and temperature distribution are shown in Fig. 2 for different rates of wettability $(\varepsilon_{wf} = \sqrt{\varepsilon_w \varepsilon_f})$. As is seen, the velocity profile is linear showing a slip at the wall and the temperature profile is parabolic performing a jump at the wall/fluid interface. The parabolic temperature distribution and the linear velocity distribution are quite expectable because the shear rate is constant in the entire domain in our simulation. Figure 2 also presents the velocity and temperature profiles for different wettability magnitudes. As is observed, the velocity slip and the temperature jump decrease as the wettability increases. This is because of increase in the interaction strength. An increase in the interaction strength shows a higher influence of wall molecules on the fluid molecules and this is why the velocity slip and temperature jump decrease. Heat is dissipated from the wall molecules because of imposing the thermostat model, and therefore imposing a strong wettability. We observe that a strong interaction between the fluid and wall cause a higher dissipation. As is seen in Fig. 2, there is a lower temperature magnitude for imposing a higher wettability condition. It is because of a higher dissipation rate there.

Figure 3 shows the velocity and temperature profiles for different bonding stiffness magnitudes. As the bonding stiffness increases the velocity slip and temperature jump increase as well. Imposing a high bonding stiffness magnitude, the dissipation is faded and the temperature jump increases at the fluid-wall interface.

Sampling is required to obtain the flow variables. In this paper, we use 1×13 grid for sampling. In other words, the simulation domain is divided in 13 sampling bins in the y direction. For each bin, sampling is based on the averaging on the atoms that crossed that bin over the sampling period. The simulation ran 100000 steps before the start of sampling.



a)

b)

Figure 2. Velocity and temperature profiles for different wettability magnitudes, K=0.01 (10^{-14} *gr/mole fs^2*)

3 POISEUILLE FLOW SIMULATION ON NANOSCALE WITH CONSTANT TEMPERATURE WALLS

In this section, we present the MD simulation results for treating the Poiseuille flow. The simulation domain is as the one in the previous section while the walls are stationary and that the wall temperatures are set at 120 K. We apply the interactive thermal walls and that liquid argon is in a condition with $\rho = 0.8$. In the streamwise direction, we apply the periodic boundary condition. To move the molecules in the flow direction, we impose body force to all inlet molecules. The magnitude of this force is 5.86× 10^{-7} ($10^3 N/mole\, fs^2$). The work done by this external force is converted into heat, which must be removed from the fluid through the channel walls to avoid a temperature raise. We use scaling thermostat for setting the temperature of walls at the target temperature. Figures 4 and 5 show the temperature and velocity profiles for the Poiseuille flow considering different rates of wettability and bonding stiffness, respectively. To finalize the velocity and temperature profiles, we use 13 slab bins that are parallel to the walls, similar to the previous section. The velocity and temperature values at each bin are calculated by averaging the data recorded for all the samples. The velocity profiles are parabolic and this is quite expectable for the Poiseuille flow. Similar to the previous section, Figure 4 shows that a high wettability magnitude can cause higher velocity slip and temperature jump magnitudes in shear driven flows.

