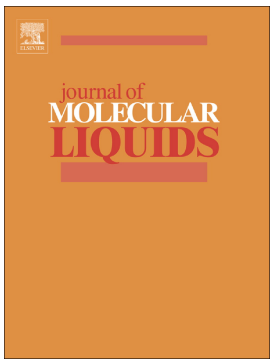
Journal Pre-proof




# Effects of surface roughness with the spherical shape on the fluid flow of Argon atoms flowing into the microchannel, under boiling condition using molecular dynamic simulation

Yeping Peng, Majid Zarringhalam, Azeez A. Barzinjy, Davood Toghraie, Masoud Afrand

PII: S0167-7322(19)33014-4

DOI: https://doi.org/10.1016/j.molliq.2019.111650

Reference: MOLLIQ 111650

To appear in: *Journal of Molecular Liquids*

Received date: 27 May 2019

Revised date: 19 July 2019

Accepted date: 26 August 2019

Please cite this article as: Y. Peng, M. Zarringhalam, A.A. Barzinjy, et al., Effects of surface roughness with the spherical shape on the fluid flow of Argon atoms flowing into the microchannel, under boiling condition using molecular dynamic simulation, *Journal of Molecular Liquids*(2019), https://doi.org/10.1016/j.molliq.2019.111650

This is a PDF file of an article that has undergone enhancements after acceptance, such as the addition of a cover page and metadata, and formatting for readability, but it is not yet the definitive version of record. This version will undergo additional copyediting, typesetting and review before it is published in its final form, but we are providing this version to give early visibility of the article. Please note that, during the production process, errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

© 2019 Published by Elsevier.

Journal Pre-proof

# Effects of surface roughness with the spherical shape on the fluid flow of Argon atoms flowing into the microchannel, under boiling condition using molecular dynamic simulation

Yeping Peng [1], Majid Zarringhalam [2], Azeez A. Barzinjy [3,4], Davood Toghraie[5], Masoud Afrand[6,7,*]

1-Shenzhen Key Laboratory of Electromagnetic Control, College of Mechatronics and Control Engineering, Shenzhen University, Shenzhen 518060, China

2- Department of Mechanical Engineering, South Tehran Branch, Islamic Azad University, Tehran, Iran

3- Physics Education Department, Tishk International University TIU, Erbil, Kurdistan Region – Iraq

4- Physics Department, College of Education, Salahaddin University-Erbil, Kurdistan Region – Iraq

5- Department of Mechanical Engineering, Khomeinishahr Branch, Islamic Azad University, Khomeinishahr, Iran

6-Laboratory of Magnetism and Magnetic Materials, Advanced Institute of Materials Science, Ton Duc Thang University, Ho Chi Minh City, Vietnam

7- Faculty of Applied Sciences, Ton Duc Thang University, Ho Chi Minh City, Vietnam

**Corresponding author at: Ton Duc Thang University, Ho Chi Minh City, Vietnam*

Email: masoud.afrand@tdtu.edu.vn (M. Afrand)

Journal Pre-proof

**Abstract**

This paper presents influences of roughness components with the spherical shape on the 10 million Argon atoms flowing inside the microchannel, under boiling condition using molecular dynamic simulation method. Microchannels are with cubic perspective in size of 10000*5000*5000 $A^3$ with roughened and smooth surfaces to be comparable in results by statistical method. Constant boiling temperature of 108 K is fixed in walls of microchannels to be transferred on the Argon fluid atoms are enforced at the inlet region of microchannels by different external driving forces in the range of 0.002 to 0.02 eV/Angstrom. A statistical approach is employed to analyses the effects of external force on the roughened and smooth surfaces. Finally, it is concluded that the spherical shape of roughness elements brings no destructive effect on the flow behavior when the external driving force is in the range of 0.002 to 0.01 eV/Angstrom. Therefore, preparing smooth surfaces by removing this type of roughness elements can be accounted as the wasted cost for real usage suchlike pharmaceutical microprobes to eradicate maladaptive or diseased cells of liver, prostate, lung and oral cancers.

**Keywords:** Microchannel, External force effects, Spherical roughness, MDS Method

**Nomenclature**

$F_{ij}$ Intermolecular force on molecule *i* by molecule *j*

$F_{ext}$ External applied force

$m$ Molecule mass

$r_c$ Cutoff distance

$r_{ij}$ Position between molecules *i* and *j*

$T$ Temperature

$V_i$ Velocity of molecule *i*

$N_{bin}$ Number of bins

$N_{atom}$ Number of atoms

$k_B$ Boltzmann Constant

a acceleration

**Greek symbols**

$\varepsilon$ Energy parameter in Lennard-Jones (LJ) potential

$\varepsilon_s$ Energy parameter for solid

$\sigma$ Length parameter of LJ potential

$\sigma_s$ Length parameter for solid

$\rho$ Density

$\phi$ Interaction potential

$\phi_w$ Wall potential function

δ Delta deviation

δt Time step

$\nabla$ Dell Gradient

**Subscripts**

f Liquid

s Solid

c Cut off

i $i_{th}$

w Wall

t Time

$A_r$ Argon fluid

$P_t$ Platinum

## 1- Introduction

Generally, the CFD method with Euler & Navier–Stokes formulation is the known tool for flow simulation. Although, for flows tiny systems, the continuum pattern credit is not authentic [1]. So, the MD method [2] is replaced. Molecular Dynamics (MD) is a computer simulation method to excavate the physical translocations of particles. The particles are allowed to interact for appropriated time, giving a view of the dynamic evolution of the system. Newton's formula of motion is the basis of the molecular dynamics simulation method. It means that acceleration of particles into the system is determined by knowledge of applied force on particles. Then, integration of the motion formulation can describe the position, velocity, and acceleration of the atoms as they vary with time. Molecular dynamics simulations are deterministic; once the position and velocity of each particle is determined, the system state is estimated at any time in the future or the past. Although MD abilities to

compute and anatomize atomistic simulations by 20 billion atoms is demonstrated by pioneering work [3, 4], this approach is time-consuming and computationally expensive. Therefore, it is reliable only for tiny systems. Nowadays, most of the published papers using the MDS method present study on the nanoflows [5-9]. Moreover, fluid flow is mostly flowing inside the channel are in nanoscale with the limited number of atoms. Also, atoms are mostly in single phase of gas or liquid. Therefore, the statistical approach in present MDS study with huge number of Argon atoms, under phase change condition shall be interested in the researcher to extend their researches. Because it reduces the gap between theoretical activities of previous works to real usage suchlike pharmaceutical microprobes to eradicate maladaptive or diseased cells of the body.

Liakopoulos et al. [10] using molecular dynamics simulation studied the Darcy-Weisbach coefficient of nanoflow into circular nanochannel and reported that theoretical form of this theory has an acceptable match with the results of MDS study. Cao et al. [11] using molecular dynamics simulation method, investigated the influences of surface barriers on the Argon gas flow inside Platinum microchannels. Surface roughness geometries were modeled in order of triangular, rectangular & sinusoidal waveform. Their simulation showed slipping and non-slipping boundary conditions of velocity pertain not only to the Kn number but also; it depends on the shape of barriers. Ziarani and Mohammad [12] used molecular dynamics method to simulate the turbulent Poiseuille flow in a nanochannel. In this study, different types of turbulent external forces were applied to the flow to investigate their effect on total energy, kinetic energy, temperature profiles. Their results showed that increasing the amount of applied external force lead to an increase in the kinetic energy and total energy of the system. Martini et al. [13] using unbalanced molecular dynamics simulation studied the molecular mechanisms of slip condition in Couette flow. They employed Nose- Hoover Thermostat to control the boundary temperature and reported that slip condition can enhance

in the number of slipping particle, which results in increasing length of the slip. They also reported that for a large amount of force, the slip length would be a fixed value, which results following the results of MD simulation. Kucaba et al. [14] employed using MDS method to investigate the flow of water fluid inside a nanochannel with different widths and different wall material types. They also considered the physical properties of the material and the potential for electrostatic interaction and obtained the velocity and density profiles for their different simulations. Their report revealed that slip condition on the nanochannel wall surfaces depends on the degree of fluid-wall interaction. Heidarinejad et al. [15] used the molecular dynamics method to study the effects of wall force on temperature distribution in nanochannels containing argon gas. They concluded that to eliminate the effect of boundaries on the results and their independency the channel dimensions in the periodic directions should be at least equal with the distance of the gas molecular free path. Liu and Li [16] proposed a composite nanochannel system in which liquid Argon was steadily moving under the influence of symmetric temperature gradient (thermal creep flow). In their proposed system, a composite channel was composed of two parallel wall planes which were consisted of two parts, the first part was made of low surface energy, while; the second part was made of relatively high surface energy. Using molecular dynamics simulation, they showed that the proposed scheme can create a thermal creep. Pengfei et al. [17] studied the evaporation and condensation of argon fluid within the copper nanochannel with nine types of surface structure, using a molecular dynamics simulation. The evaporation conditions were investigated in two stages of accelerated boiling and explosive boiling at 130 and 300 Kelvin, respectively. They reported that the arrangement of roughness elements and their interval distance are effective parameters for improving heat transfer. Zhang et al. [18], using the MDS method, investigated the explosive boiling of Argon fluid inside rectangular nanochannel with different height. they reported that increasing the height of the nanochannel

