Numerical Simulation Of Nanofluid Viscosity Using Molecular Dynamics

Amir haghighatkhah
Master of Mechanical Engineering
Tehran, Iran
haghighatkhah.eng@gmail.com

Milad Abdollahi Kahriz
Tehran, Iran
Miladmak@yahoo.com

Hossein Ahmadi-Danesh-Ashtiani
Islamic azad university, PhD ,Department of
Mechanical Engineering, South Tehran Branch,
Islamic Azad University, Tehran, Iran
h_a_danesh@azad.ac.ir
hdanesh1381@yahoo.com

Kourosh Amiraslani
Islamic azad university, PhD ,Department of
Mechanical Engineering   South Tehran Branch,
Islamic Azad University, Tehran, Iran
k_amiraslani@azad.ac.ir

Abstract—**Due to the growing need of industries for heat transfer with higher efficiency and in smaller volumes, researchers have studied the use of nanofluids as a substitute for conventional fluids for heat transfer. In the present paper, viscosity as one of the key thermophysical properties of a fluid has been investigated using molecular dynamics simulations. To perform molecular dynamics simulations, Lamps software has been used. A complete description of the theory of interaction between fluid and nanofluid particles has been investigated in order to achieve the key parameters of nanofluid. A detailed description of the relationships and equations governing phenomena such as potential force applied to various fluid particles and nanoparticles is provided. The validity of the obtained numbers and ratios for the viscosity of nanofluids with different nanoparticle characteristics and pure fluid is measured using the fluctuations of stress correlation functions. Analysis of shear stress correlation function and the results show that the presence of nanoscale particles in the base fluid leads to significant changes in the amount of nanofluid viscosity compared to the base fluid. The ratio of nanofluid viscosity to base fluid viscosity varies in different nanofluids, but it can be seen that on average the minimum viscosity increase is about 1.2 times that of the base fluid. Finally, the results obtained from molecular dynamics simulations are compared with the values obtained from experimental results and existing theories, and comparison charts containing the results are presented.**

Keywords—Molecular dynamics, Nanofluid, Lamps, Numerical simulation, Viscosity

I. Introduction

In addition to many of the macroscopic models proposed to describe the static and dynamic thermophysical properties of nanofluids, equal and unequal simulations are useful tools for providing a detailed view of the physical mechanisms governing intermolecular interference at the nanoscale [1].

Brownian motion has been shown to play a weak role in heat transfer and microscopic heat transfer calculations [2]. These observations have been confirmed by other researchers [4,3]. Also, various researchers have investigated the simulation of molecular dynamics to support experimental results such as volume concentration, the important role of nanoparticles and temperature in increasing heat transfer and viscosity of nanofluids [5-8]. Contrary to the complex data obtained, subsequent molecular dynamics studies focused on understanding the effect of nanoparticles on increasing the heat transfer of nanofluids. For example, it was suggested that particle-fluid interaction plays a key role in transmitting temperature characteristics and thus improving nanofluid heat transfer [9]. This point was investigated by other researchers and it was found that both wet and non-wet regimes affect the temperature resistance in the liquid-solid interaction [10]. Further studies on liquid-solid interferences showed that the liquid near the surface has higher heat transfer values compared to the bulk fluid and the ratio of capillary resistance thickness to nanoparticle diameter is significant [12,11]. It was shown that a dynamic layer is formed at the nanoparticle surface by which potential energies are exchanged between solid and liquid [13]. It is with the help of this dynamic layer that a permeable network is created in the nanofluid system in which the transferred energy potentials are maximized [14]. Research has shown that the collision-collision function of the collision of liquid molecules near the nanoparticle surface (hydration layer) is the dominant factor in improving the heat transfer of the nanoparticle-water theory system [15]. The combination of potential-kinetic relationship is the dominant relationship in thermal conductivity calculations [16]. Viscosity depends on two factors, the concentration and diameter of nanoparticles [17], although the shear behavior of nanofluids decreases sharply in two cases, which are the ratio of size and mass of nanoparticles to fluid larger than one and

increasing the volume ratio with size ratios and Mass greater than one [17].

