



Investigation Dynamic Viscosity of Water-Single Wall Carbon Nanotube Nanofluid and Its Effective Factors by Molecular Dynamics Simulation

F. Jabbari^{1*}, A. Rajabpour², S. Saedodin¹

¹ Department of Mechanical Engineering, Semnan University, Semnan, Iran

² Department of Mechanical Engineering, Imam Khomeini International University, Qazvin, Iran

ABSTRACT: Nanofluids as new groups of the heat transfer environments with unique and special properties have attracted particular attention in recent decades. Knowing the characteristics of the nanofluid is the first step in the nanofluid study, which is very important in describing its behavior. Although many attempts have been made to modeling the thermodynamic properties of nanofluids, a comprehensive model for predicting these properties has not yet been provided. In this work the dynamic viscosity of water-single wall carbon nanotube nanofluid and the effect of volume fraction and size of nanoparticles and nanofluid temperature on it in ranging from 25°C to 65°C with an interval of 10 °C and 0.125% to 0.734% (0.125%, 0.25%, 0.5%, and 0.734%) have been studied, respectively. After the full explanation of the interaction between base fluid and nanoparticle atoms, the results show that the presence of nanoparticles in the base fluid and the addition of its, reducing the temperature, as well as reducing the size and diameter of the carbon nanotubes, increase the dynamic viscosity of nanofluids. Finally, the interpretation and conclusion of the results are discussed.

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1- Introduction

Nanofluids have unique and special features relative to conventional fluids such as water, ethylene glycol and motor oil. These features include a higher thermal conductivity and a higher shear viscosity and a lower pressure drop that results in better heat transfer in cooling and thermal fluxes equipment. Despite the extensive research using various methods, including analytical, experimental and numerical methods were done, the researchers still failed to understand the exact behavior of nanofluids and present comprehensive model for predicting the thermophysical properties at different temperatures and volume fraction of nanoparticles [1-3].

The use of new technologies and the accuracy of their results cannot be ignored. The results of computer simulations such as molecular dynamics can enhance our understanding about how the nanofluid behavior is and the physical phenomena governing them at the atomic and molecular levels. The basis of the molecular dynamics simulation is determination of the atoms and molecules path by solving Newton's equations of motion, while the potential energy between the particles is calculated by means of the interatomic potential function or the molecular mechanical force field.

With the advent of computer simulation methods, and especially the molecular dynamics simulation, many researchers tried to investigate the rheological behavior of nanofluids with this technique at the atomic level. Therefore, some studies have been done in the field of studying the viscosity of nanofluid by molecular dynamics simulation and investigation of the effect of various parameters such as nanofluid temperature, volume fraction, size and aggregation

of nanoparticles. The viscosity of nanofluid in systems containing Al_2O_3 nanoparticles in water and ethylene glycol, water-gold nanofluid, and aluminum and lithium nanoparticles in liquid argon has been investigated with molecular dynamic simulation methods by Lu and Fan [4], Lu et al. [5] and Rudyak et al. [6, 7], respectively. According to their results, the shear viscosity of the nanofluids increases by adding nanoparticles and increasing the volume fraction of nanoparticles, which shows a higher viscosity increase at lower temperatures. In addition, the viscosity decreases with increasing temperature, as the temperature increases, the bond between the nanoparticles and the base fluid becomes weaker and leads to lower viscosity at higher temperatures.

Water as the most widely used and available chemical material in nature [8] and carbon nanotubes, due to its distinctive thermal properties compared to other nanoparticles, can provide a suitable nanofluid for heat transfer applications. Given the previous studies in this regard, that no research has been conducted on simulating of viscosity of nanofluids containing water-based Single-Walled Carbon Nano Tube (SWCNT) using molecular dynamics simulation. This has made us interested in investigate the water-SWCNT nanofluid system by equilibrium molecular dynamics simulation at the atomic and molecular level. The studied volume fraction and temperature are 0.125-0.734% (0.125, 0.25, 0.5 and 0.734%) and 25°C- 65°C, respectively. In the following, the results of this molecular dynamic simulation are presented in detail.