causes to increase explosion of argon fluid particles which brings sooner equilibrium state of the system. Barisik and Beskok [19] used the MDS method to study the influences of wall force on the shear stress distribution in the fluid. They showed that increasing the density causes to increase tension between fluid particles. Also, they showed the non-homogeneous distribution of vertical stress adjacent walls of microchannel. Barisik and Beskok [20] studied the flow of Argon gas in three-dimensional nanochannel using the molecular dynamics method. They compared their results with the results of the kinetic theory of gases. Their results showed that for finite values of dimensionless parameter β (which is defined as the length of the wall force penetration to the channel width), the dynamic similarity method between the gas flow in low-pressure conditions and the small dimensions are abolished. Bakhshan and Shadloo [21] studied molecular dynamics simulation of the effects of physical properties of the surface on the fluid flow behavior inside nanochannel. The results showed that the hydrodynamic characteristics of the flow and shear stress of the wall depend on roughness and wall dents. Also, the results showed that the roughness on the lower wall have a great effect on the velocity and density profiles. Also, the roughness on the lower wall increases the shear stress of the lower wall and decreases the shear stress of the upper wall. Nourian et al. [22] investigated the effects of nano-channel roughness with cubic and spherical forms using MDS. The fluid in their study was Argon, and height of roughness component was various. They showed that increasing height the roughness causes to decrease density and velocity. Because roughness has a direct impact on the intermolecular forces and leads to increase repulsive force and decrease attractive force in the domain of fluid flow is in the exposure of roughness element. Isfahani et al. [23] compared the thermal and hydrodynamic solutions obtained from the Boltzmann grid model which was developed for Argon gas with the result of that by molecular dynamics method in nano dimensions and porous media. They suggested a model to increase the accuracy of the solution significantly.

They also showed that their model reduces the time of calculations. Rahmatipour et al. [24] using molecular dynamics simulation studied the effects of the geometric shape of the barriers on the steady Couette flow behavior of Argon fluid inside smooth and roughened nanochannels. They reported that increasing channel height reduces the slip velocity of the fluid. Also, they showed that the reduction of density on the walls causes to reduce the slip velocity. Also, references [25–32] present phase change of Argon fluid into small nanochannels and references [33–46] are related to microchannel flows and influences of suspending nanoparticle into fluids to empower their properties.

A literature review indicated that the study of molecular dynamic simulation is limited to the small number of particles in nanoflows. Also, the lack of comprehensive study in phase change condition with roughness elements effects leads us to present this paper which investigates the effect of spherical roughness components on the 10 million Argon atoms under boiling condition inside the microchannel. Also, fluid atoms are considered under influences of applying external driving forces in wide range to be applicatory for real usage.

## 2- Simulation method

Present molecular dynamics simulation was performed by LAMMPS software [47]. LAMMPS is abbreviated from Large-scale Atomic/Molecular Massively Parallel Simulator which is a molecular dynamics program from Sandia National Laboratories. This software is supported by Message Passing Interface (MPI) for parallel communication and is free and open-source software, distributed under the terms of the GNU General Public License. In other words, it is a widely used free software license, which guarantees end users the freedom to run, study, share, and modify the software. LAMMPS employs neighbor lists to keep track of nearby atoms. It integrates Newton's equations of motion for a collection of interacting atoms. Sequences of simulations were in order of the following procedure.

Two Platinum microchannel with square cross-section were simulated in accordance with perspective view as shown schematically in Fig. 1. Dimensions of both microchannels were 10000*5000*5000 $(A°)^3$ in X, Y, and Z directions respectively. Internal surfaces of one of them were roughened by spherical roughness elements by the front view in Fig. 1. Then, Argon fluid atoms were structured on the surfaces of both microchannels. Argon atoms were placed under boiling condition which was prepared by boundary constant temperature of 108 Kelvin on the walls of both microchannels. Afterward, external driving forces were enforced on the Argon atoms in order of 0.002, 0.01 and 0.02 eV/Angstrom in X direction. Microchannel height was divided into 2200 bin in Z direction. Structure of atoms was Face Center Cubic (FCC) with lattice constant of 5.26 A°.

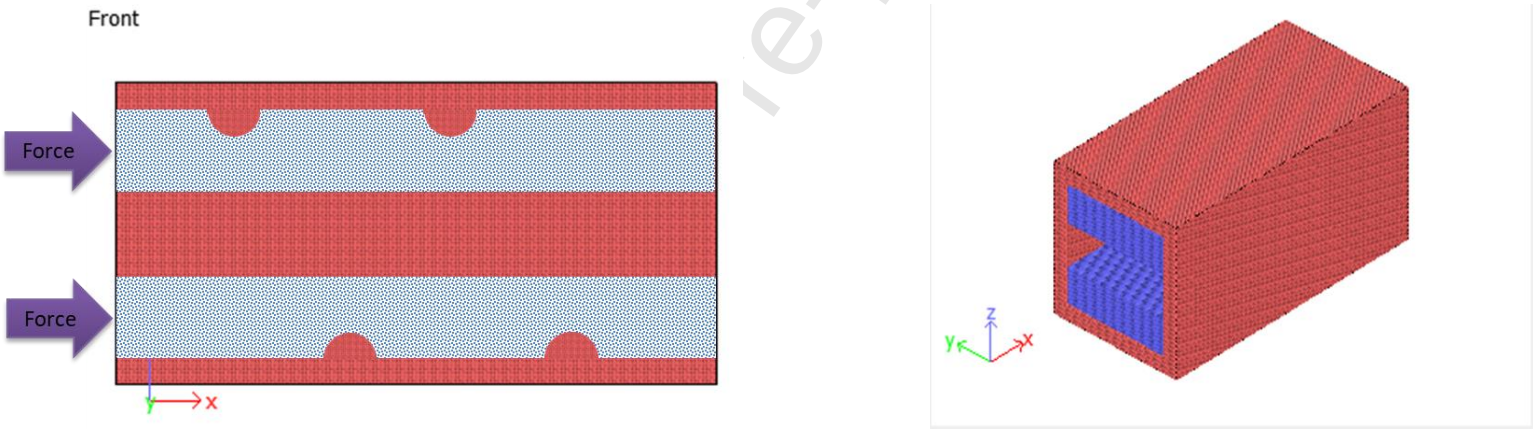



**Fig. 1:** Front & perspective views of roughened microchannel

Roughness barriers were simulated in the arrangement of X: 2000, 4000, 6000 & 8000 A°. The dimensions of each of element were 500 and 50 $A^3$ in order of diameter and height. These dimensions were selected to save on time of running and reduce interference.

Periodic boundary conditions is applied along X directions while in Y and Z directions are non-periodic.

The interaction of fluids atoms are computerized on the basis of LJ potential function as following equation [48, 49]:

$$\phi\,(r_{ij}) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right] \qquad r_{ij} \le r_c \tag{1}$$

where $r_{ij}$ defines the interatomic track from atom i and j and energy parameter was introduced by $\varepsilon$ as the depth of the potential well, next cut-off radius is shown by $r_c$ which was as much as 8.5125 Angstrom. The atomic mass, diameter, and potential depth of Argon atoms were defined respectively as $m=m_f=m_{Ar}=39.95$ grams/mole, $\sigma=\sigma_f=\sigma_{Ar}=3.405$ A° and $\mathcal{E}=\mathcal{E}_f=\mathcal{E}_{Ar}=1.67*10^{-21}$J. Next, for the Platinum atoms, parameters were accounted as following values: atomic mass $m_s=m_{pt}=195.08$ grams/mole, diameter $\sigma_s=\sigma_{pt}=$ 2.475A°, and potential depth $\mathcal{E}_s=\mathcal{E}_{pt}=8.35*10^{-20}$J. Also, solid-fluid interactions were computed based on the modified L-J equation, pairing with Lorentz–Berthelot equations as following [48, 49]:

$$\phi_w(r_{ij}) = 4\varepsilon_{sf}\left[\left(\frac{\sigma_{sf}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{sf}}{r_{ij}}\right)^{6}\right] \qquad r_{ij} \le r_c \tag{2}$$

$$\varepsilon_{sf} = \sqrt{\varepsilon_s \varepsilon_s} \qquad \sigma_{sf} = \frac{\sigma_s + \sigma_f}{2} \tag{3}$$

To propagate the system's motion through time, Newton's second law at the atomic level was offered as the gradient of the potential function as below equation [51].

$$\overrightarrow{Fi} = \sum_{i \ne j} Fij = m_i \frac{d^2 \vec{r_i}}{dt^2} = m_i \frac{d\vec{v_i}}{dt} \tag{4}$$

Then, the temperature is determined by Gaussian distribution as below formula [51].

$$\frac{1}{N_{atm}} \sum_{i=1}^{N_{atm}} \frac{1}{2} m \left| v_i^{\,2} \right| = \frac{3}{2} k_B T \tag{5}$$

Association of previous functions to integrate the Newton equation was performed by the velocity Verlet method as following formulations [50].

$$v(t+\delta t) = v(t) + a(t)\delta t \quad (7)$$

$$r(t+\delta t) = r(t) + v(t)\delta t \quad (8)$$

Equilibrium state was showed roundabout 200000 time step and computations were continued until 1000000 time step.

## 3- Results and Discussion

The effect of different external driving forces on the behavior of Argon was studied inside a cubic microchannel with ideal & roughened surfaces [52-55]. Also, to draw influences of spherical geometry of roughness elements on the flow condition, the results of both microchannels were compared. Comparisons are mostly based on the statistical approach.