It is shown that the viscosity of the nanofluid depends on the mass of the particle and the field of effect of the nanoparticle is half the diameter of the particle [18]. It was also shown that the ocular motion of nanoparticles and its strong effect on a large volume of surrounding fluid are factors that cause a significant increase in viscosity in the nanofluid system [19].

II. MOLECULAR DYNAMICS SIMULATION

The hypothesis of the energy part is written as follows:

$$\sum_{i=1}^{N} \frac{P_i^2}{m_i} = 2 < K > = 3NK_BT$$

(1)

In the above relation <K> represents the total energy of a system with N particles, P represents the motion of a particle, m is the mass of a particle, T is the absolute temperature and K_B is the Boltzmann constant. Using this rule, the instantaneous temperature (T_{ins}) can be determined by calculating the instantaneous kinetic energy (K_{ins}). Based on this, the instantaneous temperature for a set containing N atoms can be calculated as follows:

$$T_{ins} = \frac{K_{ins}}{3NK_B} = \frac{1}{3NK_B}\sum_{i=1}^{N}\frac{P_i^2}{m_i}$$

(2)

According to the virial hypothesis, the total virial is composed of two components, the internal and external virials. As a result, the instantaneous pressure is calculated from the following equation:

$$P_{ins} = \frac{2K_{ins}}{3V} + \frac{1}{3V}\sum_{i=1}^{N}\sum_j r_{ij}\cdot f_{ij} = \frac{1}{3V}\sum_{i=1}^{N}\frac{P_i^2}{m_i} + \sum_{i=1}^{N}\sum_j r_{ij}\cdot f_{ij}$$

(3)

In the above relation, r_{ij} represents the distance between two atoms i and j and f_{ij} is the force between two atoms. P represents pressure and V represents volume. An important result of the above equation can be expressed as the pressure in a N atomic system consists of an additional part over the kinetic part that is formed by the interaction between atoms.

Classical molecular dynamics simulations involve calculating the trajectories of N atoms interacting with each other, which are limited in volume and form a nanometer set. Basic information in this case includes the location and velocity of the atoms. Differential equations for the motion of a set consisting of N atoms are solved by various methods of finite difference so that the forces on the atoms can be calculated by inter-atomic potential functions.

For a particle N system, the motion equations under consideration can include 6N first-order Hamiltonian equations or 3N quadratic Newtonian equations, which are usually used to solve quadratic Newtonian equations. The travel paths can be calculated by a finite difference method, which uses a velocity algorithm. According to this algorithm, the r_i locations and v_i velocities of atoms with mass m_i in each time interval δt are expressed as follows:

$$r_i(t + \delta t) = r_i(t) + \delta t v_i + \frac{1}{2}\delta t^2 a_i(t)$$

(4)

$$v_i\left(t + \frac{1}{2}\delta t\right) = v_i(t) + \frac{1}{2}\delta t a_i(t)$$

(5)

$$v_i(t + \delta t) = v_i\left(t + \frac{1}{2}\delta t\right) + \frac{1}{2}\delta t a_i(t + \delta t)$$

(6)

In the above relation:

$$a_i(t) = -\left(\frac{1}{m}\right)\Delta V(r_i(t))$$

(7)

In the above relation, acceleration is directly related to the particle location through the potential function gradient.

In the direct velocity scaling method, the velocity components of the particles are scaled according to the instantaneous temperature difference with the canonical shear temperature. In this regard, the following equation can be used.

$$V_i^{new} = v_i\sqrt{\frac{T_D}{T_A}}$$

(8)

In the above relation, T_D represents the current particle temperature and T_A represents the predetermined temperature. The numbers in molecular dynamics simulation programs sometimes differ so much in scale that this makes calculations impossible. To solve this problem, new units must be produced for the length, energy and mass of a new system of units in which the numbers in this system differ by a smaller order. With this view, r calculations can be performed in a new system of units and finally the simulation results can be converted into real numbers.