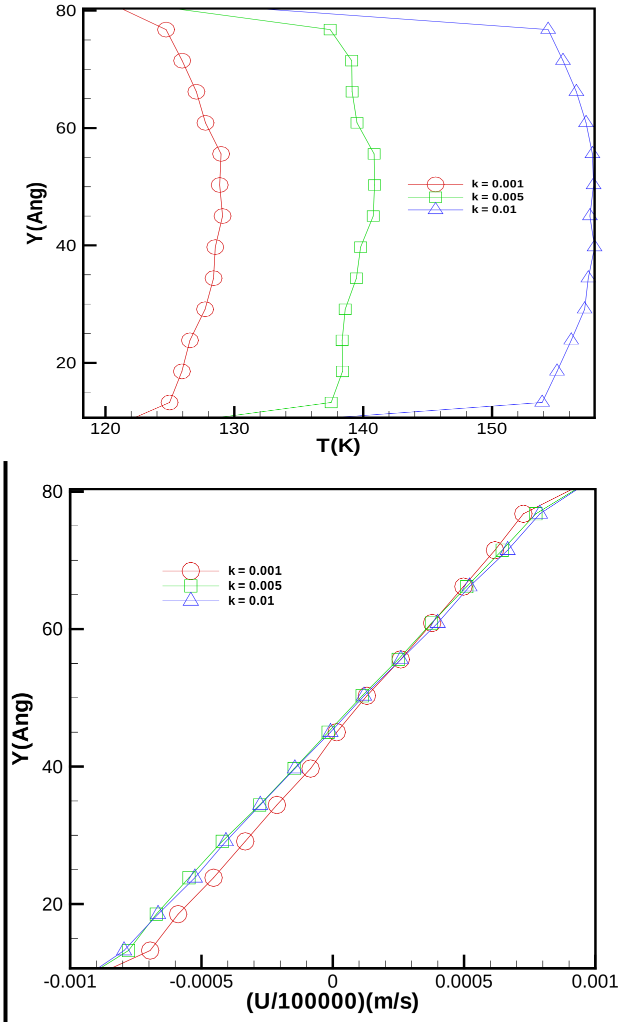
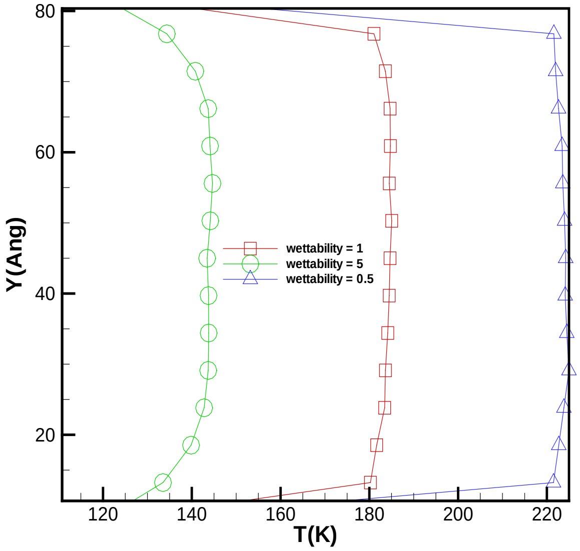
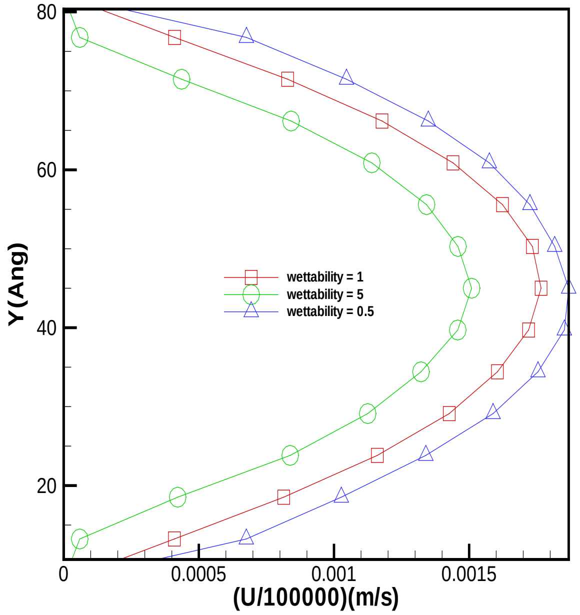


Figure 3. Velocity and temperature profiles for different bonding stiffnesses (10^{-14} *gr/mole fs*^{2}), $\varepsilon_{wf} = 1$.



a)Temperature profile

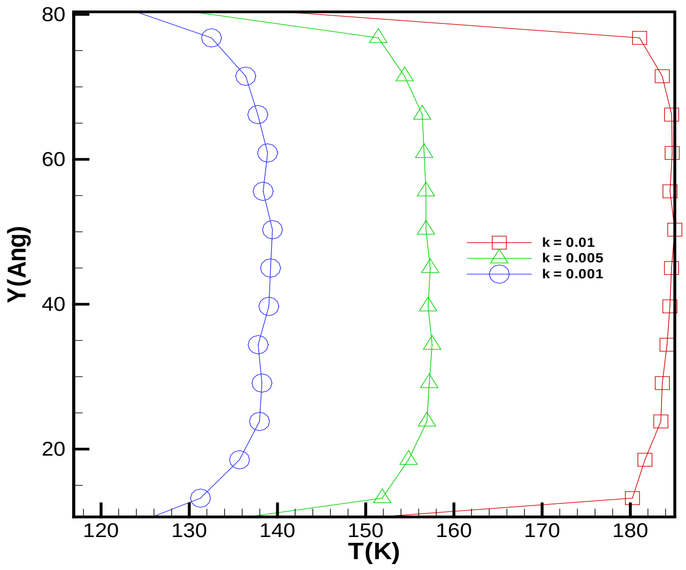


b)Velocity profile

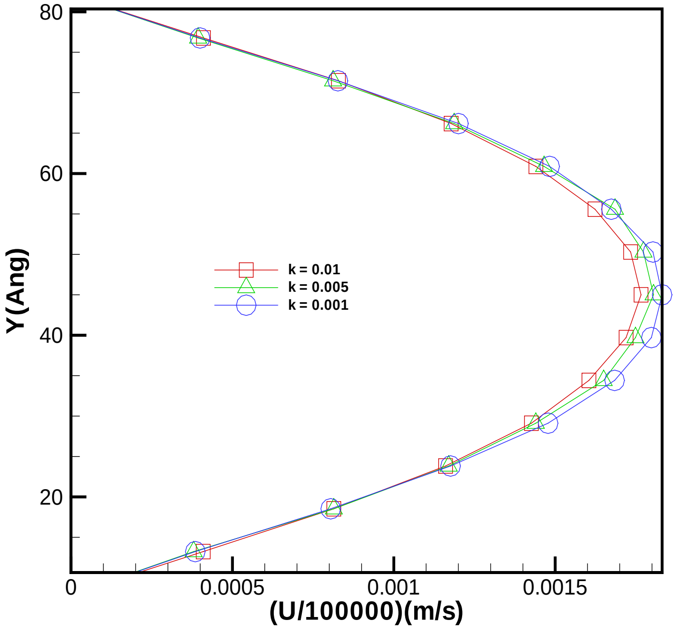
Figure 4. Velocity and temperature profiles for different wettability magnitudes, K=0.01, (10^{-14} *gr/mole fs*^{2}).