Journal Pre-proof

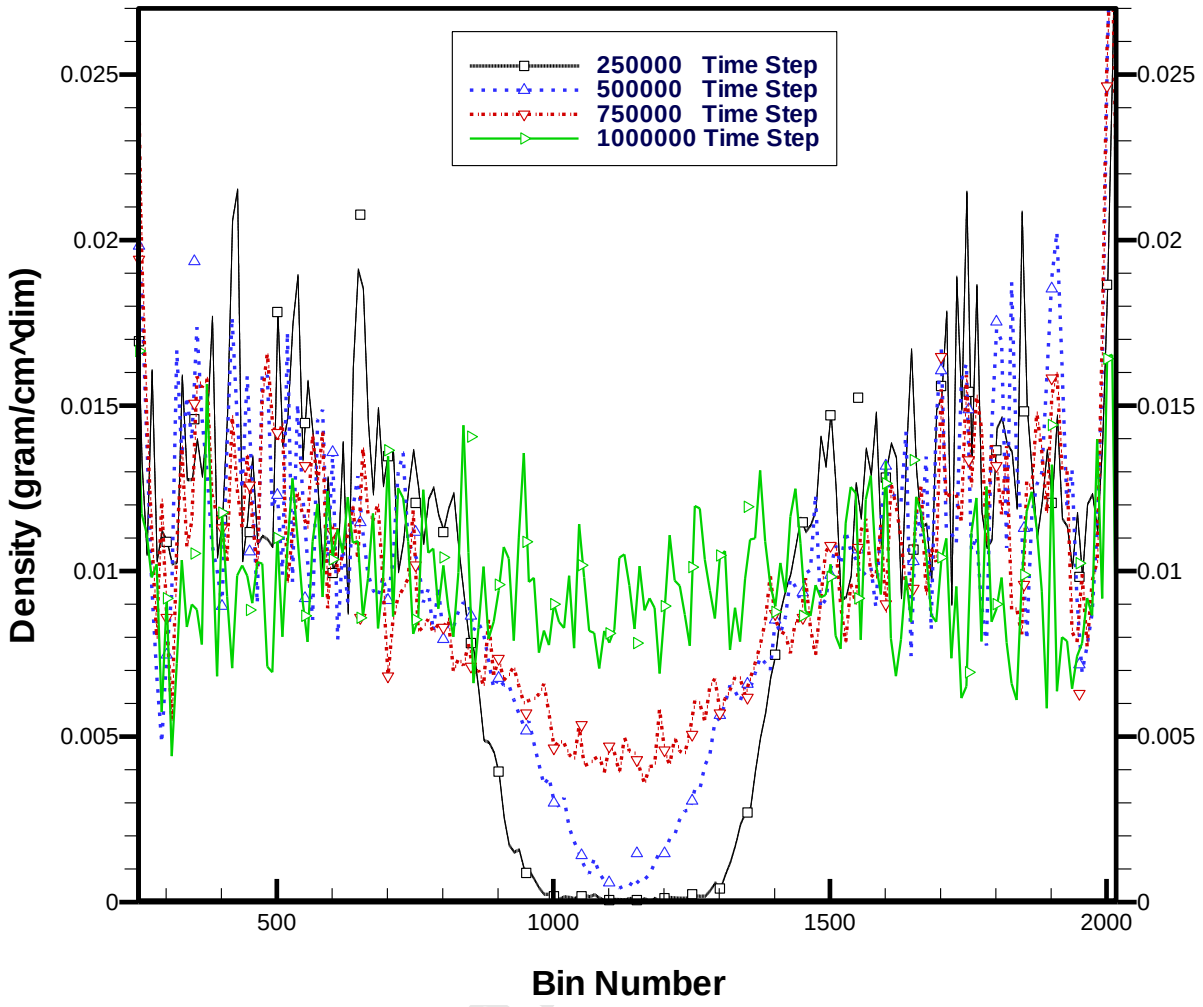



**Fig. 2:** Density of roughened microchannel under external force 0.002 eV/Angstrom

Journal

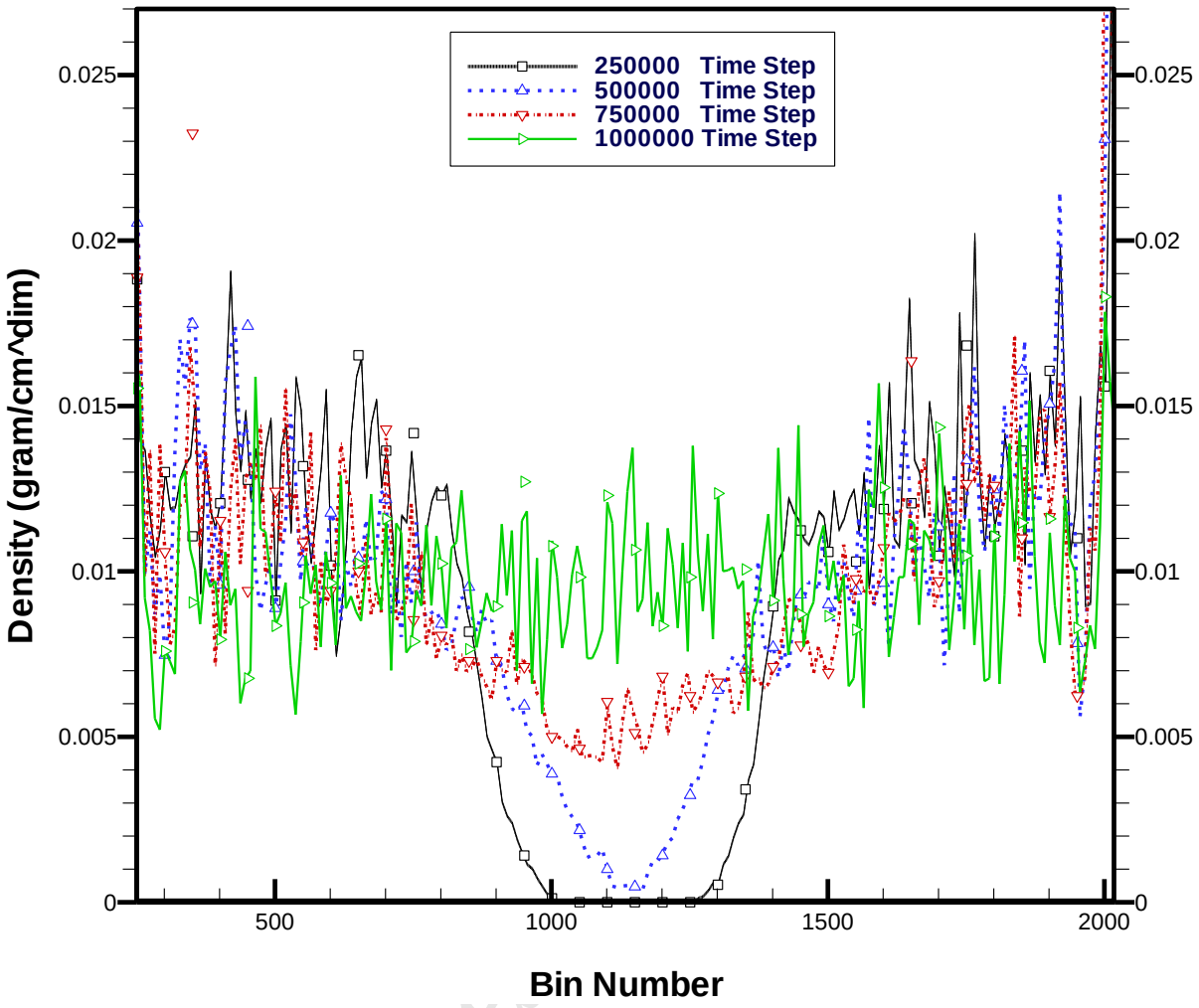



**Fig. 3:** Density of ideal microchannel under external force 0.002 eV/Angstrom

Journal

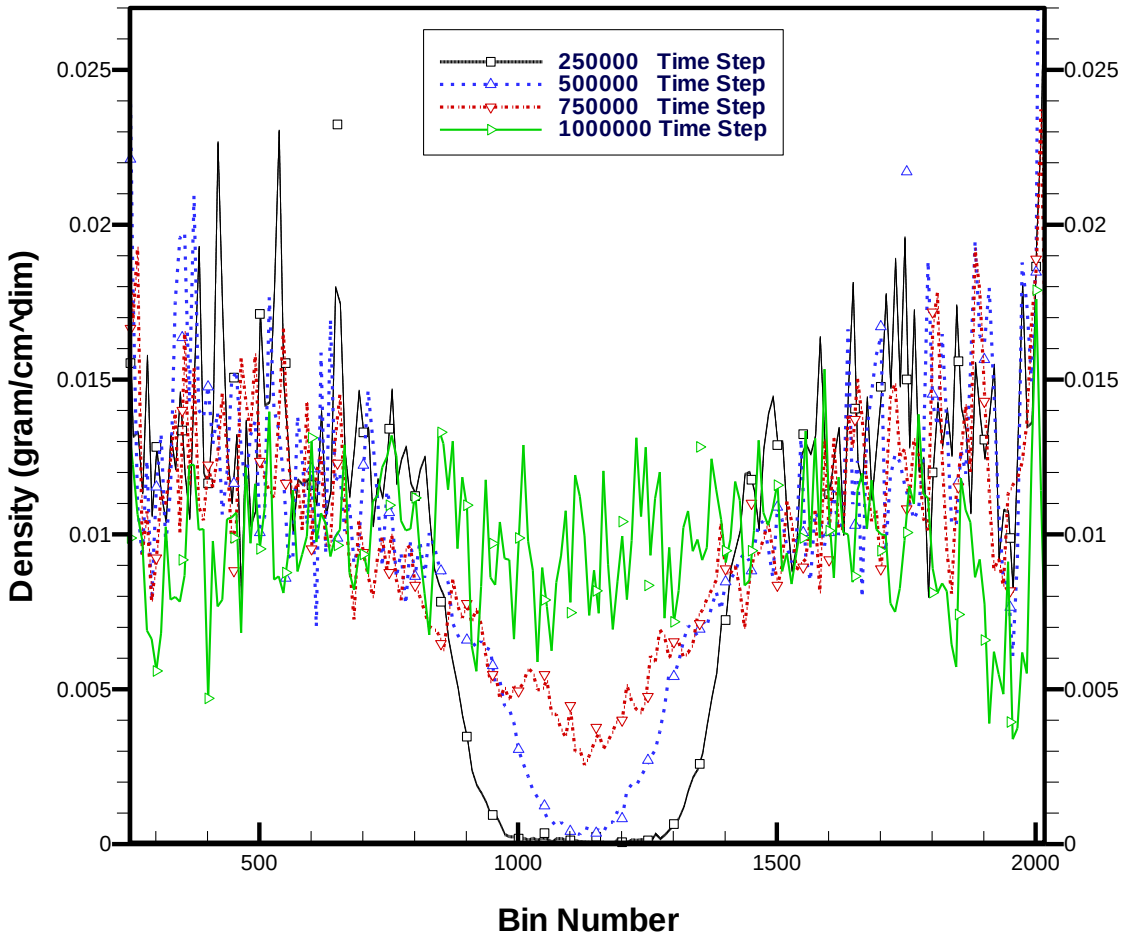



**Fig. 4:** Density of roughened microchannel under external force 0.01 eV/Angstrom

Journal

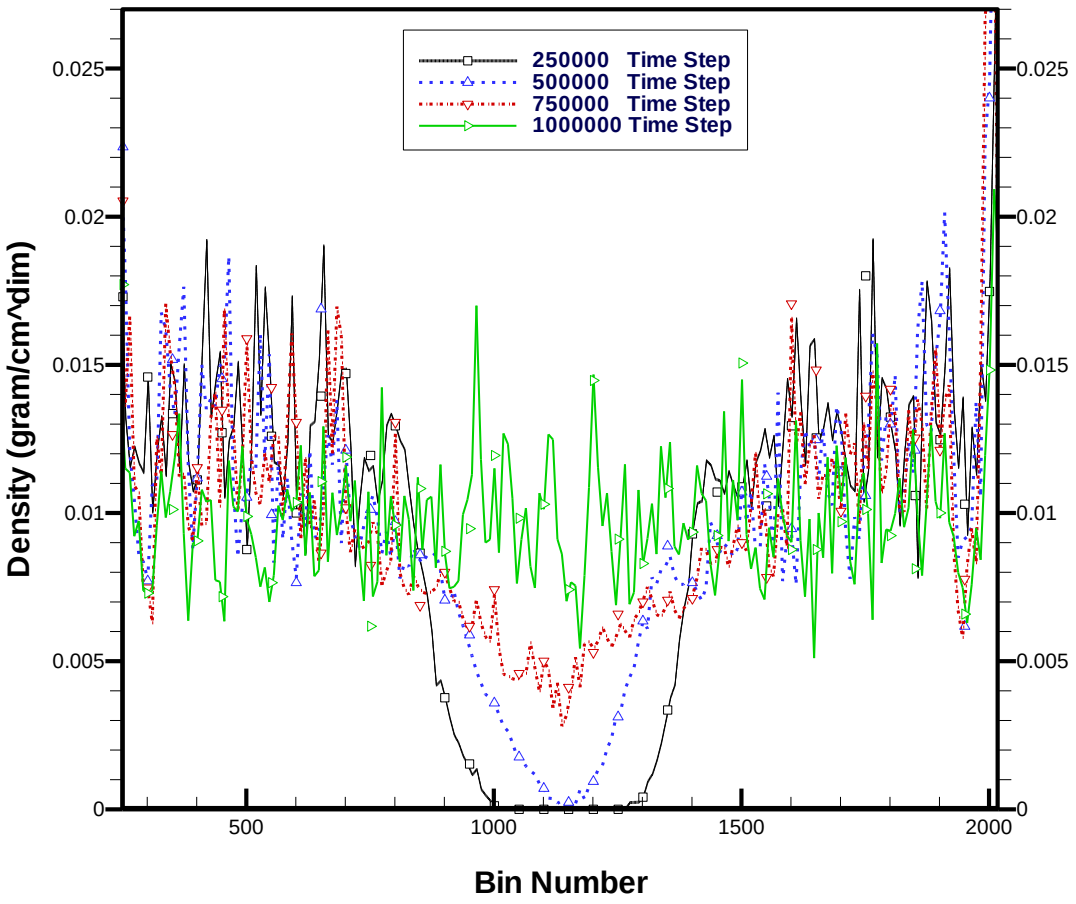



**Fig. 5:** Density of ideal microchannel under external force 0.01 eV/Angstrom

Journal Pre-proof

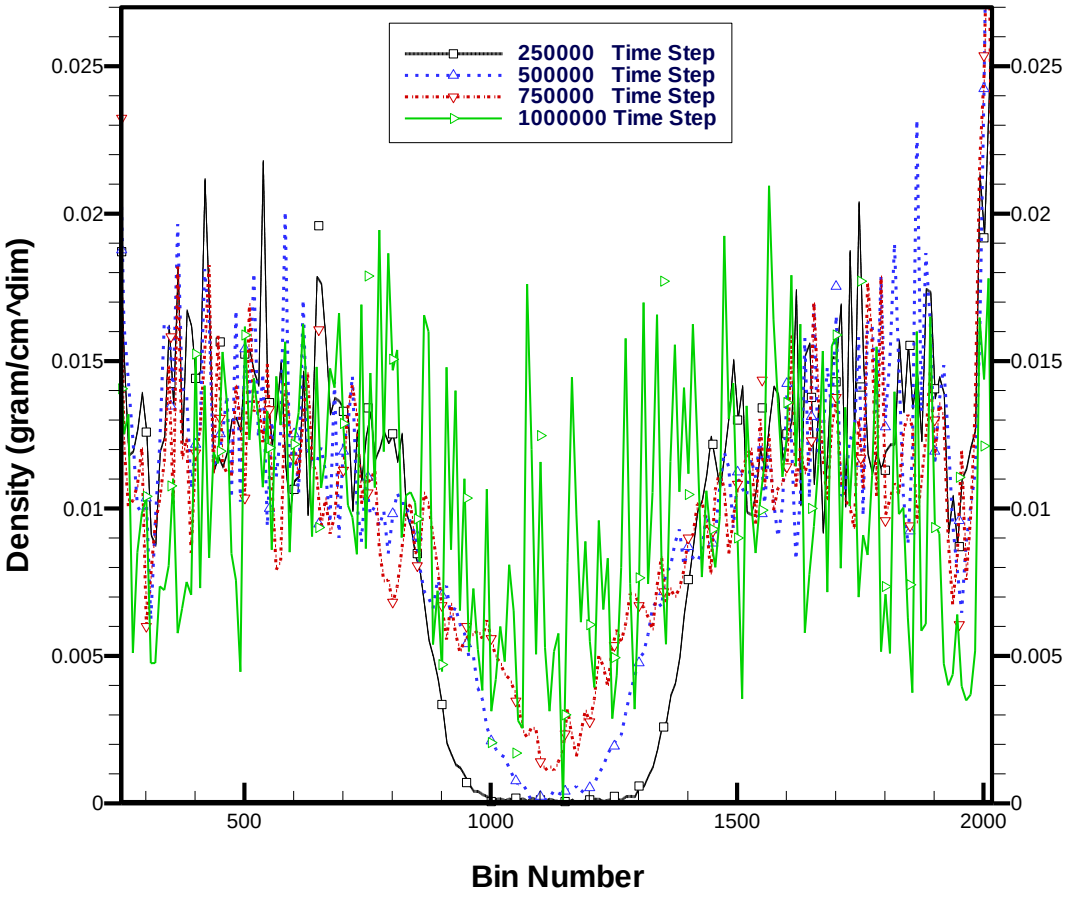



**Fig. 6:** Density of roughened microchannel under external force 0.02 eV/Angstrom

Journal Pre-proof

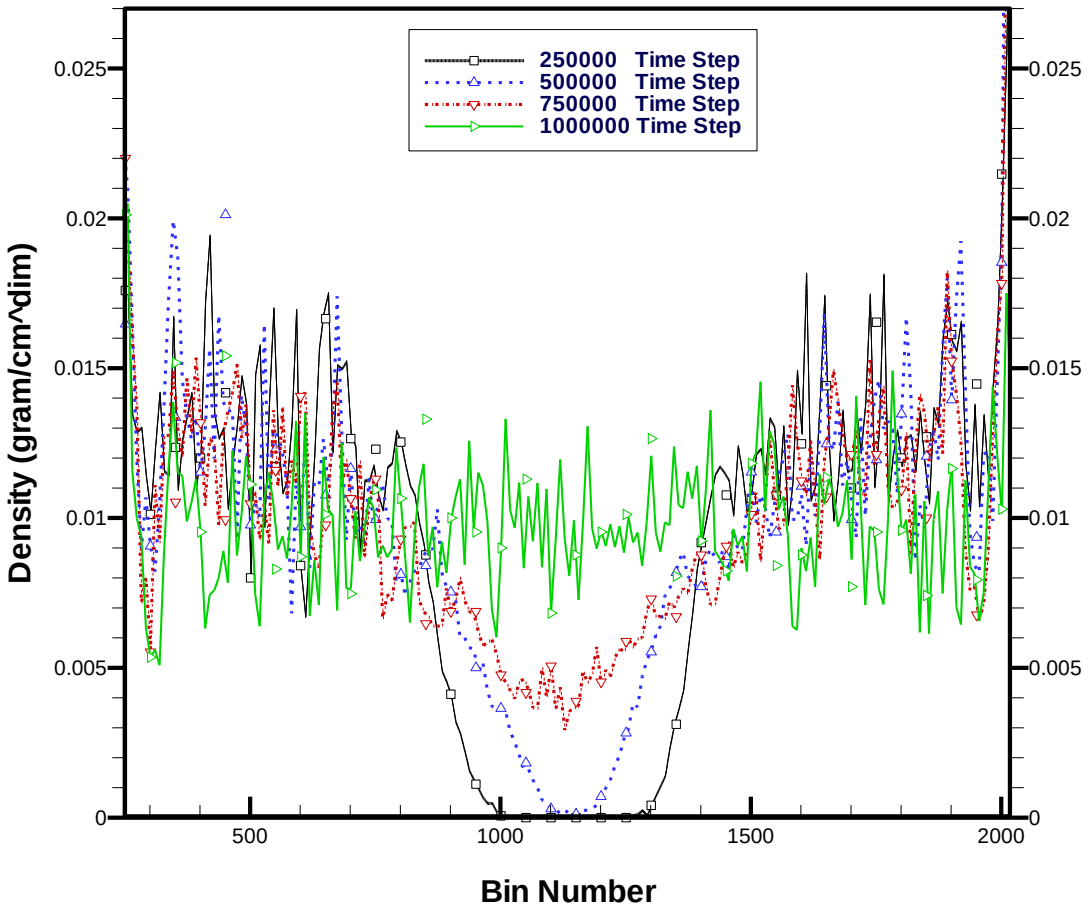



**Fig. 7:** Density of ideal microchannel under external force 0.02 eV/Angstrom

Figs. 2 to 7 present density of Argon flow into smooth & roughened microchannels, which are under different external driving forces. For all the above figures, vertical axes are graded to indicate density values, versus 2200 bin numbers in horizontal axe. Each figure is included four graphs to exhibit results of density at 4 regular time steps of 250000, 500000, 750000 and 1000000. Figs. 2, 4 & 6 are relevant to roughened microchannel by spherical components and Figs. 3, 5, and 7 are belonged to smooth microchannel.

As can be seen from Figs. 2 and 3, spherical roughness components don't change density graphs of ideal surfaces noticeably under exerting the force of 0.002 eV/Angstrom. Nevertheless, comparison of these two figures, indicated oscillation in density profiles of rough microchannel (see Fig. 2) is higher than that of ideal microchannel (see Fig. 3) at time