III. THE MAXIMUM LENGTH OF THE PAPER

To achieve the dynamic properties of an equilibrium system, non-equilibrium thermodynamics must be used. In fact, macroscopic dynamic properties can be obtained from the microscopic values of the equilibrium system using the first and second laws of thermodynamics. According to the non-equilibrium theory, viscosity is calculated as follows:

$$\eta = \frac{V}{K_BT}\int_0^\infty < P_{xy}(0)P_{xy}(\tau) > d\tau$$

(9)

$$P_{xy}(\tau) = \sum_i \frac{P_x^i P_y^i}{m^i} - \frac{1}{2}\sum_i r_x^{ij} F_y^{ij}$$

(10)

In the above relations, m and P represent the mass and momentum of a particle, respectively, r and F,

respectively, the distance and force vector between two particles.

The local equilibrium of the selected physical system is defined provided that the state values in the selected volume are negligible and are larger than the longest free distance of the average constituent particles. Molecular dynamics simulations are performed within these volumes with local equilibrium. It is not possible to define the thermodynamic state of these local volumes in the molecular dynamics simulation separately and it must be obtained from the statistical average of one of the possible microstates of the system. Different types of granules are used in the simulation of molecular dynamics [20]. In this study, the number of N particles, volume V and temperature T are constant values that determine the thermodynamic state and are obtained from the values calculated from experimental data. The thermodynamic conditions of the liquid argon simulated in this research are given in Table (1).

Table 1. Thermodynamic conditions of liquid argon simulated in the present study

Nanoparticle diameter(nm)	Total number of particles	Volume(cnm)	Temperature(K)
0.5	2048	95.820	87.057
1	5000	136.431	

The thermodynamic mode selected for the local volume of the simulated liquid argon in the equilibrium is assumed that the density and temperature are close to their triple point. The graph of total temperature and energy during the equilibration period in the molecular dynamics simulation of pure argon fluid is shown in Figure (1). It is observed that the temperature fluctuates around the mean value of 87.057 Kelvin and the energy converges.
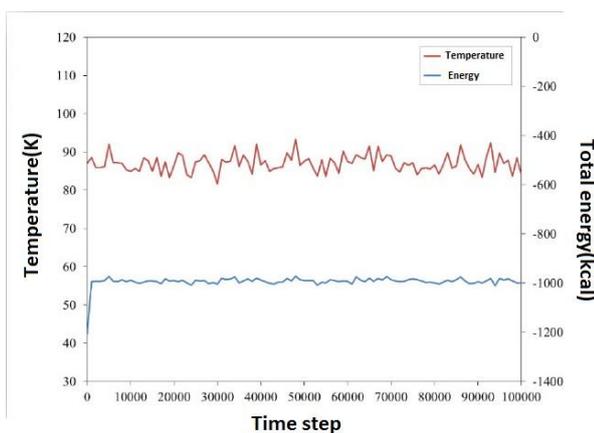
Figure 1. Values of total temperature and energy in the equilibrium process in the simulation of molecular dynamics of liquid argon

In calculating the volume ratio of nanofluids instead of directly calculating the ratio of the volume of nanoparticles to the volume of the base fluid, the volume ratios used in this research are based on

calculating the volume occupied by nanoparticles and fluid, which is calculated as follows:

$$\emptyset = \frac{N_{np}\left(\frac{4}{3}\pi r^3\right)}{vV - N_{np}\left(\frac{vV}{N_f}\right) + N_{np}\left(\frac{4}{3}\pi r^3\right)}$$
(11)

In the above relation, v is the packing atomic coefficient, which is considered for FCC structures 0.74, and N_{np} is the number of soluble nanoparticles and r is the radius of the nanoparticle.

The next step is to express the thermophysical coefficients obtained from valid experimental laws based on the microscopic values obtained from molecular dynamics simulations. While the thermophysical coefficients directly depend on the diametric values of the natural coefficient matrix (L_{ik}), it can be expressed as follows:

$$\lambda = \frac{L_{qq}}{T^2}$$
(12)

$$\eta = \frac{L}{2T}$$
(13)

The calculation of natural coefficients requires mathematical formulations derived from theoretical ideas related to non-equilibrium thermodynamics. For this purpose, the Green-Kubo relationship can be used as follows:

$$L_{ik} = \frac{V}{k_B T}\int_0^\infty <J_i(0)J_i(\tau)> d\tau$$
(14)

