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Full Length Article

# Effect of copper nanoparticles on thermal behavior of two-phase argon-copper nanofluid flow in rough nanochannels with focusing on the interface properties and heat transfer using molecular dynamics simulation

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ABSTRACT

A comparison between the efficacy of surface boundary structure and presence of nanoparticles on the condensation two-phase flow inside rough nanochannels has been accomplished by applying molecular dynamics procedure to evaluate the thermal conductivity and flow characteristics. Simulation is performed in a computational region with two copper walls containing rectangular rough elements under different saturated temperatures. The main properties of liquid–vapor interface including density and the number of liquid atoms, are obtained. It is observed that the density profile is more affected by nanoparticles than the roughness. Also, compared to the condensation of nanofluid in a smooth nanochannel, the rough wall causes a greater drop in the temperature at the early time steps and by development of liquid films, effects of the wall roughness reduce. At the first of the condensation process, adding nanoparticle causes that transferring argon particles to the liquid phase increases with a steeper slope. Furthermore, heat current autocorrelation function (HCACF) for nanofluid condensation flow over considered correlation time is analyzed and following that the thermal conductivity for different saturated conditions is calculated. It has been represented that at lower temperatures the roughness makes more significant influence on the heat transfer of two-phase flow, while at higher temperatures the importance of nanoparticles prevails.
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## 1. Introduction

Phase change processes including condensation and boiling flows in nano-sized systems have become exclusively substantial because of their application in the novel engineering fields. In such atomic levels the strong interactions between fluid-surface particles have significant impact on the flow characteristics. Compared to the nanochannel dimensions, the size of the surface structure is highlighted so that the roughness is a remarkable feature of the wall which can determine the flow behavior. The structure of the solid boundary in comparison of nanochannel dimensions and the interactions between fluid-wall atoms are the most substantial features which needs to be considered. The importance of this issue has been proofed in previous studies [1–8] that are confirmed the special emphasis of the channel width. Because of special properties of nanoparticles and nanostructures, unprecedented studies have been performed on their effects in many different applications, including medical usage [9–13]. On the other hand, the study of two-phase flows containing nanoparticles in combination with rough surfaces on the small scales can lead to interesting findings. Due to the complexities of nanoscale experimental studies, atomic simulation methods are impressive approaches in studying the multi-phase flow of nanofluids in such nanoscale systems. Molecular dynamics (MD) simulation is a computational method that can analyze complicated atomistic simulations with very high accuracy. This method is governed by solving Newton's equations with considering interatomic collisions to obtain