steps 250000, 500000, and 750000, whereas; at time step 1000000, oscillation of roughened microchannel is lower than that of ideal one. On the other side, statistical approach by density computation in 2200 bin numbers shows that maximum difference in summation of density in 800 bins in the middle of both smooth and rough microchannels (between bin numbers 701 and 1500) is accounted as much as 0.9%. Therefore, it is demonstrated that the roll of spherical roughness elements are not important when propulsion force of 0.002 eV/Angstrom is exerted on the fluid atoms at the intersection of microchannels. Also, according to Fig. 4 and Fig. 5, it can be found that increasing external driving forces from 0.002 to 0.01 eV/Angstrom, brings no significant effect on the density profiles of the rough microchannel. Because visual comparison in fluctuations of densities profiles of rough and smooth surfaces in Fig. 4 and Fig. 5 is similar to that of Fig. 2 and Fig. 3. But, their maximum difference in summation of density values for 800 layers of the central region of smooth and rough microchannels is accounted as much as 1.2% at time steps of 250000, 500000 and 750000, whereas, it reaches to 5.1% at time step 1000000. It means that physical movement of Argon atoms on the roughened surfaces is stronger than that of smooth surfaces at time step 1000000. Hence, it can be concluded from Figs. 2 to 5 that presence of spherical roughness elements on the microchannel surfaces brings no destructive effect when external forces are in the domain of 0.002 to 0.01 eV/Angstrom. But, statistical approach indicated that increasing external force can change atomic flow structure with increasing time steps due to emerging flow turbulences by the increasing contradiction of external force in the X direction and thermal driving force of boiling process in Z direction which is supported by constant wall temperature of 108 Kelvin. Moreover, increasing external forces on such micro flow, simultaneous with the presence of surface roughness can be a sign for the possibility of destroying the equilibrium state of system energy in very high time steps.

Journal Pre-proof

Figs. 6 and 7 shows the effect of propulsion force of 0.02 eV/Angstrom on the density graphs of Argon flow into roughened and smooth channels. As is clear from these figures, the density profile of the roughened surfaces is not stable at time step 1000000. It means the distribution of Argon atoms in the vapor region in the center of the microchannel is not consistent, while it is stable and normal for the smooth microchannel in accordance with Fig.7. Therefore, spherical roughness elements can destroy regular distribution of atoms under normal boiling condition. In fact, the roll of the thermal driving force of boiling condition to translocate Argon atoms from lateral layers to central layers is hidden by turbulences of the external force of 0.02 eV/Angstrom. Also, comparison of results of fluid flow inside both microchannel in summation of density values of 800 layers at time step 1000000, indicated that presence of roughness barriers causes to reduce density in the central region of microchannel as much as 9.2%. It means that barriers prevent from movement of Argon fluid atoms to translocate from lateral regions to central region of microchannel. In fact, on the one side, under normal condition, atoms can be trapped in interval distance of barriers which reduce flow density in the middle section of the channel. On the other side, barriers extend contact surface of energy transfer between solid-fluid which enhances flow density of the central region of the microchannel. But, turbulences can change the power of both effects.

