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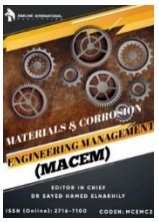

RESEARCH ARTICLE

MOLECULAR DYNAMICS SIMULATION OF THE VISCOSITY AND THERMAL CONDUCTIVITY OF AL_2O_3-H_2O NANOFLUIDS

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ABSTRACT

This research investigated Al_2O_3-H_2O nanofluids' conduction of heat and viscosity using molecular dynamics method. For nanofluids, consequences of the nanoparticles' volume fraction, temperature, size, and shape were studied. EMD computed the Al_2O_3-H_2O nanofluid viscosity, while NEMD calculated the thermal conductivity. The findings indicated the sensitivity of the nanofluid to temperature and volume fraction variations. Alongside rising volume fraction, viscosity and conduction of heat likewise rise. When the temperature rises, the viscosity will decrease, and the thermal conductivity will increase. And the variation trend is the same as the experimental value. At the same temperature, the particle size of the nanoparticles becomes smaller, the specific surface area of the particles becomes larger, and the viscosity and thermal conductivity of the nanofluids become larger. And get the shape of the nanoparticles at the time of low volume fraction of greater effects on the viscosity and thermal conductivity of nanofluids, but in the case of high-volume fraction, volume fraction increases nano fluid viscosity and thermal conductivity coefficient is bigger.

KEYWORDS

molecular dynamics simulation; nanofluid; viscosity; thermal conductivity

1. INTRODUCTION

With the development of various electronic industries, traditional heat dissipation base fluids cannot meet the required heat dissipation requirements, Choi et al. proposed to add nanoparticles into the traditional heat transfer fluid based on research (Choi et al., 2001). A base fluid's viscosity and thermal conductivity were enhanced, while nanofluid outperformed conventional heat dissipation (Sina et al., 2016). Nanoparticles and a base fluid comprise the nanofluid. Because it can enhance heat transfer, the advantages of channel blockage and wear in the channel have attracted the attention of many scholars (Duan et al.,2011; Meyer et al.,2016). They use experiments or molecular dynamics simulation (MD) transport properties nanofluids. In a very short time due to the occurrence of physical phenomena by molecular dynamics simulation cannot be observed in practical tests, especially the microscopic details of the phenomenon, molecular dynamics can be directly observed by using this tool, enabling the development of molecular dynamics (Phillpot et al.,1995).

At present, there are two main research methods, namely equilibrium molecular dynamics (EMD) and non-equilibrium molecular dynamics (NEMD). The EMD method is used to simulate the transfer coefficient, such as thermal conductivity and shear viscosity, the transfer coefficient of nanofluid can be expressed as the general form of Green-Kubo formula, but the EMD calculation method has a large amount of calculation (Green 2004; Babaei et al.,2012). Ikeshoji and Hafskjold put forward NEMD, in the simulation, two heat sources and heat sinks were established (Ikeshoji and Hafskjold, 1994). The system attained a constant state through periodic exchange, given a temperature gradient and an energy flux (Cerbelaud et al., 2017). Muller-Plathe proposed the anti-perturbation nonequilibrium dynamics (RNEMD) method, which uses the exchange of atomic centroid velocities at different locations to result in the formation of hot and cold regions in the simulated system, obtaining the temperature gradient and calculating the thermal conductivity of the nanofluids (Florian,1997).

Mehdi et al. discovered based on simulation how Ar-Cu nanofluids' conduction of heat increased progressively alongside temperature (Mehdi et al., 2018). Seyed et al. likewise provided a simulation of the effects of water-based Ag nanofluids on nanofluid viscosity considering the various configurations of Ag nanoparticles (Mirmohammadi et al., 2019). Rudyak et al. presented how nanoparticles' conduction of heat relied on particle size, rising as particle size increased (Rudyak and Krasnolutskii, 2015; Rudyak and Krasnolutskii, 2017). It also indicated that some nanoparticles with small particle size may make the thermal conductivity of the nanofluid less than the base liquid. Nguyen et al. showed that when water-based copper oxide and alumina were used, the influence of temperature and particle size on nanofluid viscosity was studied experimentally (Essajai et al., 2019). Lou et al. used Clayff force field in the study of nanofluids with Al_2O_3, and demonstrated by density functional method that the interaction between Al_2O_3 molecules and H_2O molecules is greater than that between water molecules (Lou and Yang, 2015; Cygan et al., 2004).

Nanofluids are influenced by volume fraction, temperature, nanoparticle size and shape, and other aspects. Temperature and volume fraction are the two most influential factors on nanofluid thermal conductivity and viscosity, but there are few papers combining these factors into consideration. In this paper, Al_2O_3- H_2O nanofluid is used to analyze the influence of several different factors on nanofluid and compared with the experimental value (Esfe et al., 2014; Satapathy, 2011; Ghodsinezhad et al., 2016).