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the path of the system. In this approach using statistical mechanics several features of the complicated simulations can be calculated. MD has pioneering procedure for modeling interface dominated phenomena such as condensation and boiling flows. Different studies have focused on the application of MD to survey nanofluid flows [14]. Aminfar *et al.* [15] studied the simulation of nanofluid flow behavior in the nanochannels using MD. It was declared that due to the attendance of nanoparticles, velocity and slip length increased. Also, nanoparticles moved the fluid atoms to the center of the channel. Sun *et al.* [16] accomplished simulation of nanofluid shear flow to examine the thermal conductivity using molecular dynamics approach. It was concluded that velocity gradient in the flow increased thermal conductivity value. Moreover, in less volume fraction of nanoparticles, the higher values of thermal conductivity were obtained. Honarkhaha *et al.* [17] simulated thermal properties of the nanofluid influenced by various parameters inside a nanochannel using molecular dynamics approach. It was expressed that although the specific heat increased with increasing the nanoparticle size, the thermal conductivity decreased. Cui *et al.* [18] considered disparate shear velocities to simulation of nanofluid flow inside nanochannels by MD method. They concluded that increasing shear velocity enhanced the rotation of nanofluid. Kang *et al.* [19] perused MD simulation of argon- copper nanofluid with considering heat conduction using Green–Kubo relation. They declared that variations in the thermal conductivity with volume fraction had a linear trend. From another perspective, molecular dynamics simulation has been utilized in various researches to consider the effects of roughness on the behavior of different flows. Kamali and Kharazmi [20] investigated Poiseuille flow under the influence of surface roughness by placing roughness on the bottom surface of nanochannel using MD simulation. The results of their simulation showed that wall-fluid interactions as well as surface roughness are key parameters that should put under consideration in determining nanostructures and flow profiles in the nanochannels. Tohidi and Toghraie [21] accomplished Couette flow simulation to consider the impact of roughness geometry of nanochannel walls and the number of nanoparticles using molecular dynamics method. It was stated that enhancement of rough element height leaded to reduction of self-diffusion coefficient adjacent to the upper wall. Rahmatipour *et al.* [22] examined MD simulation of Couette flow in the nanochannels by locating two different roughness shape. It was shown that rough elements reduced the fluid slip and it was more obvious at higher height. Alipour *et al.* [23] carried out Poiseuille flow simulation inside a nanochannel with various surface structures using molecular dynamics. It was revealed that the rough elements increased the velocity and the roughness with rectangular shape had the most impact on the flow characteristics. Nikolaos and Dimitri [24] surveyed Poiseuille flow simulation inside rough nanochannels by MD method. It was declared that rough elements changed the solid–liquid interface characteristics. Moreover, density layering close to the walls was intensified due to the increasing the height of roughness. Toghraie *et al.* [25] applied MD simulation to study the Couette and Poiseuille flow of nanofluids in rough nanochannels. It was declared that nanoparticles created oscillations in the central region because of surface impact on the nanoparticles compared to the base fluid. Gao *et al.* [26] examined the flow passing through rough nanochannels with considering rectangular roughness on the surfaces using MD simulation. It was expressed that the rough elements reduced the density fluctuations. Also, there was a critical value above that the slip length was not affected by the confined scale. Kim and Darve [27] simulated electro-osmotic flow inside the nanochannels using MD. The results confirmed that surface roughness affected the near wall layering. Also, raising the roughness height caused lower rate of flow. Plus, molecular dynamics simulations of condensation and boiling two-phase flows have been performed in the studies of some researchers. Rashidi *et al.* [28] simulated condensation phenomenon in rough nanochannels with attaching barriers on the bottom surface using MD procedure. It was affirmed that the influence of surface structure on the condensation flow was more evident at the higher height of the barriers. Moreover, roughened surface caused to reduction of density fluctuations near the rough wall. Kuri *et al.* [29] simulated two-phase flow of evaporation and condensation with locating nanostructures on the walls using molecular dynamics approach. They concluded that adding nanostructures on the walls cased to reduction of mass flux. Ghahremanian *et al.* [30] carried out a MD simulation to assay the condensation process of nanofluid in the nanochannels. The effect of increasing the nanoparticle diameter on the thermal conductivity was greater compared to the increasing the number of nanoparticles. Li *et al.* [31] perused MD simulation of vaporization and condensation between cold and hot walls with adding nano-barriers on the cold wall. The results demonstrated that barriers empowered condensation phase change and raised the number of liquid atoms. He *et al.* [32] carried out the simulation of condensation process over solid surfaces using MD method. The results portended that enhancement of the temperature caused to increase the liquid layering and temperature gradient. Liao and Duan [33] performed MD simulation of evaporation and condensation on the surfaces including nanostructures. It was reported that larger nanostructure groove increased the number of liquid atoms and groove dimensions affected the condensation rate as well as heat transfer. Review of literatures confirms that although many studies have been performed on the simulation of nanofluids and the influence of surface structure under single- and two-phase flows by molecular dynamics method, modeling of nanofluid condensation process in rough nanochannels is neglected. Therefore, this paper provides simulation of condensation phase change of argon-copper nanofluid inside nanochannels besides considering rough walls to compare the significance of nanoparticles and roughness on the interface properties as well as thermal conductivity. Molecular dynamics simulation has been accomplished with rectangular roughness configurations and density, velocity and temperature profiles as well as heat flux and thermal conductivity under different saturated temperature conditions have been obtained.

## 2. Simulation method

The MD procedure is applied to simulation of annular condensation of argon-copper nanofluid inside rough nanochannels to compare the efficacy of nanoparticles and surface roughness on the flow behavior and heat transfer of condensation process. The simulation is fulfilled in a nanochannel with dimensions of $l_x \times l_y \times l_z = 5 \times 5 \times 22$ considering rough elements on the upper and lower walls according to the Fig. 1. The solid walls are located at $z = 0$ and $z = l_z$, including four layers of copper atoms. The initial arrangement of the particles is considered in face-centered cubic (FCC) crystal structure with lattice constant of 11 for argon and 3.597 for copper particles. In this way 1620 argon atoms are generated between the walls consisting of 1458 copper atoms so that each wall is decorated with two rectangular rough elements which contain 98 Copper particles. For creation of nanoparticle a spherical crystal is carved out with considering diameter of 0.5 nm so that the 48 copper atoms are located in the bulk region.