2- Methodology

2- 1- Calculation method for viscosity of the nanofluid

The results presented in this study are also obtained using the equilibrium method and the Green-Kubo formula. The

Corresponding author, E-mail: Fj_jabbari@semnan.ac.ir

viscosity can be obtained from Eq. (1) according to the Green-Kubo relation [9].

$$\mu = \frac{V}{k_B T} \int_0^\infty \tau_{ij}(t) \tau_{ij}(0) dt \quad (1)$$

Where μ , V , k_B , T , and τ_{ij} are viscosity, system volume, Boltzmann constant, temperature, and an element of stress tensor, respectively. The stress tensor can be calculated by Eq. (2).

$$\tau_{ij} = \frac{1}{V} \left[\sum_n m_n v_{ni} v_{nj} + \frac{1}{2} \sum_{m \neq n} r_{mn} f_{mj} \right] \quad (2)$$

In the above equation, m_n is the n th atomic mass, r_{mn} is the distance between the m th and n th atoms, and f_{mj} indicates the force acting on the atom or molecule by neighboring particles that follows the reaction potential function.

2- 2- Simulation systems

In the present simulation, the studied nanofluid system consists of pure water and SWCNT with chiral vector of (12,0) and zigzag type, which has the equivalent diameter of 0.951nm based on the governing relationships in the nanotubes. The number of water atoms in this simulation is considered to be 12240 atoms, which are located randomly in a box with 5nm×5nm×5nm dimensions.

All the presented results in this study were done using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code and applying the periodic boundary condition in all three computational directions. To calculate the nanofluid viscosity, first the nanofluid system must reach equilibrium condition. In this study, the system reaches equilibrium after about 300 ps in the Micro canonical ensemble (NVE) with Langevin thermostat, the constant temperature- constant pressure ensembles (NPT) with a Nosé-Hoover thermostat and barostat [10, 11], and canonical ensemble (NVT). After the system has reached balance, Newton's motion equations are solved by velocity Verlet algorithm and with a time step of 1fs for 4ns simulation time. In this study, the reaction between water molecules follows the TIP4P/2005 model [12]. The reaction between carbon atoms in the carbon nanotubes and the reaction between

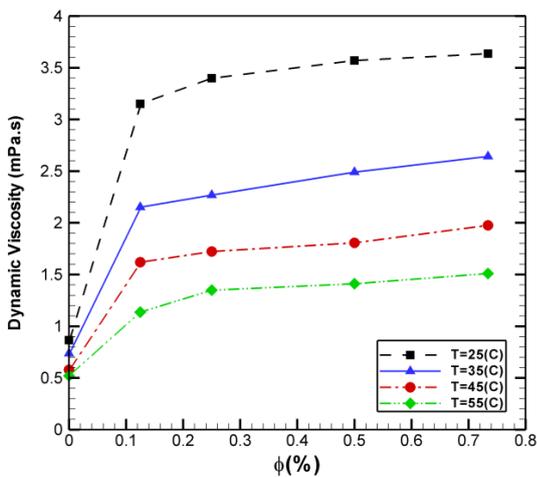


Fig. 1. Viscosity variation of the aqueous nanofluid including SWCNT in different volume fractions

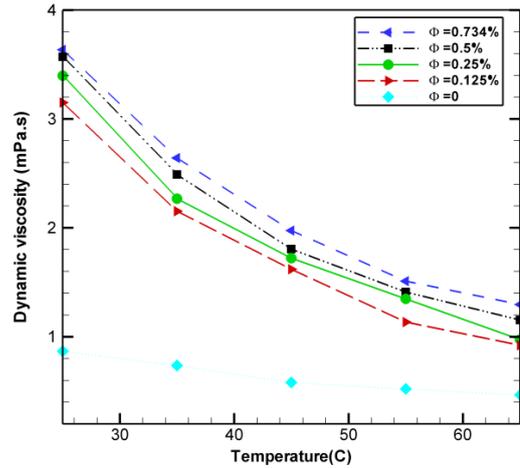


Fig. 2. Viscosity variation of the aqueous nanofluid including SWCNT in different temperatures

water and carbon nanotubes follow the Tersoff potential and Lennard Jones potential, respectively.