2. THEORETICAL MODELS

The SPC/E model used in the water molecule model in this paper, its expression:

$$U(r_{ij}) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right] + \frac{q_i q_j}{r_{ij}} \quad (1)$$

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In formula (1), $\varepsilon$and$\sigma$are the L-J potential parameters, r_{ij} represents the distance between two atoms (Sirk et al., 2013). The CLAYFF force field is used as the force between Al_2O_3 nanoparticles. According to the Lorentz-Berthelot formula, the potential parameters of the interaction between different kinds of atoms are calculated to describe the interaction between different kinds of atoms. The Lorentz-Berthelot table is the formula:

$$\sigma_{12} = \frac{1}{2}(\sigma_1 + \sigma_2) \quad (2)$$

$$\varepsilon_{12} = \sqrt{\varepsilon_1 \varepsilon_2} \quad (3)$$

In formula (2-3), 1 and 2 represent different types of atoms. After several simulations of the physical parameters of the base fluid-water, it is found that the EMD method is more accurate when calculating the viscosity. The NEMD method is preferable for thermal conductivity calculation. Normal temperature and pressure are determined using two distinct methodologies. From base fluid's viscosity and thermal conductivity, the simulated and experimental viscosity values are not substantially varied. The simulated value of the EMD method is lower by 7.53%, and the NEMD method is lower by 11.48%. However, when calculating the thermal conductivity of the base fluid, the EMD method simulates the value is 30.67% higher, and the NEMD method is 5.50% higher, as shown in Table 1. Therefore, to make the simulation results more accurate, the EMD method is used to calculate the viscosity and the NEMD method is used to calculate the thermal conductivity. In this table, η represents viscosity, λ represents thermal conductivity, **sim** represents simulated value, **exp** represents experimental value.

Table 1: Base Fluid-Water Viscosity and Thermal Conductivity At 300K Temperature

Method& Error rate	η (mPa •S)		λ (W/mK)	
	EMD	**NEMD**	**EMD**	**NEMD**
sim	0.7902	0.7564	0.7883	0.6383
exp	0.8545		0.6032	
Error rate	7.53%	11.48%	30.67%	5.50%

2.1 Equilibrium Molecular Dynamics (EMD)

The Green-Kubo (G-K) formula derived based on the wave dissipation theorem and the linear response theory. This formula relates the shear viscosity to the autocorrelation function (PACF) of the off-diagonal component of the stress tensor P:

$$\eta_{\mu\nu} = \frac{V}{3k_BT}\int_0^\alpha < P_{\mu\nu}(t)P_{\mu\nu}(0) > dt \quad (4)$$

In formula (4), V is the volume, T is the temperature, and k_B is the Boltzmann constant, $P_{\mu\nu}(t)$ represents the shear stress on $\mu\nu$plane at time t, and the components of shear stress on xy, xz, yz are calculated in the simulation calculation. $<P_{\mu\nu}(0)P_{\mu\nu}(t)>$is the pressure autocorrelation function. Angle brackets indicate the overall average, which is the average of the total simulation time.

2.2 Non-Equilibrium Molecular Dynamics (NEMD)

Figure 1 shows the model NEMD applied temperature gradient and heat flow, the purpose of periodic boundary conditions is to simulate a bounded infinite system with a finite number of particles. The NEMD simulation of the external heating flow applies a preset energy to the thermal domain at regular intervals, while extracting equal energy from the cold domain to keep the heat flow constant in the system. By adjusting the heat, momentum of the particle and the cold field is applied to achieve energy extraction, the calculation formula is as follows:

$$J = -\lambda \nabla T \quad (5)$$

In formula (5), J is the heat flux density, and ∇T is the temperature gradient.

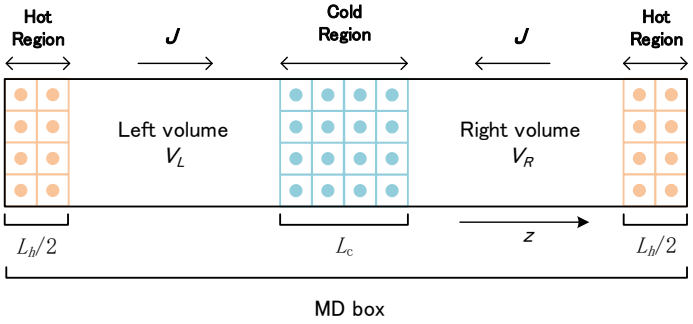


Figure 1: NEMD model of external heating flow with periodic boundary conditions

2.3 Model

The nanofluid is a water-based alumina nanofluid with periodic boundaries. In the MD simulation, the nanoparticles are randomly placed in the constructed simulation system. As shown in Figure 2, the density of the system is 1g/cm3, Fill the remaining part with water molecules according to the density. The number of nanoparticles is used to construct nanofluids with different volume fractions. Figure 3 shows the simulation system.