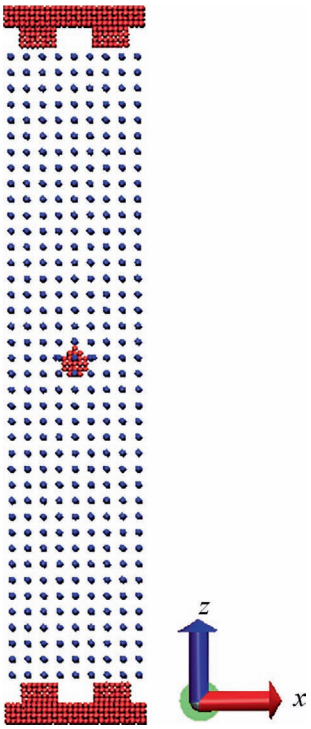


**Fig. 1.** Initial placement of nanofluid particles in nanochannels with rough walls.

The periodic boundary condition is exerted through the $x$ and $y$ directions.

In MD simulation a potential function is selected according to the type of the intended atom, and the exerted forces on the atoms are obtained using Eq. (1),

$$\boldsymbol{F}_{ij} = -\nabla(\phi + \phi_{\mathrm{w}}) \tag{1}$$

$$\boldsymbol{F}_i = \sum_{i \neq j} F_{ij} = m_i \frac{\mathrm{d}^2 \boldsymbol{r}_i}{\mathrm{d}t^2} = m_i \frac{\mathrm{d}\boldsymbol{v}_i}{\mathrm{d}t} \tag{2}$$

The recommended modified Lennard-Jones potential function [34] is considered for interaction of argon atoms as following equation:

$$\begin{aligned}\phi(r_{ij}) = &\left\{4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right]\right\} + \\ &\left\{4\varepsilon\left[6\left(\frac{\sigma}{r_{\mathrm{c}}}\right)^{12} - 3\left(\frac{\sigma}{r_{\mathrm{c}}}\right)^{6}\right]\right\}\left(\frac{r_{ij}}{r_{\mathrm{c}}}\right)^{2} - \\ &\left\{4\varepsilon\left[7\left(\frac{\sigma}{r_{\mathrm{c}}}\right)^{12} - 4\left(\frac{\sigma}{r_{\mathrm{c}}}\right)^{6}\right]\right\}\end{aligned} \tag{3}$$

where $\varepsilon$ and $\sigma$ represent the strength of interaction and atom diameter respectively, $r_{ij}$ mentions the interval between $i$ and $j$ atoms and $r_{\mathrm{c}}$ is the cut-off radius.

The interaction of argon and copper particles is modeled by Stoddard-Ford potential function combining with Lorentz-Berthlot mixing rule [35] so that $\varepsilon$ and $\sigma$ are replaced with $\varepsilon_{\mathrm{sf}}$ and $\sigma_{sf}$:

$$\varepsilon_{\mathrm{sf}} = \sqrt{\varepsilon_{\mathrm{s}}\varepsilon_{\mathrm{f}}}\sigma_{\mathrm{sf}} = \frac{\sigma_{\mathrm{s}} + \sigma_{\mathrm{f}}}{2} \tag{4}$$

The values of $\varepsilon$ and $\sigma$ for argon and copper are represented in Table 1.

For modeling the copper–copper interaction, EAM potential function is applied as follow [36]

**Table 1**
ε and σ values for argon and copper

| Material | $\varepsilon$/J | $\sigma$/m |
|---|---|---|
| Argon | $1.67 \times 10^{-21}$ | $3.4 \times 10^{-10}$ |
| Copper | $65.5815 \times 10^{-21}$ | $2.338 \times 10^{-10}$ |

$$E_i = F_i\left(\sum_{j \neq i} \rho_i(r_{ij})\right) + \frac{1}{2}\sum_{j \neq i} \phi_{ij}(r_{ij}) \tag{5}$$

For solving equation of motion to obtain particle path, velocity - Verlet algorithm [37] is utilized according to following relations:

$$r(t + \delta t) = r(t) + v(t)\delta t + \frac{1}{2}a(t)\delta t^2 \tag{6}$$

$$v(t + \delta t) = v(t) + \frac{1}{2}[a(t) + a(t + \delta t)]\delta t \tag{7}$$

Velocities are assigned random values. For determination of initial velocities of particles, Gaussian distribution method is employed:

$$\frac{1}{N_{\mathrm{atm}}}\sum_{i=1}^{N_{\mathrm{atm}}} \frac{1}{2}m\left|v_i^2\right| = \frac{3}{2}K_{\mathrm{B}}T \tag{8}$$

