Rheological Behavior of Water-Ethylene Glycol Based Graphene Oxide Nanofluids

Izadkhah, Mir-Shahabeddin; Erfan-Niya, Hamid*[+]; Moradkhani, Hamed

Faculty of Chemical and Petroleum Engineering, University of Tabriz, P.O. Box 5166616471 Tabriz, I.R. IRAN

ABSTRACT: *Traditionally water-ethylene glycol mixture based nanofluids are used in cold regions as a coolant in the car radiators. In the present study, the rheological properties of water-ethylene glycol based graphene oxide nanofluid are studied using Non-Equilibrium Molecular Dynamics (NEMD) method at different temperatures, volume concentrations, and shear rates. NEMD simulations are performed with considering 75/25, 60/40, and 40/60 ratios of water/ethylene glycol as the base fluids at volume concentrations of 3%, 4%, and 5% graphene oxide nanosheets. The results, which demonstrated good agreement with experimental data, show that the viscosity and density of base fluids significantly decrease with temperature and increases with ethylene glycol volume fraction. Also, the viscosity and density of nanofluids depends directly on the volume concentrations of nanoparticles and decreases with increasing temperature. For example, at 289.85 K, the viscosity of water (75%)-ethylene glycol (25%) based nanofluids containing 3%, 4% and 5% volume concentrations of nanoparticles increased by 33%, 43%, and 56%, respectively. Similarly, the density of the same nanofluids increased by 1%, 1.7%, and 2.2%, respectively. Moreover, the theoretical models confirm the obtained results. According to the shear rate analysis, the water-ethylene glycol based graphene oxide nanofluid behaves as a non-Newtonian fluid.*

KEYWORDS: *Nanofluid; Graphene oxide; Rheological properties; Non-equilibrium molecular dynamics simulation; Shear rate.*

INTRODUCTION

Nanofluids are two phase mixtures including solid nanoparticles with sizes varying generally from 1 to 100 nm suspended in liquids with the heat transfer application such as water, ethylene glycol, light oil, and etc. [1, 2]. This term was coined by *Choi* [3] in 1995 at Argonne National laboratory of USA [4, 5]. Nanofluid is more stable and has acceptable viscosity and better wetting, spreading and adhesion behavior on the solid surface [6-9]. Using the dispersed nanoparticles can be considered as a positive point to promote heat transfer efficiency of lubricants and fluids [10-12]. On the other hand, friction caused by metal contact between hard surfaces can be a restriction for improving friction behavior of such fluids. Thus, it is essential to confine friction properties by using particles with idealized surfaces. Using such nanoparticles can prevent erosion encountered in internal systems by changing the sliding friction to rolling friction [13-16].

Ethylene glycol-water mixtures at different volume

** To whom correspondence should be addressed.*
+ E-mail: herfan@tabrizu.ac.ir
1021-9986/2018/5/177-187 11/$/6.01

percentages are suitable to lower the freezing point of the aqueous heat transfer medium. Therefore, in cold regions of the world, it is common to utilize water-ethylene glycol in varied volume fractions as heat transfer fluids in heating systems such as automobile radiators and heat exchangers [17-20].

Carbon nanostructures are well dispersed with respect to metals and metal oxides in an aqueous medium due to their low density [21]. Graphene oxide is a suitable case which is a derivative of graphite. Graphite powder is converted to graphene oxide nanosheets by some chemical methods [22]. Graphene oxide's water dispersity and hydrophilicity has been mainly on account of the ionizable groups (–COOH) at the edge [23-26] and its low density is attributed to strong C–C covalent bonds and phonon scattering [27].