The time step in the simulation process is 1fs. First, run the NPT ensemble for 1ns. Because of the force of the potential function, the ensemble can make the volume and density of the model reach a more appropriate situation, which will cause the volume of the simulation box changes. Secondly, under the action of the NVT of the ensemble, the volume remains unchanged, so that the simulation box is in a balanced state.

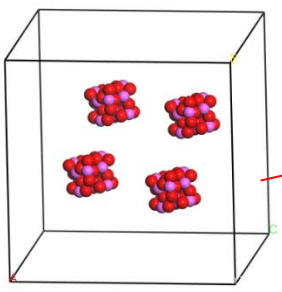


Figure 2: Nanoparticle model

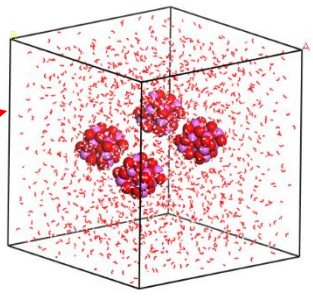


Figure 3: Nanofluid model diagram

3. Viscosity of Nanofluid

3.1 Viscosity of The Base Liquid (Water)

When using the G-K method to calculate the viscosity, using the NVE ensemble output data, the running time is 2ns. The Nose-Hoover thermostat was used during the simulation. Before calculating the viscosity of the nanofluid, first verify the base liquid(water). The simulation temperature is between 290K ~360K, and the temperature interval is 10K. Since it is a periodic boundary, the data obtained from the stress tensors under the three off-diagonal vectors are averaged to obtain the final viscosity value, as shown in Figure 4.

In the process of simulating the properties of the base liquid, different correlation lengths such as 10fs, 15fs, 20fs and 25fs were selected, as shown in Figure 5. It can be seen from the figure that the temperature increases with the increase of temperature. Compared with the experimental value shown in Figure 6, it is found that the viscosity value at 290K has the largest difference with the experimental value, with a difference of 0.11mPa •S and a relative error of 11.20%, within the allowable margin of error. It is proved that the EMD method is feasible to calculate the viscosity of nanofluids. This approach was used to investigate the consequences of temperature, volume fraction, as well as shape variations on water-based alumina nanofluids' viscosity. The subscript f represents basic fluids, whereas the subscript nf represents nanofluids.