The temperature is defined according to equipartition theorem that states temperature of a system is pertained to its average kinetic energy:

$$T = \frac{\sum_{i=1}^{N_{\mathrm{atm}}} \frac{1}{2}m(v_{xi}^2 + v_{yi}^2 + v_{zi}^2)}{3K_{\mathrm{B}}N_{\mathrm{atm}}} \tag{9}$$

where $K_{\mathrm{B}}$ is the Boltzmann constant and $N_{\mathrm{atm}}$ is the number of atoms.

To discern the boundary between the liquid and vapor phases, the density is calculated using the cell method. In this method, the nanochannel is partitioned into 400 bins in the direction of phase change ($z$-axis) so that the particles in each bin at each time step is counted and divided to the volume of the bin which is considered as density. Considering these conditions, the density can be obtained from the following equation:

$$\rho(z) = \frac{N_{\mathrm{zi}}(z)m\sigma^3 M}{N_{\mathrm{sample}}L_x L_y \Delta z \sigma^3 N_{\mathrm{A}}} \tag{10}$$

where $L_x$ and $L_y$ demonstrate the dimension in $x$ and $y$-direction, m refers to particle mass, $N_{\mathrm{zi}}(z)$ and $N_{\mathrm{sample}}$ signify the number of molecules in $i^{\mathrm{th}}$ bin and sampling atoms, respectively.

Thermal conductivity is calculated as follow [9]:

$$\lambda = \frac{V}{3K_{\mathrm{B}}T^2}\int \langle \boldsymbol{J}(\boldsymbol{t}) \cdot \boldsymbol{J}(0)\rangle \mathrm{d}t \tag{11}$$

where $\boldsymbol{J}$ is the heat flux distribution that can be determined the following relation:

$$\boldsymbol{J}(\boldsymbol{t}) = \frac{1}{V}\sum_i \left[(E_{K\cdot i} + E_{P\cdot i} - \langle h_i\rangle)\boldsymbol{v_i} + \sum_{j\, j \neq i}(\boldsymbol{f_{ij}} \cdot \boldsymbol{r_{ij}})\boldsymbol{v_j}\right] \tag{12}$$

The first expression expresses the energy due to the self-diffusion where $\langle h_i\rangle = \langle E_{K\cdot i}\rangle + \langle E_{P\cdot i}\rangle$ is the sum of the average of the potential and kinetic energies which is related to the attendance of nanoparticles. The $\langle \boldsymbol{J}(\boldsymbol{t}) \cdot \boldsymbol{J}(0)\rangle$ term demonstrates heat flux autocorrelation function (HFACF) that by considering appropriate correlation time should tend to zero. In such a case its integral is correspond to the thermal conductivity.

The simulation is started by setting all argon particles at desired saturated temperature using Berendsen thermostat coupling with NVE microcanonical ensemble. The system takes 100,000 time steps to reach equilibrium. After equilibrium step the temperature of walls is adjusted at $T_{topwall} = T_{bottomwall} = T_{sat} - \Delta T$ and because of the interaction between fluid particles with the wall, phase change process occurs and liquid film forms on the walls. The system has been allowed to simulate during 1,000,000 time steps so that the sampling is done in each 100 time steps.

## 3. Results and discussion

The results of density calculation for saturated temperature of 102 K are plotted in Fig. 2. The figure demonstrates density profile for argon condensation with a nanoparticle in the smooth and rough nanochannels and for pure argon inside the rough nanochannel. During the condensation of nanofluid, the fluctuation in the middle region is due to the increasing the surface-to-volume ratio in this area as the presence of nanoparticle, which does not change much compared to the simulation without nanoparticle. The greatest effect of nanoparticle is on the density near the wall. According to the results, it is observed that the addition of nanoparticle to the fluid in both smooth and rough nanochannels causes asymmetry and non-uniform oscillations and moves the liquid film towards the walls relative to the middle of the nanochannel. However, even in the presence of nanoparticle, the rough elements restrict the free movement of fluid particles and reduce the magnitude of fluctuations in the proximity of the walls relative to the nanofluid condensation flow in the smooth nanochannel. Also, because during the condensation of nanofluid inside the rough nanochannel, the copper nanoparticle spends most of its time near the bottom wall and finally is placed in the liquid film formed on this wall, more fluctuations are apperceived on the liquid density profile in the left side. Comparing the results, generally the impact of nanoparticles on the density profile is greater than the adding rough elements on the walls.

