Effect of bounding wall vibrations on a flow of simple fluid passing through flat nano – channels

Andrey K. Abramyan and Leonid V. Mirantsev

Institute for Problems of Mechanical Engineering, Russian Academy of Sciences, St. Petersburg, Russia

Abstract:

We present results of molecular dynamics simulations of a fluid flow in flat nano - channels of the width of the order of 10 molecular diameters and with vibrating walls. Both cases of crystalline and amorphous walls are considered. It is shown that these vibrations have an essential influence on the structure and the flow of the fluid. In particular, the vibrations of the walls with crystalline structure strongly enhance a positional order in the fluid and give rise to significant changes in the fluid flow rate. It is shown that a fluid flow through the flat nano-channel can be efficiently controlled by high frequency vibrations of one of the channel's bounding wall.

Numerous experiments that have been performed for the last two decades [1-3] revealed significant differences in static and dynamic behavior of fluid in micro volumes (10 or less molecular diameters in size) from the behavior predicted by the classic continual theories. Therefore, computer simulation methods, namely, molecular dynamics (MD) simulations [4-10], which take into account the atomic (molecular) structure of fluids, are extremely important for description of the fluid flow in nano – channels. However, up to now MD simulations of the fluid flow in such channels have been performed under the fixed bounding walls condition, i.e. at the constant channel cross-section. It is interesting to perform MD simulations of a fluid flow in nano-channels with vibrating bounding walls. First of all, such vibrations periodically change the distance between the bounding walls, and, as shown in [1-2],a structure of the fluid confined between two solid bounding surfaces displaced at a distance of the order of 10 or less molecular diameters from each other is essentially dependent on this distance. It means that the nano-channel wall vibrations can cause a periodical change in the structure of the confined fluid, and, therefore, in its viscous-elastic properties. Secondly, the wall vibrations can have a significant effect on the surface layer structure of the confined fluid, and, hence, on the molecular slipping effect near solid bounding surfaces, which is greatly dependent on the above mentioned structure [6,7]. Thus, inducing the nano-channel wall vibrations, we can control the fluid flow in the channel. Finally, the devices allowing to induce high-frequency ($10^9 - 10^{10}$ Gz) vibrations of the nano-channel walls have been recently developed [11]. In the present paper we report results of MD simulations of a model fluid behavior in flat nano-channels with vibrating walls. We have considered flat nano-channels with parallel bounding solid walls disposed at the distance of 10 - 20 molecular diameters from each other along **z** axis and infinitely extended in **x** and **y** directions. One of the walls was fixed and the other could vibrate along **z** axis. The fluid atoms could move freely in all three directions (x, y, z) and the bounding walls were assumed to consist of fixed atoms. For the solid walls with a crystal structure, the atoms were rigidly fixed in the face-centered cubic lattice sites. As for the amorphous bounding walls, the spatial positions of their constituent atoms were fixed in a random manner. Vibration of one of the bounding walls was simulated by purely kinematic oscillations of all its atoms along z-axis with the same amplitude and frequency. The interactions between the fluid atoms and between the fluid atoms and wall atoms were modelled by the well known Lennard-Jones pair potential [12] :

$$V_{ij}(r_{ij}) = 4\varepsilon[(r_{ij}/\sigma)^{-12} - [(r_{ij}/\sigma)^{-6}], \qquad (1)$$

where r_{ij} is a distance between atoms i and j, ε is their interaction constant, σ is the characteristic interaction length determining effective size of the interesting atoms. The motion of fluid particles was described by the Newton's second law, i.e

$$d^2\mathbf{r}_i/dt^2 = \mathbf{f}_i/m, \qquad (2)$$

where m is the i- th particle mass , and $\mathbf{f}_{ij}$ is the total force acting on it by the other fluid particles and wall atoms. It is equal to :

$$\mathbf{f}_i = \Sigma_j \, \mathbf{f}_{ij}\,, \qquad (3)$$

where $\mathbf{f}_{ij}$ is the force acting on i-th particle by j-th particle. It can be determined as:

$$\mathbf{f}_{ij} = \mathbf{-}\ \mathbf{(}\partial V_{ij}/r_{ij}\mathbf{)}\mathbf{e}_{ij}\,;\ \ \mathbf{e}_{ij} = \mathbf{r}_{ij}/r_{ij},$$