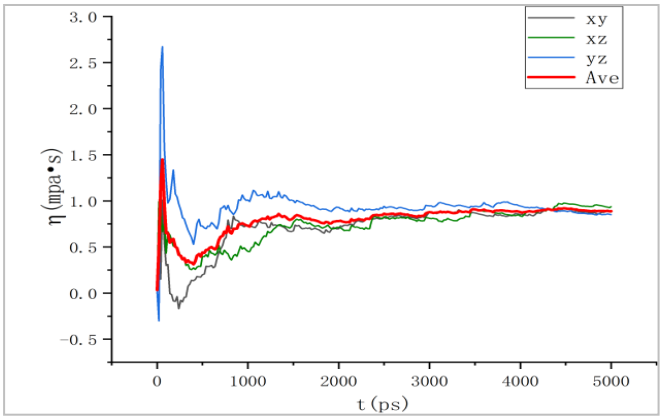


Figure 4: Base fluid viscosity and average viscosity under different stresses

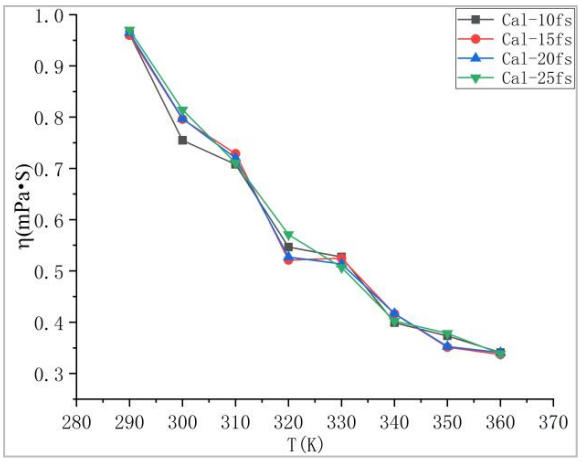


Figure 5: Simulation value of base fluid viscosity

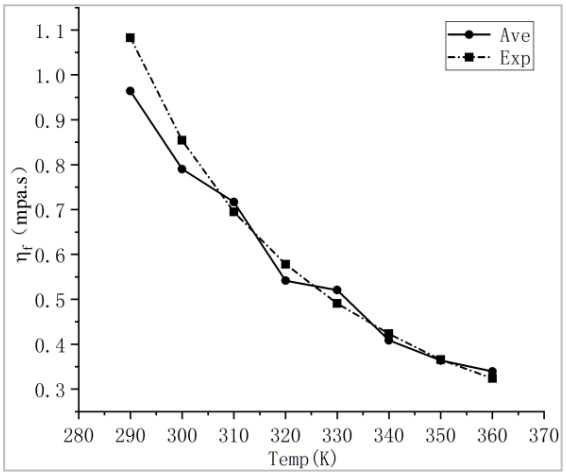


Figure 6: Experimental value and simulated value of base fluid viscosity

3.2 Viscosity of Nanofluids

Spherical nanoparticles were used to investigate the effects of different temperatures and volume fractions on the viscosity of nanofluids, and the viscosity of nanofluids with different volume fractions was calculated, as shown in Figure 7. For example, at a temperature of 300K, the viscosity of the base fluid is 0.7952mPa•S, After adding nanoparticles, the nanofluid's thermal conductivity with a 2.48% volume fraction is 1.7614 mPa•S, the relative base fluid's rise in viscosity ratio is 2.22, the nanofluid's viscosity reduces with a rise in temperature, and the base fluid's viscosity follows

the same trend. When distinct volume fractions of nanofluid rise within the same temperature, the decline rate becomes steeper as the volume fraction increases.

At constant temperature, the nanofluid's viscosity rises with increasing volume fraction, as determined by relative viscosity (η_{nf}/η_f). As shown in Figure 8, nanofluid-to-water viscosity ratio can be used to further infer changes in nanofluid viscosity and determine the nanofluid's relative viscosity under various volume fractions and temperatures. With a lower volume fraction, the nanofluid's viscosity becomes sensitive to volume fraction variations. The volume fraction is from 1.24% to 2.48%, the viscosity increases in the range of 0.4875~0.8491mPa •S, but the volume fraction is from 3.72% to 4.96%, the viscosity increase range is 0.2036~0.4597mPa •S. The temperature affects the relative viscosity of the nanofluid to a small extent, so it can be explained that the interaction between the nanoparticle and the base fluid in the figure will increase the viscosity of the nanofluid. The more nanoparticles, the larger the contact area with the base fluid, the force between the particles and the base fluid will increase.

In the simulation process, not only the influence of temperature and volume fraction on the viscosity of the nanofluid, but also the influence of the shape and size of the nanoparticle on the viscosity of the system must be considered. Several different shapes of nanoparticles are extracted from the alumina unit cell, and the specific parameters are shown in Table2. S in Table 2 represents the specific surface area of nanoparticles.

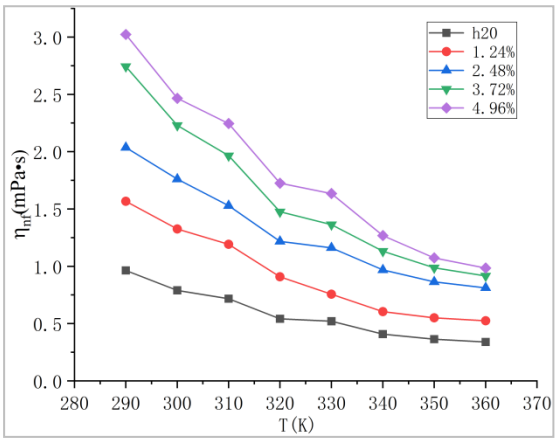


Figure 7: Viscosity of different volume fractions

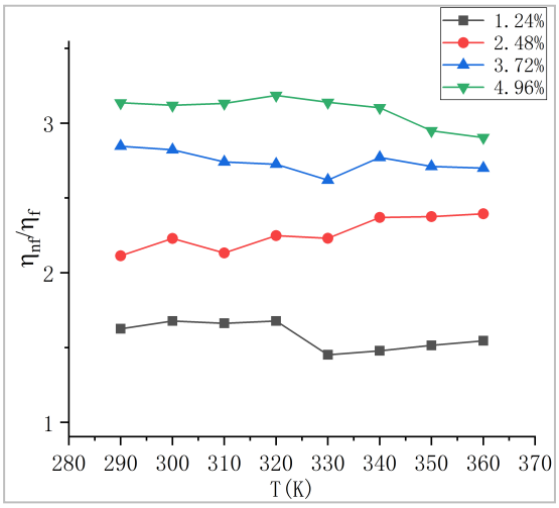
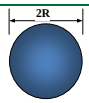
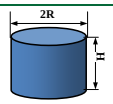
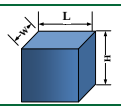


Figure 8: Relative viscosity of different volume fractions

Table 2: Nanoparticle Parameters

	2R/L(Å)	H(Å)	W(Å)	Aspect ratio	S (Å^{-1})
	10.858	---	---	---	0.5525
	10.330	---	8	1.549	0.6372
	11.930	---	6	1.005	0.6686
	14.610	---	4	1.826	0.7737
	8.743	8.743	8.743	1.000	0.6863
	13.880	6.938	6.938	2.002	0.7195
	20.000	5.780	5.780	3.460	0.7921