Fig. 3 illustrates the fluid temperature profile for $T_{sat} = 102$ K along the $z$-axis inside a rough nanochannel with and without nanoparticle. It is apperceived that in the neighborhood of the walls, which are at lower temperature than the saturated temperature of argon, the local temperature of the fluid has decreased. However, due to the application of the thermostat, by moving away from the walls the temperature of the fluid increases and fluctuates around the saturated value. Placement of nanoparticle on the lower wall at the end of the simulation time causes a greater drop in the fluid temperature and increases the fluctuations in the adjacency of the lower wall compared to the temperature conditions of pure argon condensation, which results in the asymmetry in the temperature profile of nanofluid.

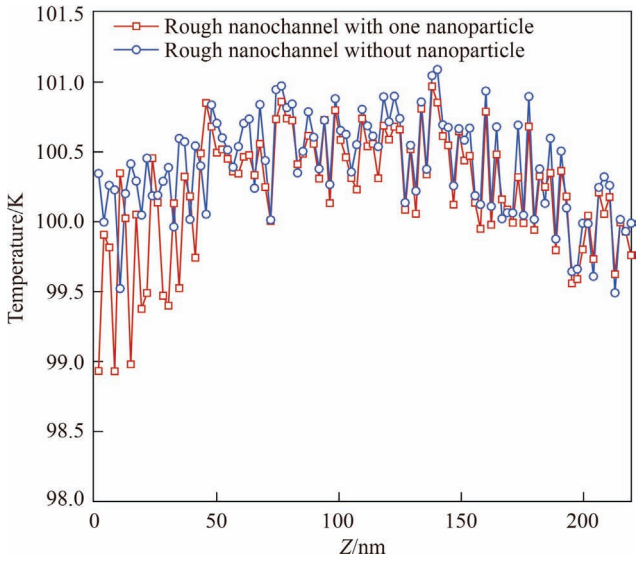


**Fig. 3.** Fluid temperature profile along the $z$-axis inside a rough nanochannel with and without nanoparticle at $T_{sat} = 102$ K.

The average temperature profile at $T_{sat} = 102$ K during the simulation time inside smooth and rough nanochannels is depicted in Fig. 4. This profile shows the influence of wall surface structure on the nanofluid temperature changes during phase change time. With starting the simulation, due to the local drop in the temperature near the walls, the average temperature of the fluid decreases, but over the time with formation of the condensation process and due to the application of thermostat, the temperature increases to near saturated value and fluctuates around it. It is declared that the influence of wall roughness on the temperature