In the models that have been introduced to simulate the molecular dynamics of nanofluids so far, the Lenard-Jones potential has been used to describe the interaction effects of nanoparticles and fluid. But this model often gives inaccurate results for calculating nanofluid conductivity. Hence the colloidal model is presented. In this model, nanoparticles are considered as a solid sphere whose diameter is larger than the diameter of fluid particles. The equilibrium between the fluid and the nanoparticle is calculated using the Gay-Byrne potential for two spherical particles, one of which is assumed to have a radius of zero, as follows:

$$U = \frac{2a^3\sigma^3 A_{cs}}{9(a^2-r^2)^3}\left[1 - \frac{(5a^6+45a^4r^2+63a^2r^4+15r^6)\sigma^6}{15(a-r)^6(a+r)^6}\right]$$
(15)

In the above relation σ the size of the Lennard-Jones solvent particle, a is the radius of the colloidal particle and A_{cs} is the constant consonant.

IV. RESULTS

To calculate the viscosity of copper-argon nanofluid, it is first necessary to calculate the viscosity of liquid argon. In calculating the viscosity of argon, it should be taken into account that with increasing the diameter of the nanofluid, the volume of the simulation box also increases, so the viscosity of liquid argon in

different volumes should be calculated. The average viscosity of pure argon fluid at 87 K in volumes of 0.5 and 1 nm nanofluids is 268.25 µPa.s, which is consistent with the number 299.37 µPa.s presented in various references.

Figure (2) shows the dimensionless autocorrelation function related to the average viscosity of pure argon in different volumes.
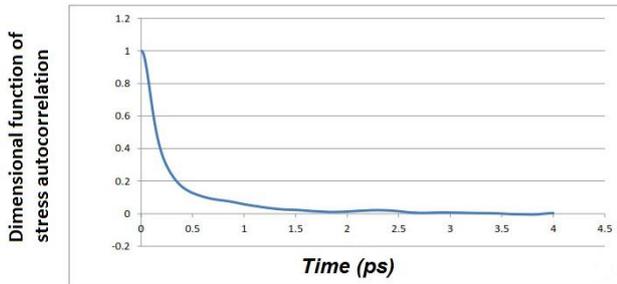
Figure 2. Dimensional function of mean stress self-correlation for pure argon in different volumes

Figure (2) well shows the absence of excess stress or residue in the fluid.

By changing the diameter of the nanoparticles or changing the volume of the simulation box, the volume percentage of the nanoparticles changes to the total volume of the fluid. Figure (3) shows the changes in the viscosity of aluminum-argon nanofluid with a nanoparticle diameter of 0.5 nm in different volume percentages.
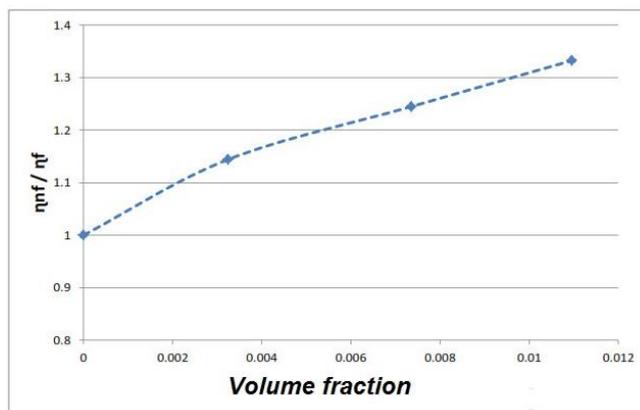
Figure 3. Effect of volume ratio on the viscosity of nanofluid with nanoparticles with a diameter of 0.5 nm

According to Figure (3), with increasing the volume percentage of nanofluid, which is done by reducing the dimensions of the simulation box, the viscosity ratio of nanofluid to the base fluid increases. Of course, this increase in the maximum case in the volume percentage of 0.01096 is about 30%.