To study the influence of different shapes on the viscosity of nanofluids, calculate the changes in the case of four volume fractions at a temperature of 300K, and plot the data as Figure 9, the nanofluid viscosity of the nanoparticles in seven different shapes. The data in the figure shows that the greater the specific surface area of the nanoparticle, the greater the viscosity of the nanofluid, which proves that the viscosity of the nanofluid mentioned above will be affected by the contact area between the base fluid and the particle surface. It is determined that the temperature of the simulation system is 300K and the volume fraction is 2.48%. For example, the viscosity of the cylindrical S-0.6372 nanoparticle is 1.8226mPa•S, and the viscosity of the rectangular parallelepiped S-0.6863 is 1.8444mPa•S. To clearly observe the influence of the shape of the nanoparticle on the viscosity of the nanofluid, compare the viscosity of the nanofluid with the viscosity of the base fluid to obtain the relative viscosity increase rate. As shown in Figure 10, the smaller the volume fraction, the more the shape is the viscosity of the nanofluid is more affected. For example, when the volume fraction is 1.24%, the relative viscosity increases rate of the cylinder S-0.6686 is 1.88, which is 20% different from the spherical

viscosity increase rate; when the volume fraction is 3.72%, the relative viscosity increases rate of cylinder S-0.6686 is 2.90, which is 8% different from the spherical viscosity increase rate. As the volume fraction increases, the main reason for the increase in the viscosity of the nanofluid will become the increase in the number of particles in the nanofluid.

To investigate system viscosity effect by the size of the particles, the viscosities of nanoparticle nanofluids with varying particle sizes were determined at the same volume fraction, while determining three distinct particle sizes: there are four particle sizes in 2.48% nanofluid. The viscosity of the nanofluid with 8.62Å nanoparticles is 1.8577mPa•S, the viscosity of the nanofluid containing two nanoparticles with a particle size of 10.86Å is 1.7614mPa•S, and the nanofluid contains one nanoparticle with a particle size of 13.68Å. 1.6420 mPa•S is the resulting viscosity. A higher nanofluid viscosity entails a greater nanoparticle size. Hence, those three aspects may impact nanofluid viscosity, and that with volume fraction rise, such resulting value rises with higher specific surface area; with rising temperature, viscosity reduces its value.

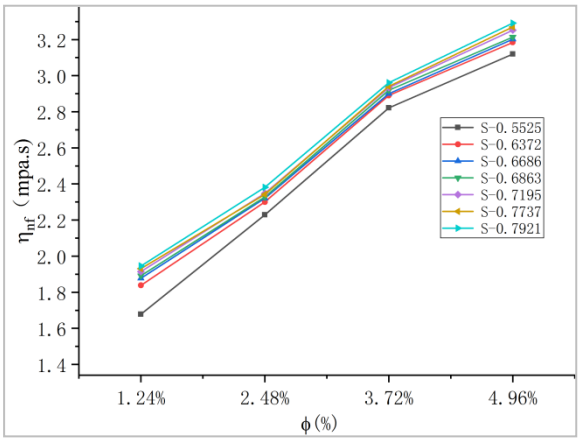


Figure 9: Viscosity of different particle shapes

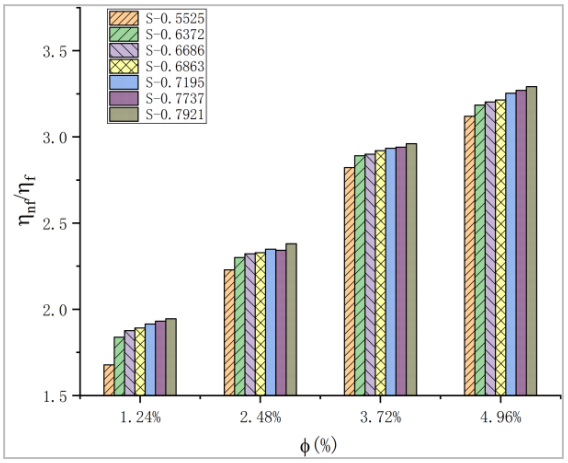


Figure 10: Relative viscosity of nanofluids with different particle shapes

4. Thermal Conductivity of Nanofluid

4.1 Thermal Conductivity of The Base Liquid (Water)

The NEMD method is used to calculate the thermal conductivity of nanofluids. Like the viscosity calculation process, the thermal conductivity of the base liquid(water) is calculated first. In a simulation box ,1/4 of the simulation box is used as the hot end to apply energy, and 3/4 of the simulation box is used as the cold end to extract energy. The simulation box is divided into 60 blocks before the simulation. The temperature gradient is calculated by the exchange of atoms at the cold and hot ends. A total of 100 groups are calculated, the temperature of one block is made into an interval graph as shown in Figure 11. The average value of each group is shown in the graph, and the temperature gradient is Divided into four intervals, the four temperature gradients generated are used to calculate the thermal conductivity of the nanofluid using the Fourier formula, and the average value is obtained as shown in Figure 12.