Journal Pre-proof

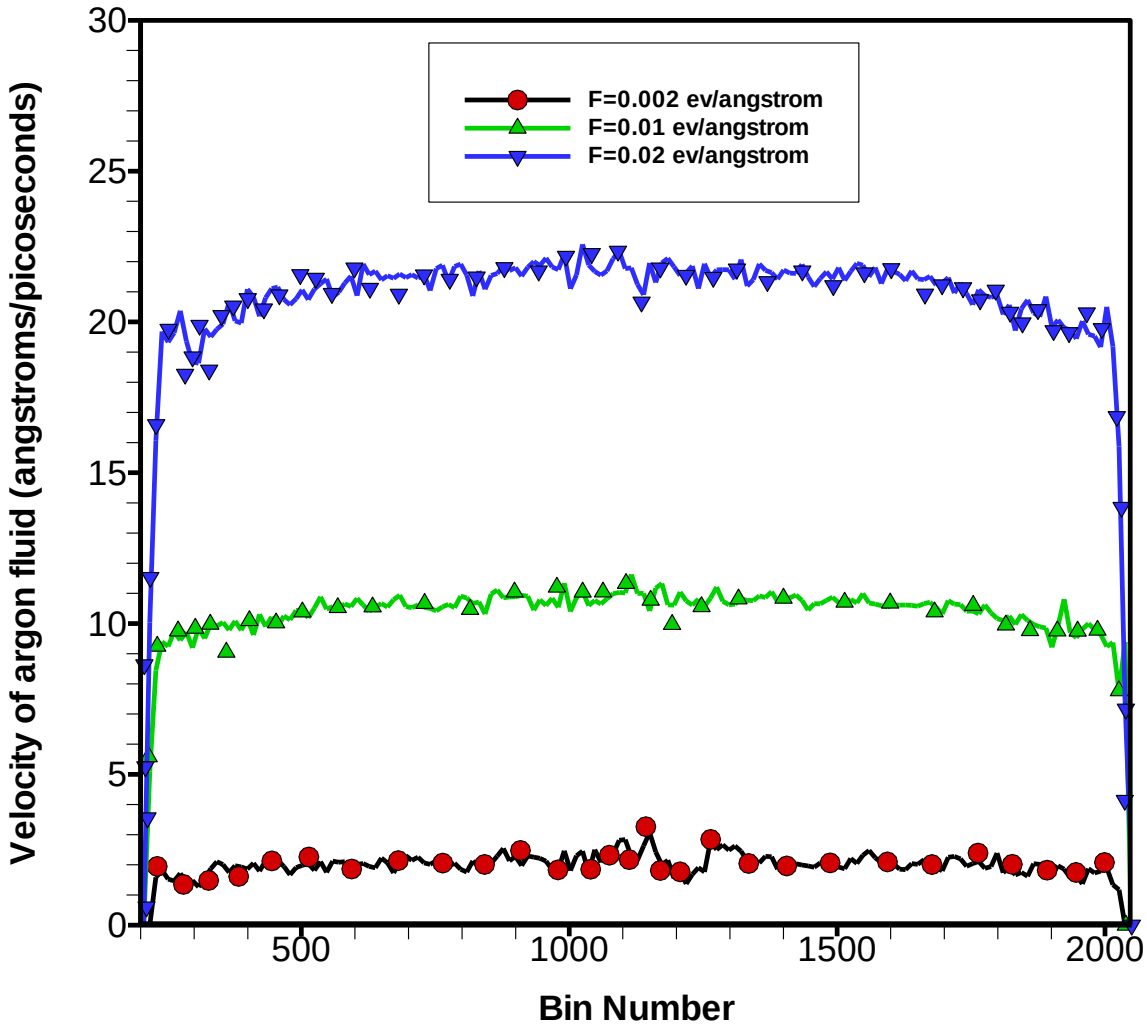



**Fig. 8:** Velocity of roughened microchannel under different external forces

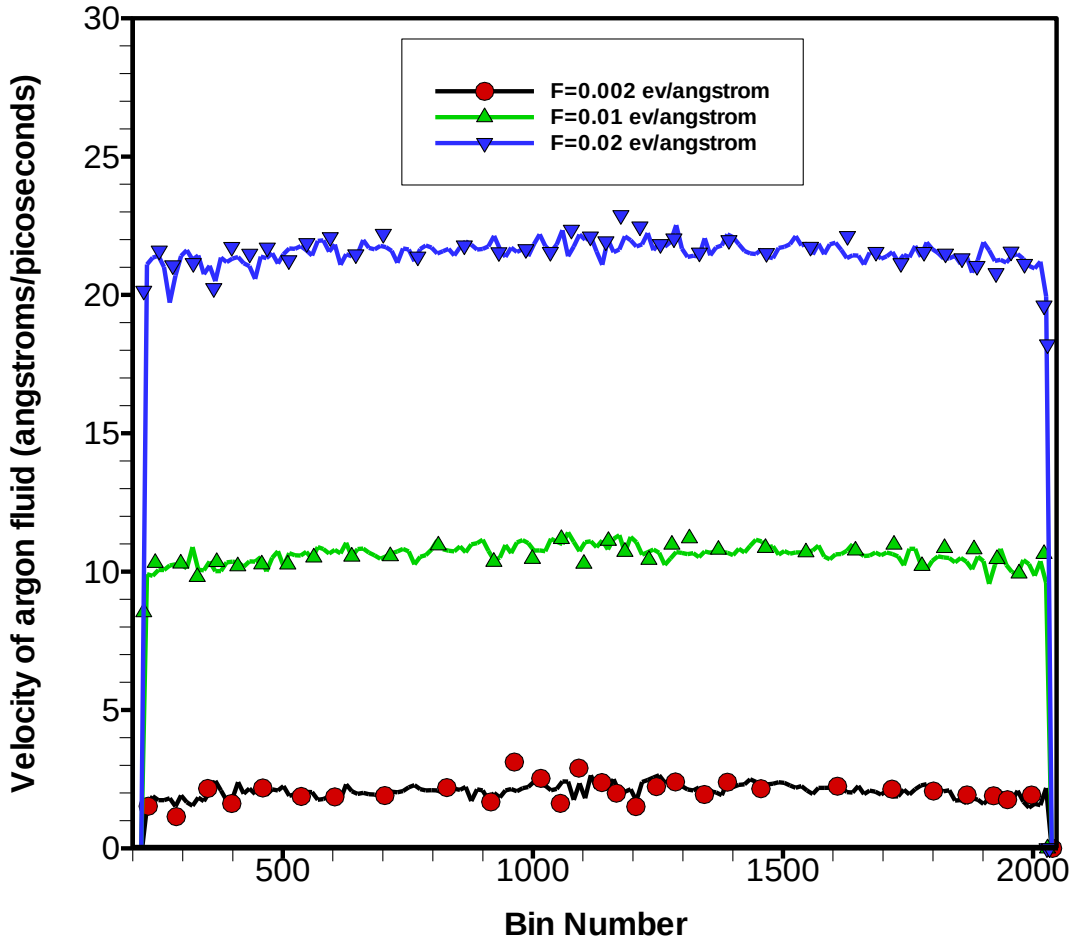



**Fig. 9:** Velocity of ideal microchannel under different external forces

Figs. 8 and 9 present velocity graphs of fluid flow into roughened and ideal microchannels respectively. Data sampling was done at time step 1000000. Each figure, exhibit 3 profiles to show the effect of applying different external driving forces of 0.002, 0.01 and 0.02 eV/Angstrom on the velocity of Argon flowing into roughened and ideal surfaces of microchannels. For both figures, vertical ax determines velocity values, versus 2200 bins as shown in horizontal ax. As can be seen from the above figures, the spherical shape of roughness elements is not effective on the velocity profiles, except in the layers are in the vicinity of microchannel walls. Because on the roughened surfaces, spherical elements are as obstacles to prevents their movements in the x direction, under pressure of external driving forces. Therefore they reduce the velocity of flow in lateral layers are in exposure of

roughness elements. Calculations in total values of velocities accounted by summation of velocity values of 2200 layers of rough and smooth microchannels show reduction as much as 1.45%, 0.7% and 1.5% in order of applying external driving forces of 0.002, 0.01 and 0.02 eV/Angstrom. Hence, adding roughness components on the surfaces of the channel causes to reduce average velocity as much as 1.22% which is exactly related to the reduction of velocity in lateral layers. Therefore statistical approach demonstrates that a consequence of the presence of barriers with spherical shape is not noticeable on the flow velocity for real usage suchlike biology and pharmaceutical equipment.