A similar study for nanoparticles with a diameter of 1 nm is given in Figure (4).
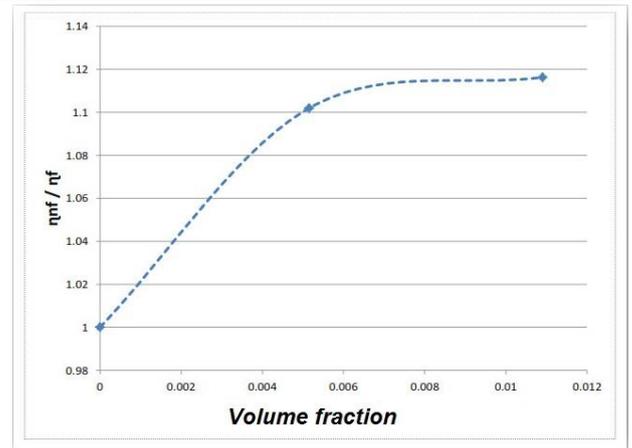
Figure 4. Effect of volume ratio on the viscosity of nanofluids with nanoparticles with a diameter of 1 nm

In order to validate the model developed in Figures (5) and (6), the amount of argon viscosity increase with increasing nanoparticle diameter and the increase of aluminum oxide nanofluid viscosity in different volume ratios with different volume models have been compared, respectively.
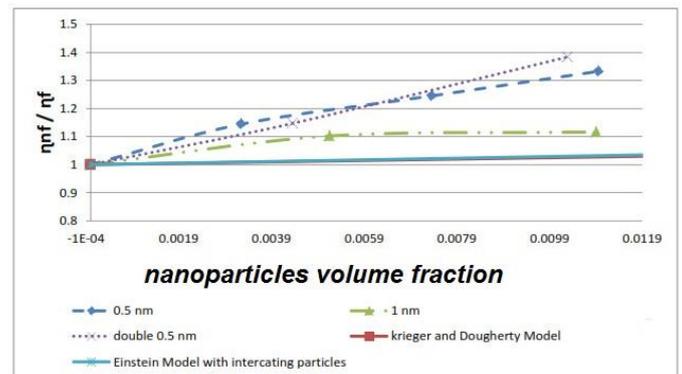
Figure 5. Increase of viscosity in argon fluid by increasing the nanoparticle diameter compared to theoretical models
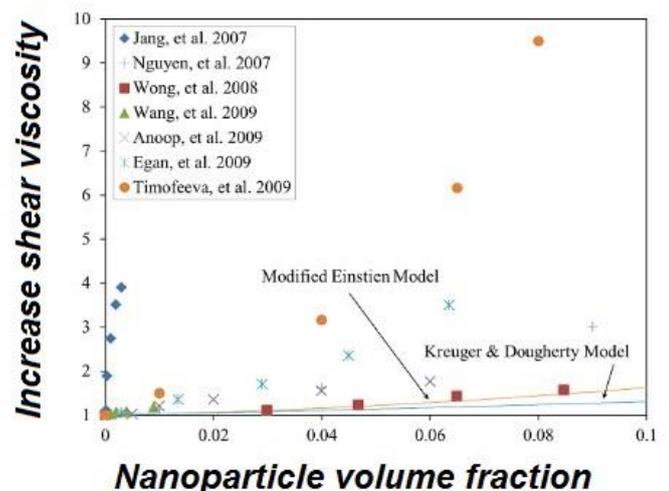
Figure 6. Increase the viscosity of aluminum oxide nanofluids in different volume ratios

It is observed that the viscosity of the nanofluid may be higher than the viscosity of the base fluid.

The effect of nanofluid temperature on viscosity is investigated. Considering the NVT curve and the constant temperature and volume during molecular dynamic simulation, the temperature is reduced by 40 degrees Kelvin in two steps. It should be noted that at all these temperatures, argon is a liquid and the temperature change for nanoparticles with a diameter of 0.5 nm and in different volume ratios has been done. The results are shown in Figure (7).
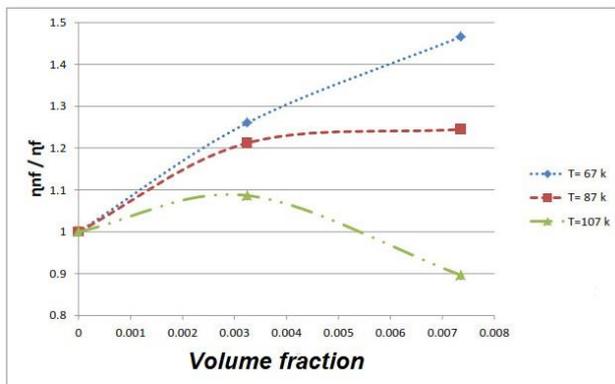
Figure 7. Investigation of the effect of temperature on the viscosity of nanofluids with nanoparticles of 0.5 nm