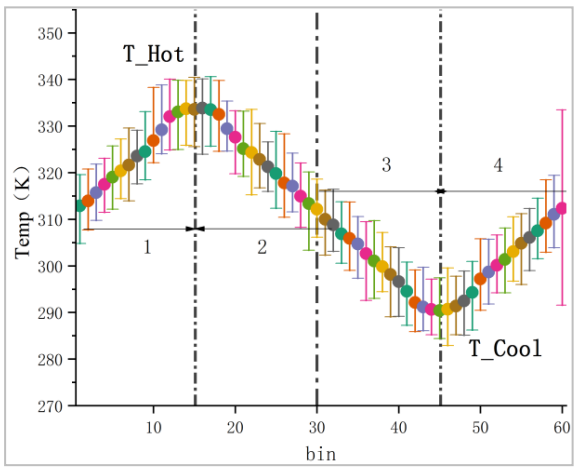


Figure 11: Temperature gradient of base fluid

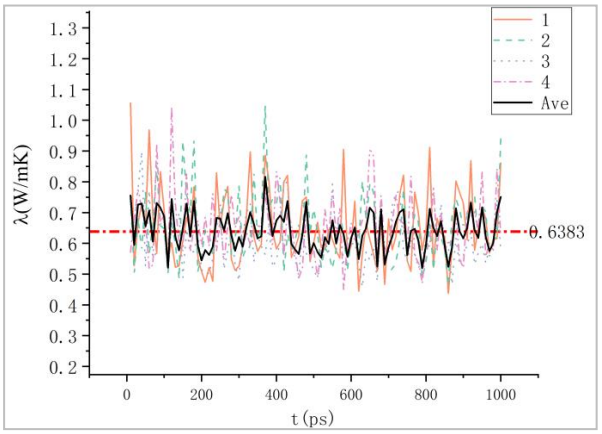


Figure 12: Thermal conductivity and average thermal conductivity under four temperature gradients

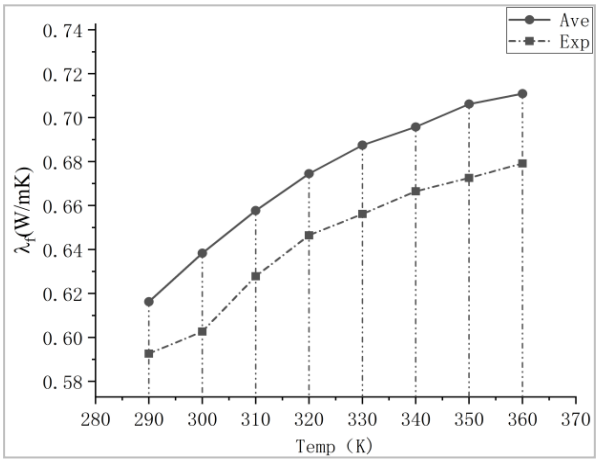


Figure 13: Experimental value and simulated value of base fluid thermal conductivity

The average of the four simulated values were compared with the experimental values, as shown in Figure 13. The difference between the viscosity value and the experimental value is the largest at 290K, with a difference of 0.0272W/mK. The error is 4.59%, which is within the allowable error range. It is proved that the NEMD method is feasible to calculate the thermal conductivity of nanofluids, and the method is suitable for nanofluids.

4.2 Thermal Conductivity of Nanofluids

Considering varying temperatures, fraction of volumes, as well as shapes regarding nanofluids' conduction of heat, they were examined in the same manner as viscosity. Figure 14 depicts temperature's impact on the nanofluid's conduction of heat. From Figure 14, thermal conductivity rises alongside temperature, in accordance with base fluid's changing trend. A smoother curve and slower thermal conductivity increase rate are alongside a higher temperature. At 290 K, for example, the base fluid's conduction of heat value is 0.6162 W/mK. After the addition of nanoparticles, the 3.72% nanofluid's thermal conductivity becomes 0.7262 W/mK, a 17.85 percent increase over the initial value. Hence, nanofluid's conduction of heat increases with temperature at various volume fractions, mirroring base fluid's behavior with temperature. From Figure 15, relative conduction of heat values of the two fluids are determined alongside various temperatures. Such values rise gradually with temperature. Figure 15 demonstrates that the nanofluid's thermal conductivity rises as the temperature rate rises; with increased volume fraction, so does the relative thermal conductivity range.

Calculate the influence of the shape and size of nanoparticles on the thermal conductivity of the system. The specific parameters are shown in Table 2. Figure 16 shows the thermal conductivity of nanofluids of seven different shapes of nanoparticles. The temperature of the simulation system is determined to be 300K. The data in the figure shows that the larger the specific surface area of the nanoparticle, the greater the thermal conductivity of the nanofluid. For example, the thermal conductivity of cylindrical S -0.6686 nanoparticles is 0.7507 W/mK, and the viscosity of rectangular parallelepiped S -0.7921 is 0.8253 W/mK. Comparing the thermal conductivity of nanofluids with different particle sizes with the base fluid, the relative thermal conductivity viscosity is shown in Figure 17.