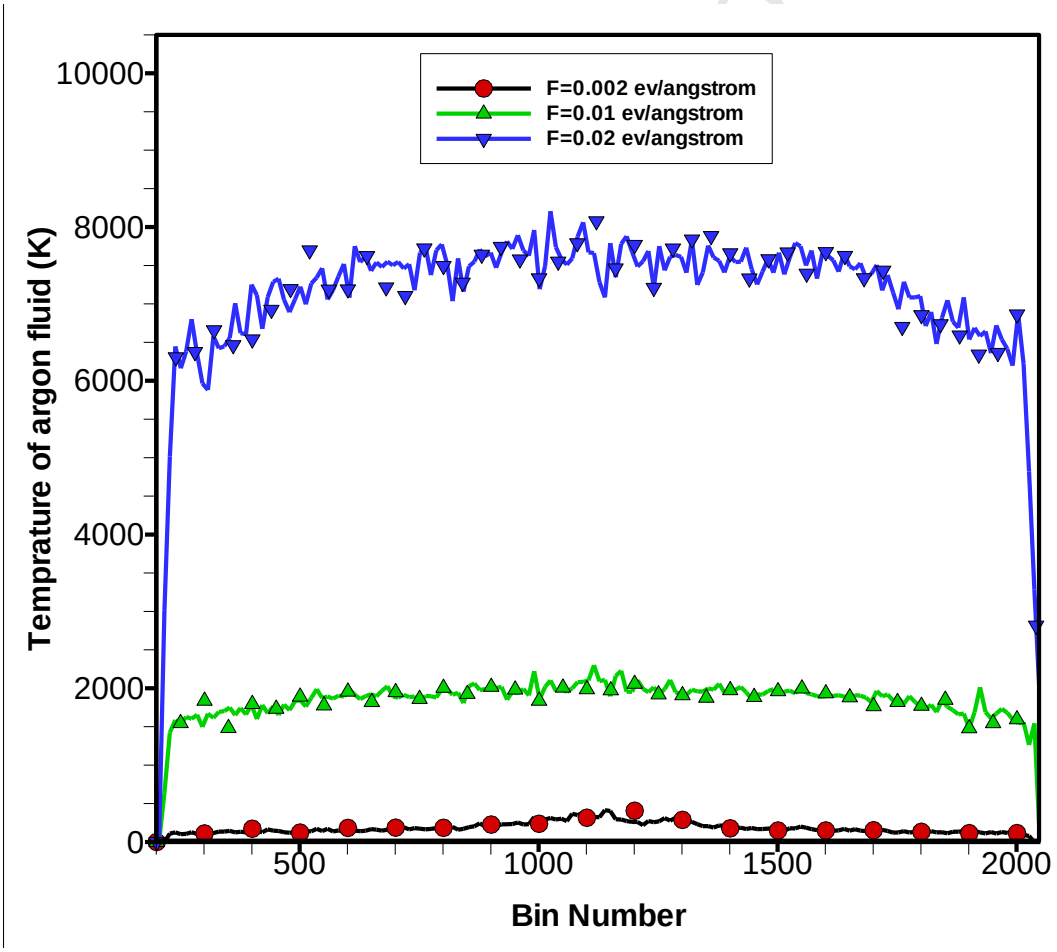



**Fig. 10:** Temperature of Argon fluid inside rough microchannel under different external forces

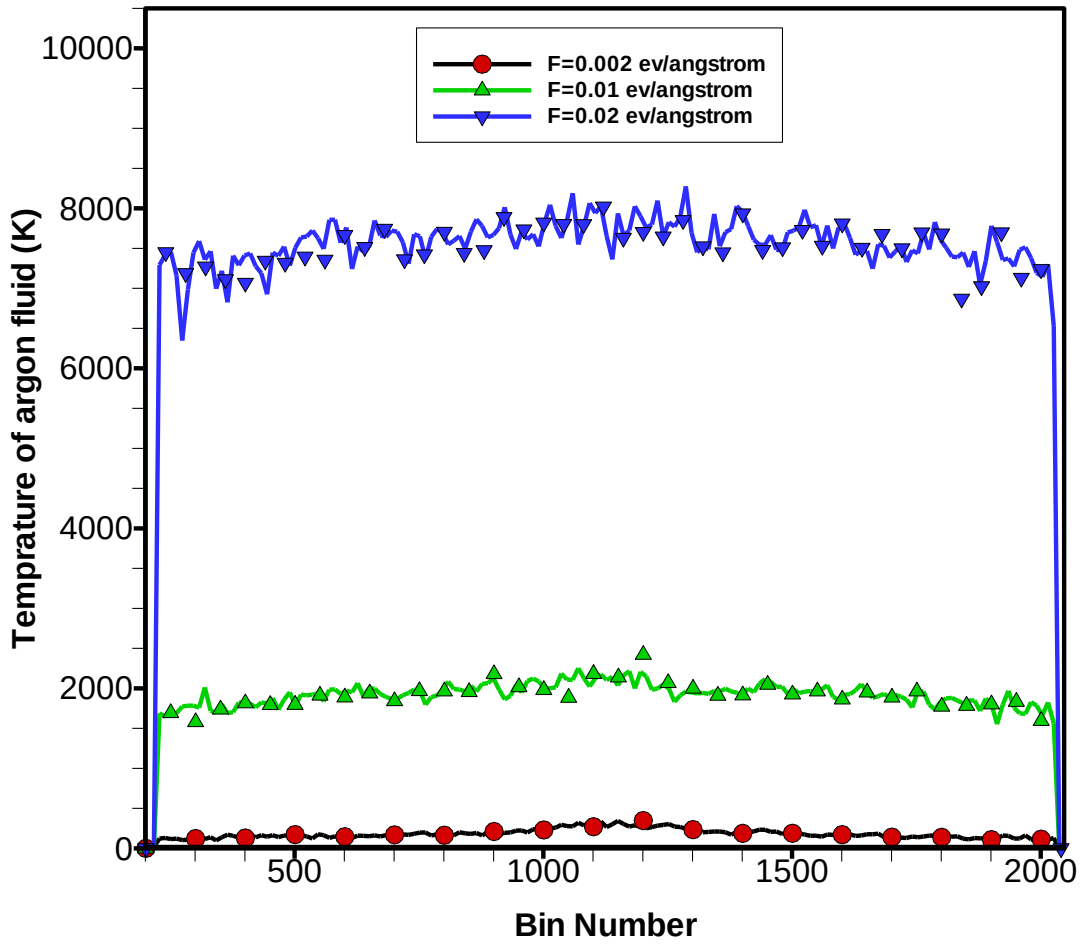



**Fig. 11:** Temperature of Argon fluid inside smooth microchannel under different external forces

Figs. 10 and 11 present temperatures graphs of flow into rough and ideal microchannels under applying different external driving forces in the range of 0.002 to 0.02 eV/Angstrom. The data sampling of these results was done at time step 1000000 from temperature values of 2200 layers. Generally, it is clear from the comparison of Fig. 10 with Fig. 11 that adding the spherical shape of roughness component on the smooth surfaces of microchannel bring no significant consequence and its only effect is seen in temperature profiles of external forces of 0.02 eV/Angstrom. Because in this case, oscillations of the temperature profile of roughened surfaces are higher than that of smooth surfaces. Also, the temperature of lateral layers of roughened surfaces is lower than that of smooth one due to the effect of roughness components in velocity, which is academically convinced by Newton's second law in

molecular dynamic simulation method. Also, the statistical approach shows that roughness elements increase the temperature of fluid flow under external forces of 0.002 eV/Angstrom around 4%. But, with the enhancement of external driving forces to 0.01 and 0.02 eV/Angstrom, barriers cause to decline temperature profiles around 2%. It means they empower boiling condition due to their role in the enhancement of contact surfaces of energy transfer from microchannel walls to Argon fluid atoms.

## 4- Conclusion

This paper investigated the effect of applying different external driving forces on the Argon atoms, flowing inside microchannel in the presence of barriers with the spherical shape. Argon fluid atoms were under boiling flow by constant wall temperature of 108 Kelvin. Finally, the results of both microchannels were compared by the statistical approach to find following key points:

- Generally, the spherical geometry of roughness elements does not affect strongly on the distribution of Argon atoms in the central section of microchannel when the range of external driving is less than 0.01 eV/Angstrom.
- Applying the external driving force of 0.02 eV/Angstrom in the presence of spherical shape of roughness elements can bring so turbulences that reduce noticeably effect boiling process in normal distribution of Argon atoms in the middle region of microchannel.
- Adding spherical geometry of roughness elements on the smooth surfaces of microchannel result in reduction of average velocity as much as 1.22%. Because they are as obstacles to trap atoms and causes to decrease the velocity of flow in lateral layers of fluid in the vicinity of microchannel walls.

Journal Pre-proof

- Presence of spherical roughness element under different external forces causes to change temperature profile of fluid flow between 2% to 4% due to the contradiction of external force and boiling force.
- The statistical approach demonstrated that roll of the spherical shape of roughness on the flow behavior is not significant when the external force is in the range of 0.002 to 0.01 eV/Angstrom. Therefore, it is never suggested to invest in removing roughness and preparing the ideal surface for practical application.
-

**Acknowledgments**

This research is partially supported by the Natural Science Foundation of Guangdong Province, China, (2018A030310522), Shenzhen Science and Technology Planning Project, China, (JCYJ20170818100522101) and Natural Science Foundation of Shenzhen University (2017032).

## 5- References

[1] Kalweit M, Drikakis D. Coupling strategies for hybrid molecular—continuum simulation methods. Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science. 2008 May 1;222(5):797-806.

[2] Allen MP. Tildesley. DJ Computer simulation of liquids.

[3] Kadau K, Germann TC, Lomdahl PS. Large-scale molecular-dynamics simulation of 19 billion particles. International Journal of Modern Physics C. 2004 Jan;15(01):193-201.

[4] Rapaport DC, Rapaport DC. The art of molecular dynamics simulation. Cambridge university press; 2004.

[5] Alipour P, Toghraie D, Karimipour A, Hajian M. Molecular dynamics simulation of fluid flow passing through a nanochannel: Effects of geometric shape of roughnesses. Journal of Molecular Liquids. 2019 Feb 1;275:192-203.

[6] Tohidi M, Toghraie D. The effect of geometrical parameters, roughness and the number of nanoparticles on the self-diffusion coefficient in Couette flow in a nanochannel by using of molecular dynamics simulation. Physica B: Condensed Matter. 2017 Aug 1;518:20-32.

[7] Rezaei M, Azimian AR, Semiromi DT. The surface charge density effect on the electro-osmotic flow in a nanochannel: a molecular dynamics study. Heat and Mass Transfer. 2015 May 1;51(5):661-70.

[8] Toghaniyan A, Zarringhalam M, Akbari OA, Shabani GA, Toghraie D. Application of lattice Boltzmann method and spinodal decomposition phenomenon for simulating two-phase thermal flows. Physica A: Statistical Mechanics and its Applications. 2018 Nov 1; 509:673-89.

[9] Semiromi DT, Azimian AR. Molecular dynamics simulation of nonodroplets with the modified Lennard-Jones potential function. Heat and mass transfer. 2011 May 1;47(5):579-88.

[10] Liakopoulos A, Sofos F, Karakasidis TE. Darcy-Weisbach friction factor at the nanoscale: From atomistic calculations to continuum models. Physics of Fluids. 2017 May 4;29(5):052003.

[11] Cao BY, Chen M, Guo ZY. Effect of surface roughness on gas flow in microchannels by molecular dynamics simulation. International Journal of Engineering Science. 2006 Aug 1;44(13-14):927-37.

[12] Ziarani AS, Mohamad AA. A molecular dynamics study of perturbed Poiseuille flow in a nanochannel. Microfluidics and Nanofluidics. 2006 Jan 1;2(1):12-20..

[13] Martini A, Roxin A, Snurr RQ, Wang Q, Lichter S. Molecular mechanisms of liquid slip. Journal of Fluid Mechanics. 2008 Apr;600:257-69..

[14] Kucaba-Pietal A, Walenta Z, Peradzyński Z. Molecular dynamics computer simulation of water flows in nanochannels. Bulletin of the Polish Academy of Sciences: Technical Sciences. 2009 Mar 1;57(1):55-61.

[15] Heidarinejad G, Rabani R, Shirani E. The effect of wall force field on temperature distribution in nanochannel contains Lennard-Jones fluid by molecular dynamic simulation. Modares Mechanical Engineering. 2017 Aug 15;17(6):23-31.

[16] Liu C, Li Z. Molecular dynamics simulation of composite nanochannels as nanopumps driven by symmetric temperature gradients. Physical review letters. 2010 Oct 18;105(17):174501.

[17] Li L, Ji P, Zhang Y. Molecular dynamics simulation of condensation on nanostructured surface in a confined space. Applied Physics A. 2016 May 1;122(5):496.

[18] Zhang S, Hao F, Chen H, Yuan W, Tang Y, Chen X. Molecular dynamics simulation on explosive boiling of liquid argon film on copper nanochannels. Applied thermal engineering. 2017 Feb 25;113:208-14.

[19] Barisik M, Beskok A. Equilibrium molecular dynamics studies on nanoscale-confined fluids. Microfluidics and nanofluidics. 2011 Sep 1;11(3):269-82.