According to Figure (7), it can be seen that with increasing temperature, the amount of viscosity decreases so that at a high volume ratio at 107K, the viscosity decreases to a lesser extent than the viscosity of the base fluid. Of course, with increasing the volume ratio, the amount of viscosity also increases, that is, with increasing the density of nanoparticles, the amount of viscosity has increased in all cases.

V. CONCLUSION

Due to the acceptable mismatch between the experimental results related to the calculation of thermophysical properties of nanofluids that play an important role in the design of heat transfer systems, the molecular dynamics of copper-argon nanofluid viscosity has been investigated in this study.

Using the size-dependent colloidal potential model to calculate the particle impact energy in the nanofluid, it was observed that the addition of nanoparticles to the base fluid is associated with a change in the viscosity of the resulting nanofluid. The calculated viscosity values for the nanofluid showed that the viscosity is strongly dependent on the interaction between the particle and the fluid. Of course, it should be noted that this dependence is very small compared to the viscosity dependence on the volume percentage of the nanofluid under study. It can be concluded that the models used to calculate and simulate the interaction between the base fluid particles do not play an effective role in calculating the overall viscosity of the nanofluid and can be used without changing the response.

Initially, the viscosity values of pure liquid argon in different volumes were calculated. Considering that by changing the size of the simulation box, the amount of

different volume ratios is obtained to simulate the molecular dynamics of nanofluids, it is necessary to calculate the viscosity of the base fluid in different volumes by changing the size of the simulation box. Then, the obtained values are compared with the values presented by reputable authorities, which has an acceptable convergence.

In the next step, by calculating the amount of viscosity for nanofluids with nanoparticles with diameters of 0.5 and 1 nm, the viscosity ratio of nanofluids to the base fluid in different volume ratios is obtained. The presented diagrams show the increase of nanofluid viscosity with increasing volume ratio of nanoparticles to base fluid. This increase is greater in nanofluids with smaller nanoparticles, which indicates an increase in viscosity in the nanoparticle concentration.

The results also showed that temperature changes have a significant effect on the viscosity of nanofluids and can increase or decrease the viscosity of nanofluids by changing the temperature in the designed system (as long as the base fluid does not leave the liquid phase). This reduction in viscosity at high temperatures can extend to less than the viscosity of the base fluid. Finally, the results can be categorized as follows:

1. Increased viscosity of the resulting nanofluid compared to pure liquid argon

2. Aluminum-Argon Oxide Nanofluid Viscosity Dependence on Nanoparticle Size Used

3. Nonlinear relationship between nanoparticle size and nanofluid viscosity

4. Changing the viscosity of the nanofluid by changing the simulated temperature conditions

REFERENCES

[1] Li, Y., Zhai, Y., Ma, M., Xuan, Z., & Wang, H. (2021). Using molecular dynamics simulations to investigate the effect of the interfacial nanolayer structure on enhancing the viscosity and thermal conductivity of nanofluids. International Communications in Heat and Mass Transfer, 122, 105181.

[2] Rudyak, V., Krasnolutskii, S., Belkin, A., & Lezhnev, E. (2021). Molecular dynamics simulation of water-based nanofluids viscosity. Journal of Thermal Analysis and Calorimetry, 145(6), 2983-2990.

[3] Zeroual, S., H. Loulijat, E. Achehal, P. Estellé, A. Hasnaoui, and S. Ouaskit. "Viscosity of Ar-Cu nanofluids by molecular dynamics simulations: effects of nanoparticle content, temperature and potential interaction." Journal of Molecular Liquids 268 (2018): 490-496.