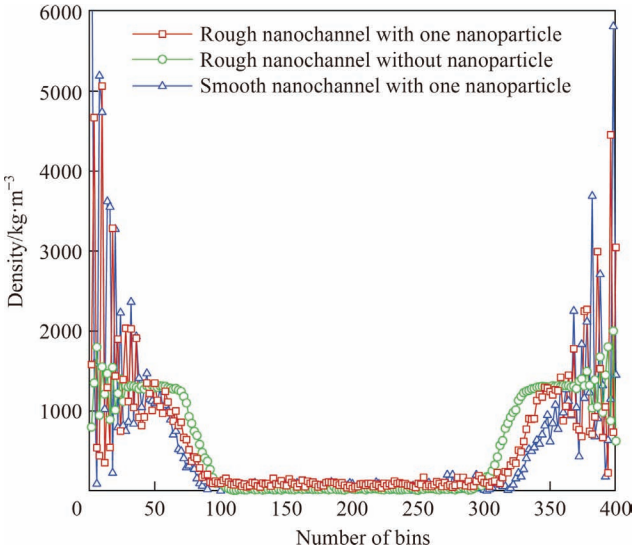


**Fig. 2.** Density profile at $T_{sat} = 102$ K in smooth and rough nanochannels.

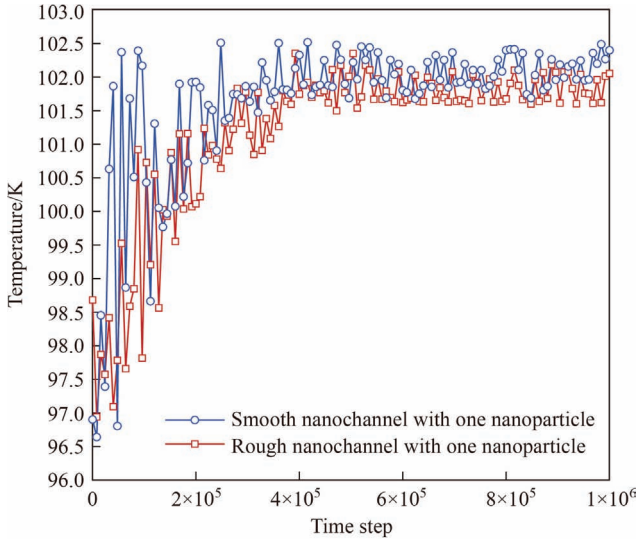


**Fig. 4.** Temperature change of nanofluid during the simulation time inside smooth and rough nanochannels at $T_{sat} = 102$ K.

profile is greater at the commencing of the simulation time and decreases during the time. As can be observed, compared to the condensation of nanofluid in a smooth nanochannel, the rough wall causes a greater drop in the temperature due to increased interaction of fluid and wall particles at the first of the condensation process so that by the formation of liquid film on the walls and locating argon particles between the rough elements, effects of the wall roughness reduce.

Fig. 5 shows the change in the number of liquid argon particles at $T_{sat} = 102$ K for the condensation process with and without the nanoparticle inside rough nanochannel, as well as in a smooth nanochannel with a nanoparticle. According to the consequences, at the commencing of the simulation time adding nanoparticle to the condensation flow inside the rough nanochannel compared to the condensation of pure argon, causes that the transferring of particles to the liquid phase increases with a steeper slope and reach a certain value. But with completing the simulation time and when the condensation process reaches a steady state, the presence of the nanoparticle in the base fluid within the rough nanochannel does not make much difference in the number of liquid particles. This is because at the primary steps, the nanoparticle is in the fluid flow and moves with the argon particles, which increases the interactions, then after a period of time, the nanoparticle is pulled towards the liquid film on the bottom wall. Also, comparing the trend of changing in the number of liquid particles during the time for condensation with a nanoparticle, it is observed that up to the time step of 400000, there is not much difference between the number of liquid particles in the smooth and rough nanochannels, but at termination of the running time, the roughness efficacy on the enhancement of the liquid particles is more significant so that has a greater increase than the nanofluid condensation in a smooth nanochannel, which is due to the gradual entrapment of argon particles between the rough elements.

Fig. 6 demonstrates the velocity profile in a rough nanochannel during the condensation of pure argon and argon-copper nanofluid for three different saturated temperatures. According to the figure, adding copper nanoparticle to pure argon fluid increases the fluctuations of the velocity profile. Furthermore, under different temperature conditions, the presence of nanoparticle increases the velocity values, especially in the middle region of the nanochannel, which is due to the increased interaction between atoms that leads to the strengthening of the condensation process and phase change.

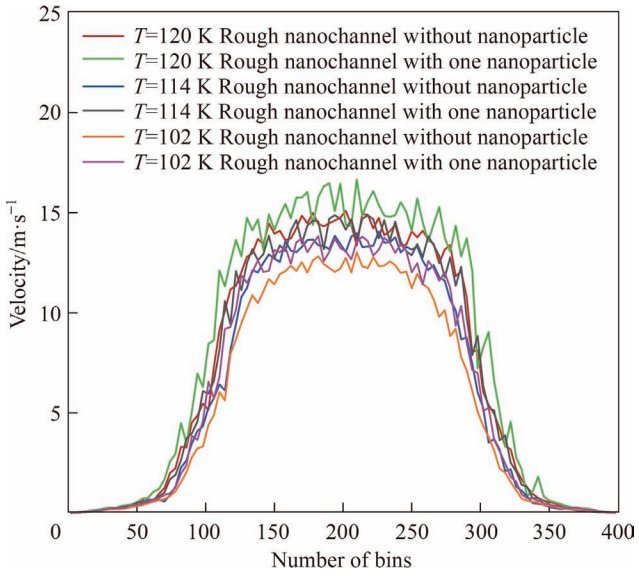


**Fig. 6.** Velocity profile in the z direction for three different saturated temperatures in the rough nanoparticles with and without nanoparticle.