summing over $j \neq i$.. The system (the fluid and the solid channel bounding walls) was placed in a simulation box, which is a rectangular parallelepiped of 18 x 18 x 24 size in reduced length units usually used for MD-simulations [13]. The total number of the system particles was 5324. 4356 of them were the fluid particles, and 968 belonged to the bounding solid walls. The MD simulations were performed under periodical boundary conditions along x and y axes that was used to imitate the infinite dimensions of the system in these directions. The volume of the simulation box and the reduced temperature $T^* = K_B T/\varepsilon$, were constant. Here, T is the absolute temperature of the system, and K_B is the Boltzmann constant. The interaction constant ε in the potential (1) was assumed to be the same for the interaction between fluid atoms as well as for interaction between the fluid atoms and atoms of the solid wall, and it was taken as the unity (in the MD dimensionless energy units [12]). The characteristic interaction length σ in the potential (1) and the fluid atomic mass m in the equation (2) were also assumed to be the unity. For each i - th fluid particle, the equation (2) was integrated numerically by using the standard MD-simulation methods [13] with the time step $\Delta t^* = 10^{-3}$ in the same reduced MD - units.

First of all, we investigated an vibration effect of one of the channel bounding walls (the other bounding wall was fixed) on a structure of the confined liquid at rest (without flow). The reduced temperature T* of the system was taken as T* = 2, and the initial width of the channel was equal to about 14 σ. The amplitude A of vibration of one of the bounding wall along z axis was equal to 2σ and the corresponding period T was set to 40 t*, where $t^* = \sigma\varepsilon^{1/2}m^{1/2}$ is the reduced time unit used in MD simulations. It is easy to calculate that if σ is equal to the water molecular size (σ = 0.3 nm), m is the water molecular mass (m $\approx 3 \cdot 10^{-26}$ kg), and the absolute temperature of the system is equal to $T^* = 300$ K (the room temperature), the vibration period T corresponds to the frequency ~ $(2 - 8)\cdot 10^{10}$Gz. Fig.1 presents the density profile of the initial state (the bounding walls are fixed) of the fluid confined in the nano-channel.

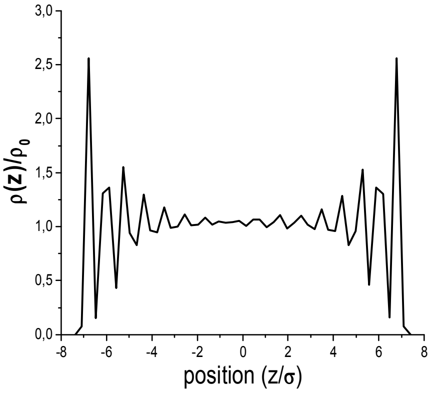

Fig.1 The relative fluid density profile within the nano - channel with fixed bounding walls

The figure shows that the fluid layer in the channel can be separated into three regions: two relatively small regions near the walls with the width of the order of 3σ, and one relatively large central region with the width ~ $8\ \sigma$. It is clearly seen that in the wide central region the fluid density is practically homogeneous (only slight oscillations around the average value of the density in the nano-channel are observed), but in the narrow regions near walls distinctive oscillations of the density can be observed. These oscillations indicate the existence of the layer structure with the translational order induced by the interactions between fluid atoms and the solid wall atoms located at the crystal lattice sites. It should be noted that the similar translational order near the solid walls regions was observed in the experiments performed by Israelashvili [2]. The existence of the wide central region in the nano-channel, where the translation ordered layering structure is not observed, suggests that the effect of the crystalline structure of the solid wall on the adjacent fluid decays very fast with the distance from the wall. This behavior is caused by the short range character of the intermolecular interactions used in our model, and due to this reason the positionally ordered regions near the walls do not overlap in the initial state of the fluid in the nano - channel.

Vibrations of one of the nano-channel walls along z-axis lead to the change in the structure of the confined fluid. The Fig. 2 shows two-dimensional xz projection of the fluid within the nano-channel after a quarter period from the oscillation's start at $A = 2\sigma$ and $T = 40\ t^*$. In this state the channel's width is minimum (12σ). The figure shows that in this state the thickness of the positionally ordered regions near the walls exceeds their thickness in the initial state, and the thickness of the central positionally disordered region decreases.

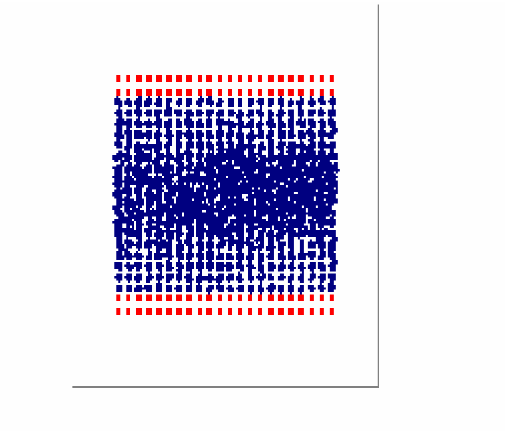

Fig.2 The lateral (xz) view at the fluid within the nano - channel after a quarter of the period of oscillations.