[4] Razmara, N., Namarvari, H., & Meneghini, J. R. (2019). A new correlation for viscosity of model water-carbon nanotube nanofluids: Molecular

dynamics simulation. Journal of Molecular Liquids, 293, 111438.

[5]   Bao, L., Zhong, C., Jie, P., & Hou, Y. (2019). The effect of nanoparticle size and nanoparticle aggregation on the flow characteristics of nanofluids by molecular dynamics simulation. Advances in Mechanical Engineering, 11(11), 1687814019889486.

[6]   Jabbari, F., Saedodin, S., & Rajabpour, A. (2018). Experimental investigation and molecular dynamics simulations of viscosity of CNT-water nanofluid at different temperatures and volume fractions of nanoparticles. Journal of Chemical & Engineering Data, 64(1), 262-272.

[7]   Heyhat, M. M., Rajabpour, A., Abbasi, M., & Arabha, S. (2018). Importance of nanolayer formation in nanofluid properties: Equilibrium molecular dynamic simulations for Ag-water nanofluid. Journal of Molecular Liquids, 264, 699-705.

[8]   Izadkhah, M. S., & Zeinali Heris, S. (2019). Influence of Al2O3 nanoparticles on the stability and viscosity of nanofluids. Journal of Thermal Analysis and Calorimetry, 138(1), 623-631.

[9]   Wu, L., Keer, L. M., Lu, J., Song, B., & Gu, L. (2018). Molecular dynamics simulations of the rheological properties of graphene–PAO nanofluids. Journal of Materials Science, 53(23), 15969-15976.

[10] Jabbari, F., Rajabpour, A., & Saedodin, S. (2019). Viscosity of carbon nanotube/water nanofluid. Journal of Thermal Analysis and Calorimetry, 135(3), 1787-1796.

[11] Wang, Z., Li, L., & Yang, M. (2020). Molecular dynamics simulation of the wetting characteristics of a nanofluid droplet on rough substrate. Journal of Molecular Liquids, 319, 114204.

[12] Vakili-Nezhaad, G. R., Al-Wadhahi, M., Gujarathi, A. M., Al-Maamari, R., & Mohammadi, M. (2019). Molecular dynamics simulation of water–graphene nanofluid. SN Applied Sciences, 1(3), 1-7.

[13] Rudyak, V. Y., & Minakov, A. V. (2018). Thermophysical properties of nanofluids. The European Physical Journal E, 41(1), 1-12.

[14] Yan, S. R., Toghraie, D., Hekmatifar, M., Miansari, M., & Rostami, S. (2020). Molecular dynamics simulation of Water-Copper nanofluid flow in a three-dimensional nanochannel with different types of surface roughness geometry for energy economic management. Journal of Molecular Liquids, 311, 113222.

[15] Rabani, R., Saidi, M. H., Joly, L., Merabia, S., & Rajabpour, A. (2021). Enhanced local viscosity around colloidal nanoparticles probed by Equilibrium Molecular Dynamics Simulations. The Journal of Chemical Physics, 155(17), 174701.

[16] Abbasi, M., Heyhat, M. M., & Rajabpour, A. (2020). Study of the effects of particle shape and base fluid type on density of nanofluids using ternary mixture formula: A molecular dynamics simulation. Journal of Molecular Liquids, 305, 112831.

[17] Mirmohammadi, S. A., Behi, M., Gan, Y., & Shen, L. (2019). Particle-shape-, temperature-, and concentration-dependent thermal conductivity and viscosity of nanofluids. Physical Review E, 99(4), 043109.

[18] Toghraie, D., Hekmatifar, M., Salehipour, Y., & Afrand, M. (2019). Molecular dynamics simulation of Couette and Poiseuille Water-Copper nanofluid flows in rough and smooth nanochannels with different roughness configurations. Chemical Physics, 527, 110505.

[19] Rudyak, V. (2019). Thermophysical characteristics of nanofluids and transport process mechanisms. Journal of Nanofluids, 8(1), 1-16.

[20] Ahmed, Z., Bhargav, A., & Mallajosyula, S. S. (2018). Estimating Al2O3–CO2 nanofluid viscosity: a molecular dynamics approach. The European Physical Journal Applied Physics, 84(3), 30902.