The changes in heat current autocorrelation function (HCACF) for nanofluid condensation over correlation time of 0.1 ps (20,000 time steps) is shown in Fig. 7. It is evident that this term tends to zero during the nanofluid condensation with oscillating behavior in all cases due to the attendance of nanoparticles, but for the flow inside the rough nanochannel, these fluctuations are more pronounced, especially at lower time steps. Comparing the results affirms that HCACF for nanofluid flow with one nanoparticle in a rough nanochannel is greater than its values for nanofluid flow with one and two nanoparticles in a smooth nanochannel and tends to almost condensation conditions with three nanoparticles in a smooth nanochannel. As the thermal conductivity is commensurate to the HCACF integral, the surface roughness leads to the larger thermal conductivity. It is also observed that rough surfaces cause HCACF to drop to zero in a shorter period of time.

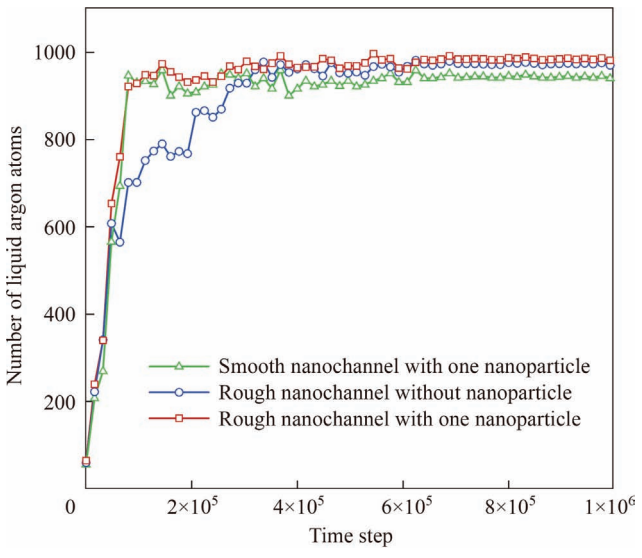


**Fig. 5.** Changing the number of liquid particles over time in smooth and rough nanochannels with and without nanoparticle at $T_{sat} = 102$ K.

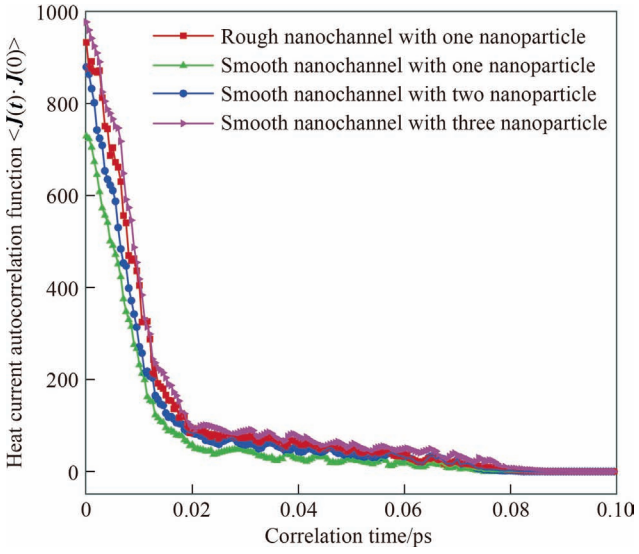


**Fig. 7.** Heat current autocorrelation function (HCACF) over correlation time for argon condensation in smooth nanochannel with different number of nanoparticles and rough nanochannels with one nanoparticle at $T_{sat} = 102$ K.

Comparison between the impact of adding copper nanoparticles and wall roughness on the values of the thermal conductivity obtained from the Green-Kubo formula at different saturated temperatures is represented in Fig. 8. From the calculated values, it is detected that both factors of adding nanoparticles and rough elements on the walls lead to increasing thermal conductivity of the condensation process. The thermal conductivity inside rough nanochannel without nanoparticles has almost the same results as the condensation inside smooth nanochannel with one nanoparticle, but by increasing the number of the nanoparticles in the smooth nanochannel, higher values of thermal conductivity can be achieved. Also, the presence of one nanoparticle in the condensation flow in the rough nanochannel has a substantial improvement on increasing the thermal conductivity relative to the flow in the nanochannel under the same conditions without nanoparticles.