The same conclusion can be derived from the Fig. 3 which presents the corresponding density profile.

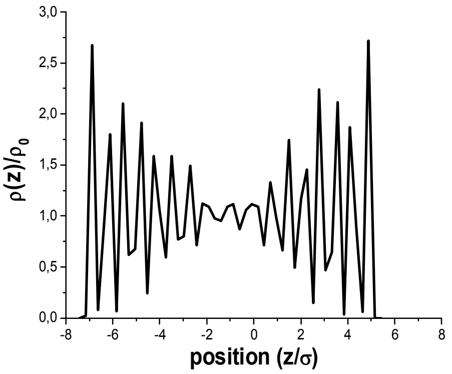

Fig.3 The density profile for the nano channel with one vibrating bounding wall corresponding to a quarter of the period of oscillations.

It is seen that in this case the width (~ 5 σ) of the regions near the walls exhibiting distinct maxima and minima of the density profile is approximately 2.5 times larger than the width (~ 2σ) of the central region demonstrating only minor oscillations of the density profile ρ(z) about its average value ρ_0. Perhaps, such change in the structure of the fluid can be attributed to the partial overlapping of the regions affected by the crystalline structure of the bounding walls. Nevertheless, it should be noted that the system under consideration is a dynamical system, and it exhibits retardation in the rearrangement of its structure. This retardation is distinctly illustrated by Fig's 4 and 5, which show the two-dimensional xz projection of the fluid within the nano-channel after three eights of the period from the oscillation's start and the corresponding density profile, respectively. Though the bounding wall is moving backwards at this moment when the nano – channel expands, the system's positional order is significantly stronger than that in the channel with minimum width (see Fig's 2 and 3).

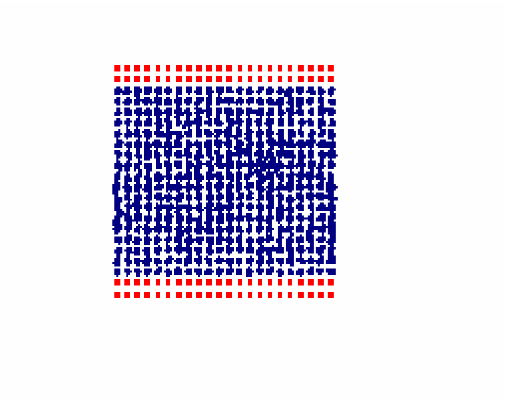

Fig.4 The lateral (xz) view at the fluid within the nano - channel after three eighth's of the period of oscillations.

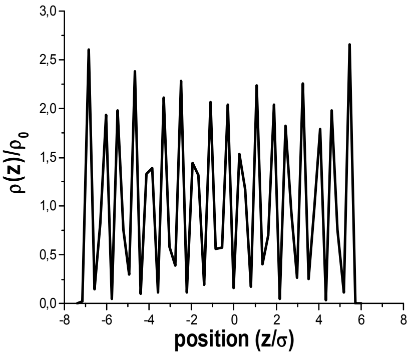

Fig.5. The density profile after three eighth's of the period of oscillations.

However, the further backward motion of the bounding wall leads to the decrease of the positional order of the fluid in the nano – channel. It is seen from the fluid density profile (Fig.6) obtained after three quarters of the period when the nano-channel width has the maximum (~16σ).

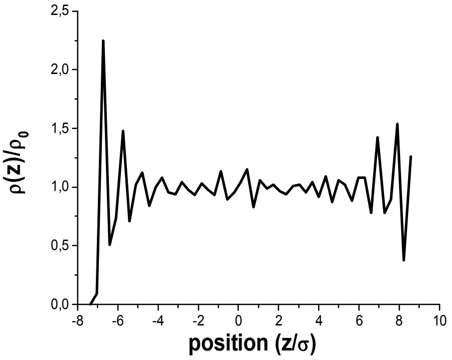

Fig.6 The relative density profile after tree quarters of the period of oscillations.

Firstly, the width of the disordered central region significantly increases (~10 σ), and, secondly, the fluid density oscillations in the regions near the walls (especially near the moving wall) are notably weakened.