In this work, the rheological properties such as viscosity and density of water-ethylene glycol based fluid in contact with graphene oxide nanosheets are studied by Molecular Dynamics (MD) simulation method. Many researchers have focused on the flow characteristics of nanofluids using MD simulation. Recently, some theoretical studies [28-30] were collaborated with molecular dynamics simulation to get a better knowledge about nanofluids. However, some theoretical models [2, 31-33] are available on the rheological properties which were validated with experimental data; but, there have not been paid enough attention to the collaborative effort of MD and theoretical approach. Mechanisms are all on the ground of physical phenomena. These phenomena are indicated by the simplified MD simulation method on the basis of Newton's second law [34]. The obtained results from MD simulations need to be confirmed by theoretical models. Theoretical models can go along with MD results to evaluate the accuracy of the simulation [35]. For the first time, *Lu et al.* [36] compared Brinkman results with numerical data obtained from MD results. They used Al_2O_3 as the nanoparticle for the system of water and ethylene glycol, separately. In their work, shear viscosity was calculated as a function of nanoparticle's diameter and then was validated with Brinkman results. According to their results, theoretical equations for calculating viscosity are not always accurate because particle size effects were not considered in these equations. Furthermore, as it has been mentioned in the article, in addition to a larger ratio of surface area to volume, nanoparticles have better viscosity improvement effects because of more excellent momentum exchange between particles and fluid. So, when this value is greater than an amount, shear viscosity becomes invariable and the obtained MD simulation results show well agreement with the results from theoretical correlations [36]. Since carbon nanosheets have a larger ratio of surface area to volume; hence, graphene oxide nanosheets can be proposed as appropriate particles.

The aim of this study is to reduce the high costs of investigations by using computational and theoretical methods besides experimental analysis. As mentioned above, many theoretical [8, 9] and experimental [1-5] studies have been done on heat transfer and flow behavior of nanofluids which show that nanofluids significantly enhance heat transfer. Nevertheless, the rheological behavior of nanofluids has not been enough analyzed using Non-Equilibrium Molecular Dynamics (NEMD) method. The obtained NEMD results can be approved by theoretical models which have not been paid enough attention to this issue in the literature. Therefore, confirmation of NEMD results by theoretical models can be considered as the novelty of this work.

THEORETICAL SECTION

Molecular dynamics simulation

Molecular dynamics simulation method [37-39] is a well-established method for predicting properties of nanofluids. Prediction of the rheological properties such as viscosity and density can be done either by equilibrium or non-equilibrium molecular dynamics. Both methods have their own advantages and disadvantages. In this paper, Non-Equilibrium Molecular Dynamics (NEMD) method is used to predict the rheological properties of water-ethylene glycol based graphene oxide nanofluid.

The MD simulations are performed using LAMMPS code [40]. LAMMPS integrates Newton's equations of motion for collections of atoms, molecules, or macroscopic particles that interact via short- or long-range forces with a variety of initial and/or boundary conditions [41, 42].

In a MD simulation, a force field which includes the functional form and parameter sets needs to be specified in order to describe the interaction between atoms or molecules, which is also called the potential energy of a system of particles. Therefore, to model the nanofluid

structures, the Consistent Valence Force Feld (CVFF) is chosen [43]. This force field has been widely used to predict the behavior of small molecules and macromolecules. The CVFF uses Morse potential to calculate bond-stretching interactions. Also, the non-bonded terms describe the van der Waals (vdW) and long-range electrostatic interactions. Lennard-Jones (LJ) potential is used to explain the van der Waals (vdW) interactions between base fluid atoms and graphene oxide [34, 44, 45].

All the atoms in the simulation model are in Face Centered Cubic (FCC) lattice with a periodic boundary condition. In the present work, total simulation time is 2 ns with a time-step of 1 fs. Canonical (NVT) and isothermal-isobaric (NPT) ensembles were applied in the simulation process. The simulation temperature and pressure controlled by Nosé-Hoover thermostat [46] and Berendsen barostat [47]. The Velocity Verlet algorithm is used to integrate Newton's equations of motion.