The quantitative results of thermal conductivity at different saturated temperatures are shown in Table 2 as percentage increase due to the appending nanoparticles and rough elements compared to the condensation without nanoparticles in smooth nanochannel. According to the obtained values, it is observed that at saturated temperatures of 96 K, 102 K, 108 K and 114 K the highest growth in the thermal conductivity of condensation of argon in the smooth nanochannel is related to the argon-copper nanofluid flow in the rough nanochannel with one nanoparticle that the maximum rate of increase at these temperatures is 109.63%, 95.69%, 106.81% and 60.31%, respectively, while at saturated temperatures of 120 K and 133 K, the highest increase is related to the condensation of nanofluid in smooth nanochannel with three nanoparticles in the flow with maximum increase of 93.07% and 54.67%, respectively. This indicates that the roughness at lower temperatures has a better effect on the heat transfer of two-phase flow, while at higher saturated temperatures the addition of nanoparticles has a greater effect on improving the thermal conductivity of condensation.

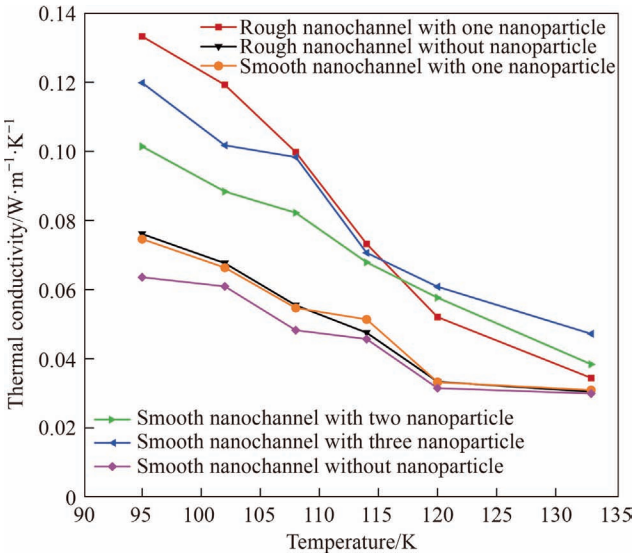


**Fig. 8.** Thermal conductivity of nanofluid condensation flow inside smooth and rough nanochannel with and without nanoparticle at different saturated temperatures.

## 4. Conclusions

In the presented study, MD simulation has been done to examine the interface properties and thermal behavior of nanofluid flow condensation inside nanochannels by attending rough surfaces. The following inferences are summarized as the most important results:

(1) The rough elements curb the free motion of argon particles and reduce the density oscillations in the proximity of the walls relative to the nanofluid condensation in the smooth nanochannels.
(2) By finishing the simulation time, the impact of roughness on the transferring the particles to the liquid films is more remarkable so that creates a greater enhancement in comparison of the nanofluid condensation in a smooth nanochannel.
(3) At the first of the simulation time, the temperature profile is most affected by the roughness and this effect decreases until the end of the simulation.
(4) The presence of nanoparticle increases the velocity values, especially in the middle region of the nanochannel.
(5) HCACF for nanofluid flow including one nanoparticle in a rough nanochannel is greater than its values for nanofluid flow with one and two nanoparticles in a smooth nanochannel and tends nearly to the values for condensation flow with three nanoparticles in a smooth nanochannel.
(6) The thermal conductivity of the condensation inside rough nanochannel without nanoparticles has almost the same results as the condensation inside smooth nanochannel with one nanoparticle.
(7) At lower temperatures, the roughness impress on the thermal behavior of condensation flow is dominant, while with increasing the temperature, the attendance of nanoparticles prevails.

## Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

**Table 2**
Percentage of increase in thermal conductivity of condensation due to the appending nanoparticles and rough elements compared to the condensation without nanoparticles in smooth nanochannels at different saturated temperatures

| Percentage increase in thermal conductivity/% | | | | | |
|---|---|---|---|---|---|
| $T_{Sat}$/K | Rough nanochannel with one nanoparticle | Rough nanochannel without nanoparticles | Smooth nanochannel with three nanoparticles | Smooth nanochannel with two nanoparticles | Smooth nanochannel with one nanoparticle |
| 96 | 109.63 | 19.70 | 88.49 | 59.51 | 17.39 |
| 102 | 95.69 | 11.01 | 66.95 | 45.008 | 8.89 |
| 108 | 106.81 | 14.97 | 103.78 | 70.49 | 13.35 |
| 114 | 60.31 | 4.04 | 54.66 | 48.63 | 12.47 |
| 120 | 65.15 | 5.91 | 93.07 | 83.01 | 5.47 |
| 133 | 14.98 | 1.68 | 57.67 | 28.16 | 3.37 |

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