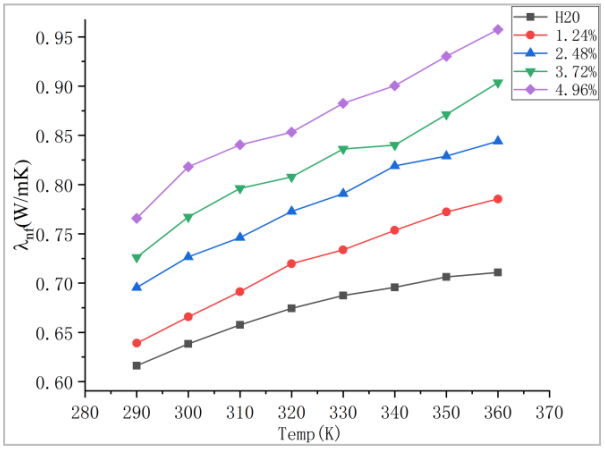


Figure 14: Thermal conductivity of different volume fractions

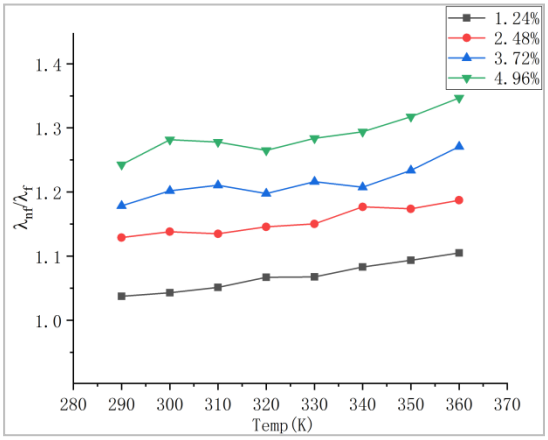


Figure 15: Relative thermal conductivity of different volume fractions

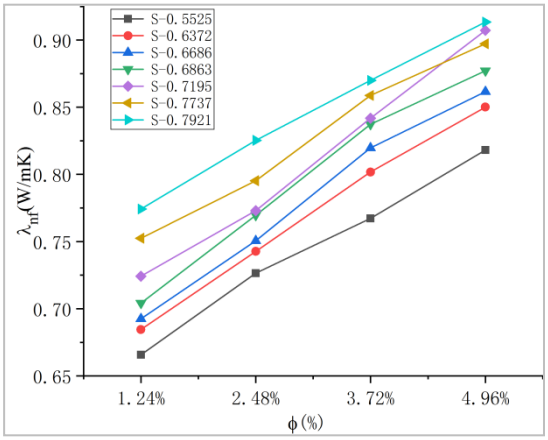


Figure 16: Thermal conductivity of different particle shapes

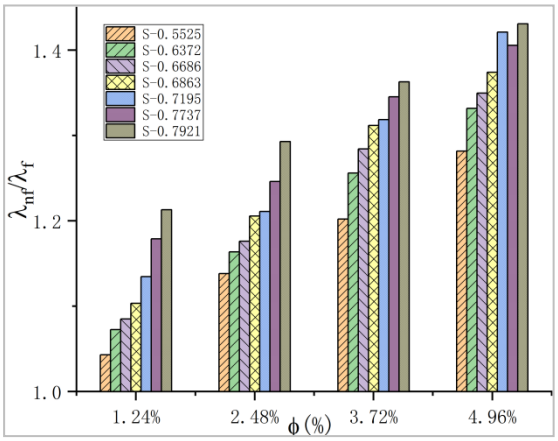


Figure 17: Thermal conductivity of nanofluid with different particle shapes and base fluid thermal conductivity

When the volume fraction is small, the shape and size of the nanoparticles have a greater impact on the thermal conductivity, but at high in the case of volume fraction, the increase in volume fraction is the main reason for the increase in the viscosity and thermal conductivity of the nanofluid. Calculate the thermal conductivity of nanofluids with particles of different particle sizes under the same volume fraction. A nanofluid's conduction of heat if there are four nanoparticles measuring 8.62 Å is 0.7428 W/mK. In a nanofluid with 300 K as the simulated temperature and 2.48% as the volume fraction, a nanofluid's thermal conductivity with two nanoparticles with a size of 10.86 Å is 0.7265 W/mK, while that with one nanoparticle with a size of 13.68 Å is 0.7265 W/mK. The data indicate that there is a rise in the viscosity of the nanofluid when particle size increases. Thus, these three variables will influence nanofluids' thermal conductivity, and that considering a rise in volume fraction, specific surface area and temperature also increase.