Non-Equilibrium Molecular Dynamics (NEMD) simulation of the shear viscosity of water and ethylene glycol mixtures were performed at nine different compositions of nanofluids (three different volume ratios of water/ethylene glycol across three nanoparticle concentrations) as discussed above. NEMD is a steady state simulation that is achieved by applying an external strain field to the fluid. This takes the system away from the equilibrium. In order to apply an external field SLLOD algorithm is used in conjunction with periodic boundary condition. In the next section, the NEMD results for the shear viscosity are compared with the results of the theoretical models.

SLLOD algorithm

The equations of motion for a system containing *N* molecules are [48]:

$$\frac{d\boldsymbol{r}_i}{dt} = \frac{\boldsymbol{p}_i}{m} + \boldsymbol{r}_i.\nabla\boldsymbol{u} \tag{1}$$

$$\frac{d\boldsymbol{p}_i}{dt} = \boldsymbol{F}_i - \boldsymbol{p}_i.\nabla\boldsymbol{u} - \lambda\boldsymbol{p}_i \tag{2}$$

Where $\boldsymbol{u}$ is the streaming velocity given by $\boldsymbol{u} = (\gamma y, 0, 0)$ in which γ is the strain rate, and also m_i, $\boldsymbol{r}_i$, $\boldsymbol{p}_i$, and $\boldsymbol{F}_i$ are mass, the position of the center of mass, peculiar translational momentum and force on the center of mass for molecule *i*, respectively.

$$\frac{d\boldsymbol{L}_i}{dt} = \boldsymbol{T}_i \tag{3}$$

$$\boldsymbol{L}_i^p = \mathbf{A}_i \boldsymbol{L}_i \tag{4}$$

$$\omega_{i\beta}^p = \frac{L_{i\beta}^p}{I_{i\beta}}, \quad \beta = x, y, z \tag{5}$$

$$\frac{d}{dt}\begin{pmatrix} q_{i1} \\ q_{i2} \\ q_{i3} \\ q_{i4} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} -q_{i3} & -q_{i4} & q_{i2} & q_{i1} \\ q_{i4} & -q_{i3} & -q_{i1} & q_{i2} \\ q_{i1} & q_{i2} & q_{i4} & q_{i3} \\ -q_{i2} & q_{i1} & -q_{i3} & q_{i4} \end{pmatrix}\begin{pmatrix} \omega_{ix}^p \\ \omega_{iy}^p \\ \omega_{iz}^p \\ 0 \end{pmatrix} \tag{6}$$

$\boldsymbol{L}_i$ represents angular momentum and the matrix $\boldsymbol{A}_i$ converts the laboratory frame coordinates of molecule *i* to molecular frame coordinates. The q_{ij}, j=1,…,4 are the quaternion orientations for molecule *i* [49]. For a homogeneous algorithm, boundary conditions must be in agreement with the equation of motion. Thus, Lees-Edwards periodic boundary condition [50] is employed to solve the equations of motion.

Lees-Edwards periodic boundary

In the Lees-Edwards periodic boundary condition the box is surrounded by the same boxes. The neighboring cells are forced to move with a specific speed V_d in the opposite direction of *x*–axis path line. In Lees-Edwards periodic boundary condition the fluid atoms will be reintroduced in to the box at non-symmetric points with a linear velocity profile. When an atom A leaves the box at point P with velocity $\vec{V}$ from the lower boundary, the atom will be reintroduced in to the box at non-symmetric point P´ with velocity $\vec{V}$ (Fig. 1) [50, 51].

$$V_x' = V_x + 2V_d \tag{7}$$
$$V_y' = V_y$$
$$V_z' = V_z$$

Theoretical models

Since there is no exact available theory to find out density and viscosity of nanofluids as yet, the classical theoretical models for the solid-liquid suspensions are used to be compared with the measured density and viscosity. In this work, the theoretical relations for calculation of density and viscosity of nanofluids