3- Results and Discussion

Fig. 1 shows the viscosity variation of the SWCNT- water nanofluid in different volume fractions and temperatures. The results show that, at a constant temperature, the viscosity is increased by increasing the volume fraction of nanoparticles. This can be explained that by increasing the number of nanoparticles, the number of water molecules that are affected by the nanotubes become more and more, and therefore higher van der waals forces are created between the particles, which prevent heat transfer between layers and consequently, increase the viscosity. It can also be seen that a water nanofluid containing SWCNT at the temperature of 25°C and volume fraction of 0.734% has a highest viscosity increase relative to the base fluid. Furthermore, it is also found that at lower temperatures, the viscosity shows a higher increase compared to higher temperatures.

Fig. 2 shows the variation in the viscosity of the SWCNT- water nanofluid in the temperature range of 25°C to 65°C

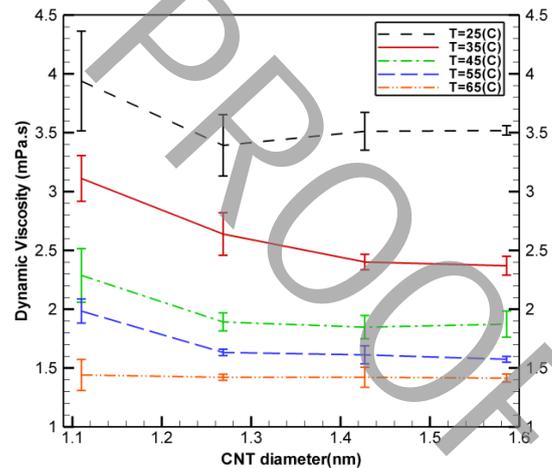


Fig. 3. Viscosity variation of the aqueous nanofluid including SWCNT in different CNT diameter

in different volume fractions. The results indicate that in a constant volume concentration, the nanofluid viscosity decreases with increasing the temperature. As the temperature increases, the reaction between the molecules and the bond between the particles is weaker and the distance between the molecules increases and leads to less effect of the molecules on each other, thereby reducing the nanofluid viscosity. Furthermore, in higher volume fractions, the viscosity increase is more than that of the base fluid.

Fig. 3 shows the viscosity variation of the SWCNT- water nanofluid in different CNT diameter and temperature. The results show that the nanofluid viscosity decreases with increasing diameter of CNT at fixed nanofluid temperature and volume fraction of nanoparticles. The reason for this is that as the nanoparticles become larger, the number of base fluid atoms in contact with the nanoparticle decreases, resulting in a reduction in the force between the particle and base fluid and, finally, the nanofluid viscosity is decreased. In addition, the relative viscosity increases with decreasing temperature.

4- Conclusions

In this study, the viscosity of SWCNT-water nanofluid is investigated by equilibrium molecular dynamic simulation and Green-Kubo formula. The volume fraction were considered between 0.125% and 0.734%, and the temperature range were considered 25°C to 65°C. In simulation, it was considered that the reaction between water molecules, the reaction between the carbon atoms in a carbon nanotube, and the reaction between water and carbon nanotubes follow the TIP4P/2005 model, Tersoff potential and Lennard-Jones potential, respectively. The results of this simulation indicate that the viscosity of nanofluids increases by increasing the volume fraction of the nanoparticles, decreasing the nanofluid temperature and CNT diameter. Furthermore, a water nanofluid containing SWCNT at the temperature of 25°C and volume fraction of 0.734% has a highest viscosity increase relative to the base fluid.

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