[20] Barisik M, Beskok A. Scale effects in gas nano flows. Physics of Fluids. 2014 May 8;26(5):052003.

[21] Bakhshan Y, Jahromi AS. Molecular Dynamics Simulation of Surface Specifics Effects on the nanoscale fluid flow. Modares Mechanical Engineering. 2015 Jul 15;15(5):176-84.

[22] Noorian H, Toghraie D, Azimian AR. Molecular dynamics simulation of Poiseuille flow in a rough nano channel with checker surface roughnesses geometry. Heat and mass transfer. 2014 Jan 1;50(1):105-13.

[23] Isfahani AM, Tasdighi I, Karimipour A, Shirani E, Afrand M. A joint lattice Boltzmann and molecular dynamics investigation for thermohydraulical simulation of nano flows through porous media. European Journal of Mechanics-B/Fluids. 2016 Jan 1;55:15-23.

[24] Rahmatipour H, Azimian AR, Atlaschian O. Study of fluid flow behavior in smooth and rough nanochannels through oscillatory wall by molecular dynamics simulation. Physica A: Statistical Mechanics and its Applications. 2017 Jan 1;465:159-74.

[25] Liakopoulos A, Sofos F, Karakasidis TE. Darcy-Weisbach friction factor at the nanoscale: From atomistic calculations to continuum models. Physics of Fluids. 2017 May 4;29(5):052003.

[26] Liakopoulos A, Sofos F, Karakasidis TE. Friction factor in nanochannel flows. Microfluidics and Nanofluidics. 2016 Jan 1;20(1):24.

[27] Semiromi DT, Azimian AR. Molecular dynamics simulation of annular flow boiling with the modified Lennard-Jones potential function. Heat and Mass Transfer. 2012 Jan 1;48(1):141-52.

[28] Zhang S, Hao F, Chen H, Yuan W, Tang Y, Chen X. Molecular dynamics simulation on explosive boiling of liquid argon film on copper nanochannels. Applied thermal engineering. 2017 Feb 25;113:208-14.

[29] Li L, Ji P, Zhang Y. Molecular dynamics simulation of condensation on nanostructured surface in a confined space. Applied Physics A. 2016 May 1;122(5):496.

[30] Ji CY, Yan YY. A molecular dynamics simulation of liquid–vapour–solid system near triple-phase contact line of flow boiling in a microchannel. Applied thermal engineering. 2008 Feb 1;28(2-3):195-202.

[31] Toghraie D, Azimian AR. Molecular Dynamics Simulation of Annular Flow Boiling in a Microchannel with 70000 Atoms. World Academy of Science, Engineering and Technology, International Journal of Mathematical, Computational, Physical, Electrical and Computer Engineering. 2011 Jun 25;5(6):831-7.

[32] Fu T, Mao Y, Tang Y, Zhang Y, Yuan W. Effect of nanostructure on rapid boiling of water on a hot copper plate: a molecular dynamics study. Heat and Mass Transfer. 2016 Aug 1;52(8):1469-78.

[33] Toghraie D, Mokhtari M, Afrand M. Molecular dynamic simulation of copper and platinum nanoparticles Poiseuille flow in a nanochannels. Physica E: Low-dimensional Systems and Nanostructures. 2016 Oct 1;84:152-61.

[34] Frank M, Drikakis D, Asproulis N. Thermal conductivity of nanofluid in nanochannels. Microfluidics and nanofluidics. 2015 Nov 1;19(5):1011-7.

[35] Cui W, Shen Z, Yang J, Wu S. Molecular dynamics simulation on flow behaviors of nanofluids confined in nanochannel. Case Studies in Thermal Engineering. 2015 Mar 1;5:114-21.

[36] Akbari OA, Safaei MR, Goodarzi M, Akbar NS, Zarringhalam M, Shabani GA, Dahari M. A modified two-phase mixture model of nanofluid flow and heat transfer in a 3-D curved microtube. Advanced Powder Technology. 2016 Sep 1;27(5):2175-85.

Journal Pre-proof

[37] Behnampour A, Akbari OA, Safaei MR, Ghavami M, Marzban A, Shabani GA, Mashayekhi R. Analysis of heat transfer and nanofluid fluid flow in microchannels with trapezoidal, rectangular and triangular shaped ribs. Physica E: Low-Dimensional Systems and Nanostructures. 2017 Jul 1;91:15-31.

[38] Bahmani MH, Sheikhzadeh G, Zarringhalam M, Akbari OA, Alrashed AA, Shabani GA, Goodarzi M. Investigation of turbulent heat transfer and nanofluid flow in a double pipe heat exchanger. Advanced Powder Technology. 2018 Feb 1;29(2):273-82.

[39] Alrashed AA, Akbari OA, Heydari A, Toghraie D, Zarringhalam M, Shabani GA, Seifi AR, Goodarzi M. The numerical modeling of water/FMWCNT nanofluid flow and heat transfer in a backward-facing contracting channel. Physica B: Condensed Matter. 2018 May 15;537:176-83.

[40] Gholami MR, Akbari OA, Marzban A, Toghraie D, Shabani GA, Zarringhalam M. The effect of rib shape on the behavior of laminar flow of oil/MWCNT nanofluid in a rectangular microchannel. Journal of Thermal Analysis and Calorimetry. 2018 Dec 1;134(3):1611-28.

[41] Rahimi Gheynani A, Ali Akbari O, Zarringhalam M, Ahmadi Sheikh Shabani G, Alnaqi AA, Goodarzi M, Toghraie D. Investigating the effect of nanoparticles diameter on turbulent flow and heat transfer properties of non-Newtonian carboxymethyl cellulose/CuO fluid in a microtube. International Journal of Numerical Methods for Heat & Fluid Flow. 2018 Oct 29.

[42] Zarringhalam M, Karimipour A, Toghraie D. Experimental study of the effect of solid volume fraction and Reynolds number on heat transfer coefficient and pressure drop of CuO–water nanofluid. Experimental Thermal and Fluid Science. 2016 Sep 1;76:342-51.

[43] Mahian O, Kolsi L, Amani M, Estellé P, Ahmadi G, Kleinstreuer C, Marshall JS, Siavashi M, Taylor RA, Niazmand H, Wongwises S. Recent advances in modeling and simulation of nanofluid flows-part I: fundamental and theory. Physics reports. 2018 Dec 6.

[44] Mahian O, Kolsi L, Amani M, Estellé P, Ahmadi G, Kleinstreuer C, Marshall JS, Taylor RA, Abu-Nada E, Rashidi S, Niazmand H. Recent advances in modeling and simulation of nanofluid flows-part II: applications. Physics reports. 2018 Dec 5.

[45] Safaei MR, Mahian O, Garoosi F, Hooman K, Karimipour A, Kazi SN, Gharehkhani S. Investigation of micro-and nanosized particle erosion in a 90 pipe bend using a two-phase discrete phase model. The scientific world journal. 2014;2014.

[46] Rashidi S, Mahian O, Languri EM. Applications of nanofluids in condensing and evaporating systems. Journal of Thermal Analysis and Calorimetry. 2018 Mar 1;131(3):2027-39.

[47] http://**lammps**.**sandia**.**gov**/**cite**.**html**

[48] Yezdimer EM, Chialvo AA, Cummings PT. Examination of chain length effects on the solubility of alkanes in near-critical and supercritical aqueous solutions. The Journal of Physical Chemistry B. 2001 Feb 1;105(4):841-7..

[49] Delhommelle J, Millié P. Inadequacy of the Lorentz-Berthelot combining rules for accurate predictions of equilibrium properties by molecular simulation. Molecular Physics. 2001 Apr 20;99(8):619-25.

[50] Haile JM, Johnston I, Mallinckrodt AJ, McKay S. Molecular dynamics simulation: elementary methods. Computers in Physics. 1993 Nov;7(6):625-.

[51] Zarringhalam M, Ahmadi-Danesh-Ashtiani H, Toghraie D, Fazaeli R. Molecular dynamic simulation to study the effects of roughness elements with cone geometry on the boiling flow inside a microchannel. International Journal of Heat and Mass Transfer. 2019 Oct 1;141:1-8.

[52] E Khodabandeh, M Bahiraei, R Mashayekhi, B Talebjedi, D Toghraie, Thermal performance of Ag–water nanofluid in tube equipped with novel conical strip inserts using two-phase method: Geometry effects and particle migration considerations, Powder technology 338, 87-100, 2018

[53] Qumars Gravndyan, Omid Ali Akbari, Davood Toghraie, Ali Marzban, Ramin Mashayekhi, Reza Karimi, Farzad Pourfattah, The effect of aspect ratios of rib on the heat transfer and laminar water/TiO2 nanofluid flow in a two-dimensional rectangular microchannel, Journal of Molecular Liquids 236, 254-265, 2017

[54] H Noorian, D Toghraie, AR Azimian, The effects of surface roughness geometry of flow undergoing Poiseuille flow by molecular dynamics simulation, Heat and Mass Transfer 50 (1), 95-104, 2014

[55] Mohammad Hemmat Esfe, Hadi Hajmohammad, Davood Toghraie, Hadi Rostamian, Omid Mahian, Somchai Wongwises, Multi-objective optimization of nanofluid flow in double tube heat exchangers for applications in energy systems, Energy 137, 160-171, 2017

Journal Pre-proof

**Highlights:**

- A statistical investigation
- Using of molecular dynamic simulation
- Forced boiling flow in a square microchannel with spherical roughness:
- Effect of external driving force

Journal Pre-proof