The above-mentioned results evidence significant changes in the structure of the fluid within the nano-channel with one vibrating bounding solid wall. One can see that the motion of the wall leads to ether increase or decrease in the reduction of the positional order in the confined fluid. It was found that such significant changes in the structure of the fluid within the nano-channel with one vibrating wall is crucially determined by the crystalline structure of the solid walls contacting to the fluid. In particular, we performed MD-simulations of analogous behavior of the same fluid confined by the nano-channel of the same width. However, the layers of the bounding walls directly contacting to the fluid had an amorphous structure. Although, the atoms of these layers were positionally fixed, they were not located in the sites of the face-centered cubic lattice, but displaced in a random manner. The results obtained in this case are drastically different from the results described above, namely, the vibrations of the bounding walls with the amorphous layers contacting to the fluid caused only the changes in the nano - channel's width, and, hence, the corresponding changes in the fluid density. No qualitative changes in the structure of the fluid were observed. The results obtained show that vibration of a flat nano-channel solid wall causes significant changes in the structure of the confined fluid, and, therefore, these vibration should lead to significant changes in effective viscoelastic properties of the fluid. Thus, these vibrations should have a significant influence on the fluid flow passing through the nano-channel caused by external pressure (Poiseuille flow) and change its characteristics, for example, the fluid flow rate. In order to check it we performed MD-simulations of the Poiseuille flow through both the nano-channel with two fixed bounding walls and the nano-channel with one fixed wall and one vibrating wall. The fluid flow passing through channels was induced as in [4-10] by some constant force equal to 0.1 (in the MD dimensionless unit system [12]) and parallel to the x-axis and applied to the each fluid particle. Otherwise, the simulation procedure was absolutely the same as described above. The main characteristic of the flow was assumed to be the rate of the flow through the nano-channel averaged over the double period of the wall vibration. It was found that the averaged flow rate for the nano-channel with one vibrating wall was only ~13% percents smaller than that for the nano-channel with the fixed walls. It can be explained by the fact that the significant increase of the effective fluid viscosity in the nano-channel during the first half of the wall oscillation period(compression of the channel) is essentially compensated by the decrease of the effective fluid viscosity during the second half of the vibration period (expansion of the channel). However, the compensation is not complete due to, perhaps, a certain time retardation in the viscoelastic properties of the fluid. We also performed simulations of the fluid flow in the nano-channel with one bounding wall vibrating in such a manner that its width either reduces or increases. The amplitude and the period of such vibrations were the same as in the above described case of the harmonic vibrations. It was found that in the first case, when the channel width reduces, the average flow rate was about 6.7 times smaller than it was for the channel with fixed walls, whereas in the second case (the channel width increases) the flow rate was approximately 1.81 times larger in comparison with that for the channel with fixed walls. It is obvious that, for the oscillations reducing the channels width, the positional order in the fluid near the walls is enforced, and, consequently the fluid effective viscosity increases, whereas, for the oscillations resulting in an increase of the channels width, the positional order is weakened in the fluid layers adjoining the bounding walls, and, hence, the effective viscosity of the fluid confined within the channel decreases. Thus, switching from one type of a boundary wall vibrations to another, one can change the average flow rate through the nano - channel in about 12 times. In other words, a fluid flow through the flat nano-channel can be efficiently controlled by high frequency vibrations of one of the channel's bounding wall.

References

[1] J.N.Israelashvili, P.M McGuiggan., A.M. Homola. “Dynamic properties of molecularly thin liquid films”.Science, 240,189-191 (1988).

[2] J.N. Israelashvili. “Intermolecular and surface forces”.2nd edn., New York, Academic Press, 1992,300.

[3] O.I. Vinogradova. “Slippage of water over hydrophobic surfaces”. Int.J.Miner Process, 56, 31 (1999).

[4] P.A. Thompson and M.O.Robbins. “Shear flow near solids: epitaxial order and flow boundary conditions”. Phys.Rev.A, 41, 6830 (1990).

[5] J. Koplik, J.R. Banavar.,and J.F. Willemsen. “Molecular dynamics of fluid flow at solid surfaces”. Fluids A., 1, 781 (1989).

[6] L. Bocquet and J.-L. Barrat. “Hydrodynamic boundary conditions, correlation functions, and Kubo relations for confined fluids” .Phys.Rev.E., 49, 3079 (1994) .

[7] J.-L. Barrat and L.Bocquet. “Large slip Effect at a nonwetting fluid – solid interface”. Phys Rev. Lett., 82, 4671 (1999).

[8] M. Cieplak, J. Koplik, and J.R. Banavar. ”Boundary conditions at a fluid – solid interface”. Phys Rev Lett., 86, 803 (2001)

[9] N.V. Priezjev. ”Rate – dependent slip boundary conditions for simple fluid”. Phys Rev. E. 75, 051605 (2007).

[10] A.S. Ziarani and A.A. Mohamad. “A molecular dynamics study of perturbed Poiseuille flow in a nanochannel”. Microfluid Nanofluid.2,12 (2005).

[11] D. Garcia-Sanchez, A. San Paulo et all.. “Mechanical detection of carbon nanotube resonator vibrations”. Phys Rev Lett. 99,085501 (2007).

[12] M.P. Allen and D.J. Tildesly. “Computer simulations of Liquids”.(Claredon, Oxford, 1989).