5. Conclusion

In this paper, the properties of hot objects are analyzed from the viscosity and thermal conductivity of nanofluids. EMD method is used to calculate the viscosity of nanofluids, and NEMD method is used to calculate the thermal conductivity of nanofluids. The numerical results and the trend of variation are consistent with the experimental data in the literature. When studying how various shapes of particles impact nanofluid properties, viscosity and conduction of heat reduce when the nanoparticle size is reduced. When the volume fraction is small, nanoparticle shape's impact on those two properties becomes magnified. In contrast, volume fraction has a greater impact when it is more significant.

References

Babaei, H., Keblinski, P., and Khodadadi, J.M., 2012. Equilibrium molecular dynamics determination of thermal conductivity for multi-component systems. Journal of Applied Physics, 112 (5), Pp. 570.

Cerbelaud, M., Laganapan, A.M., Alanissila, T., Ferrando, R., and Videcoq, A., 2017. Shear viscosity in hard-sphere and adhesive colloidal suspensions with reverse non-equilibrium molecular dynamics. Soft Matter, Pp. 13.

Choi, S.U.S., Zhang, Z.G., Yu, W., Lockwood, F.E., and Grulke, E.A., 2001. Anomalous thermal conductivity enhancement in nanotube

suspensions. Applied physics letters (14), Pp. 79.

Cygan, R.T., Liang, J.J., and Kalinichev, A.G., 2004. Molecular models of hydroxide, oxyhydroxide, and clay phases and the development of a general force field. The Journal of Physical Chemistry B, 108 (4), Pp. 1255-1266.

Duan, F., Kwek, D., and Crivoi, A., 2011. Viscosity affected by nanoparticle aggregation in Al_2O_3-water nanofluids. Nanoscale Research Letters, 6 (1), Pp. 248.

Esfe, M.H., Saedodin, S., Mahian, O., and Wongwises, S., 2014. Thermal conductivity of Al_2O_3/water nanofluids. Journal of Thermal Analysis and Calorimetry, 117 (2), Pp. 675-681.

Essajai, R., Mzerd, A., Hassanain, and Qjani, M., 2019. Thermal conductivity enhancement of nanofluids composed of rod-shaped gold nanoparticles: insights from molecular dynamics. Journal of Molecular Liquids, Pp. 293.

Florian, M.P., 1997. A simple nonequilibrium molecular dynamics method for calculating the thermal conductivity. Journal of Chemical Physics, 106 (14).

Ghodsinezhad, H., Sharifpur, M., and Meyer, J.P., 2016. Experimental investigation on cavity flow natural convection of Al_2O_3–water nanofluids. International Communications in Heat & Mass Transfer, 76(aug.), Pp. 316-324.

Green, M.S., 2004. Markoff random processes and the statistical mechanics of time-dependent phenomena. Journal of Chemical Physics, 20 (8), Pp. 1281-1295.

Ikeshoji, T., and Hafskjold, B., 1994. Non-equilibrium molecular dynamics calculation of heat conduction in liquid and through liquid-gas interface. Molecular Physics, 81 (2), Pp. 251-261.

Lou, Z., and Yang, M., 2015. Molecular dynamics simulations on the shear viscosity of Al_2O_3 nanofluids. Computers & Fluids, 117, Pp. 17-23.

Mehdi, A.E., Hicham, J., Soukaina, Z., Hamid, L., Abdellatif, H., and Said, O., 2018. Modeling and simulations of nanofluids using classical molecular dynamics: particle size and temperature effects on thermal conductivity. Advanced Powder Technology, S0921883118303005-.

Meyer, J.P., Adio, S.A., Sharifpur, M., and Nwosu, P.N., 2016. The viscosity of nanofluids: a review of the theoretical, empirical, and numerical models. Heat Transfer Engineering, 37 (5).

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

Phillpot, S.R., Wolf, D., and Gleiter, H., 1995. Molecular-dynamics study of the synthesis and characterization of a fully dense, three-dimensional nanocrystalline material. Journal of Applied Physics, 78 (2), Pp. 847-861.

Rudyak, V.Y., and Krasnolutskii, S.L., 2015. Simulation of the nanofluid viscosity coefficient by the molecular dynamics method. Technical Physics, 60 (6), Pp. 798-804.

Rudyak, V.Y., and Krasnolutskii, S.L., 2017. Simulation of the thermal conductivity of a nanofluid with small particles by molecular dynamics methods. Technical Physics, 62 (10), Pp. 1456-1465.

Satapathy, S.L.N., 2011. Al_2O_3-based nanofluids: a review. Nanoscale Research Letters.

Sina, N., Shoghl, J., Jamali, M., Keshavarzet, Moraveji, 2016. Electrical conductivity, viscosity, and density of different nanofluids: an experimental study. Experimental Thermal & Fluid Science.

Sirk, T.W., Moore, S., and Brown, E.F., 2013. Characteristics of thermal conductivity in classical water models. Journal of Chemical Physics, 138 (6), Pp. 219.