4 CONSTANT HEAT FLUX ON WALL

In this section, we provide the results of MD simulation for a flow confined between two parallel walls imposing a constant wall heat flux. The channel is shown in Fig. 1. As before, argon is chosen as the working fluid. The walls are stationary and the flow is periodic in the x direction. No force is applied to the fluid molecules and no moving walls are enforced. A heat flux is applied to the top wall and consequently a constant heat is transferred to the simulation domain. To dissipate the system energy, we apply the scaling thermostat to the bottom wall to maintain the bottom wall at a constant temperature of 120 K, which can dissipate the energy of the system. We apply constant heat flux at the wall. We have three layers in each wall; called as the top, middle and bottom layers.



a)temperature



b)velocity

Figure 5. Velocity and temperature profiles for different bonding stiffness magnitudes (10^{-14} *gr/mole fs*^{2}), $\varepsilon_{wf} = 1$

Calculating the temperature of bottom layer, we can set the temperature of middle and top layers as a function of the bottom layer temperature to achieve the target heat flux as follows:

$$T_{mid.\ layer} = T_{bottom\ \ layer} + \Delta T \tag{6}$$

$$T_{top\ layer} = T_{bottom\ \ layer} + 2\Delta T \tag{7}$$

where ΔT can be calculated considering the magnitude of the target heat flux. It is calculated from

$$q = \frac{1}{V}\left[\sum_{i=1}^{N}\left(v_i h_i + \frac{1}{2}\sum_{j=1,j\neq i}^{N} r_{ij}\left(F_{ij}.v_i\right)\right)\right] \tag{8}$$

where V is volume of the system, h_i is the total energy of molecule i, which includes the kinetic and potential energies, and F_{ij} is the force acting on the ith molecule from the jth one [2]. Figure 6 shows the variation of heat flux magnitude calculated on the top nanochannel wall during time step advancement. We present both the variation of heat flux with time for constant temperature and the constant heat flux cases to provide a better comparison for the proposed steady-state conditions of both the constant temperature and the constant heat flux cases.

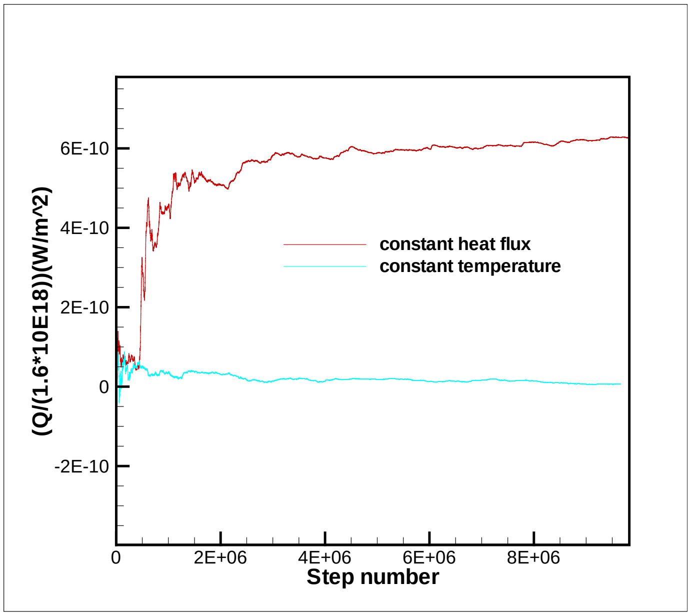


Figure 6. Variation of heat flux with time step number

Figure 6 also shows that there is a heat flux through wall in the first 2,000,000 steps in presence of a constant temperature wall. It is because of a temperature gradient between the wall and fluid molecules. However, the system shows zero heat flux after 2,000,000 steps. The figure also shows that a constant heat flux is obtained for the system after a large number of time steps. The total energy of the system will be constant because the constant energy that enters to the system is equal to the energy dissipated by the system due to a constant temperature wall enforcement.

5 CONCLUSIONS

We presented new thermal walls Nanoscale MD simulations. It can treatments for model the heat transfer in shear driven and Poiseuille flows more realistically. We applied thermal walls with thermostat to transfer the heat from domain. To simulate the thermal walls, we connected the wall molecules it resulted in to their original positions using springs. It resulted in a thermal oscillation to the wall molecules. The thermal oscillations in wall molecules enabled them to transfer heat into or out of the domain. Using this approach, we were able to dissipate the energy from the domain for shear driven flow, poiseuille flow and heat flux boundary. The results show that a strong interaction between the wall and fluid molecules (wettability) decrease the temperature jump and velocity slip at the boundaries. Because of the thermal wall effect on the fluid, we achieve desirable temperature profile for shear driven and poiseuille flows. Eventually, constant heat flux is applied as a boundary condition to the top wall of the channel.

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