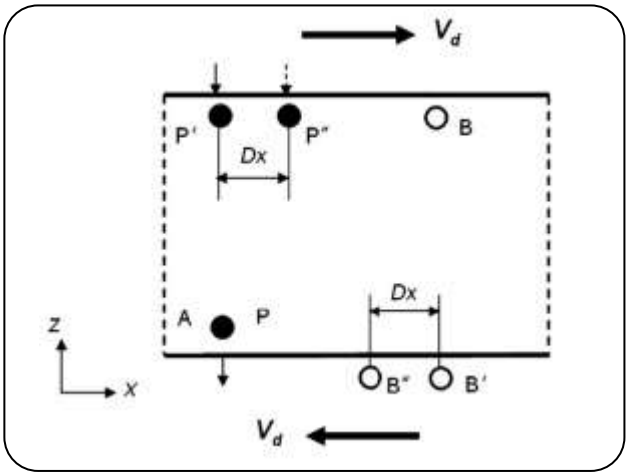

Fig. 1: Lees-Edwards periodic boundary condition box.

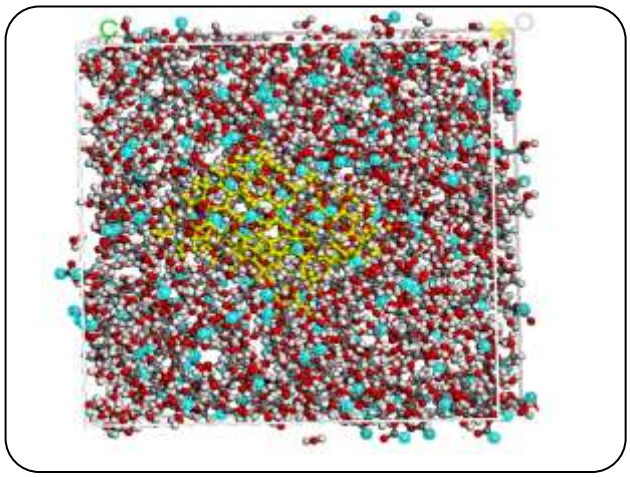

Fig. 2: The simulation cell for studying the rheological properties.

were used in order to compare with the results obtained by the molecular dynamics simulations.

In this work, the equation suggested by *Pak* and *Cho* [52] is used to calculate the density of nanofluid.

$$\rho_{nf} = (1-\varphi)\rho_{bf} + \varphi\rho_s \quad (8)$$

where ρ_{bf}, ρ_s and φ are the density of the base fluid mixture, the density of solid nanoparticle and solid volume fraction, respectively.

Theoretical relations used to calculate the value of the nanofluid viscosity are as follows:

a) In 1999, *Wang et al.* [31] suggested a model calculate the viscosity of nanofluids as the following:

$$\mu_{nf} = \mu_{bf}(1+7.3\varphi+123\varphi^2) \quad (9)$$

b) *Batchelor* [53] model is:

$$\mu_{nf} = \mu_{bf}(1+2.5\varphi+6.5\varphi^2) \quad (10)$$

where μ_{bf} , μ_{nf} and φ are the viscosity of the base fluid mixture and nanofluid, and the solid volume fraction, respectively.

RESULTS AND DISCUSSION

In the present work, a monolayer structure of graphene oxide nanosheet is used. In order to build the structure of graphene oxide nanosheet, the graphite supercell was designed and then, the functional groups were added on the structure. The functional groups are hydroxyls, carbonyls, epoxides and carboxyls [26, 54]. Fig. 2 shows one of the simulation cells used in the current work.

The first step of the simulation is the equilibration stage. This equilibration stage was run for 1 ns with a typical time-step of 1 fs. The interactions among the constituent molecules of the nanofluid lead to increasing of the energy level. This action puts the system out of the balance. Hence, the system tries to balance the simulation cell. At the second step, the model was calculated for 1 ns to obtain viscosity and density of nanofluids.

Figs. 3 and 4 show the experimental [55] and NEMD results for density and viscosity of water-ethylene glycol mixtures at different volume ratios of water/ethylene glycol, respectively.

The molecular dynamics simulation results indicate that the density and viscosity of the base fluids significantly decrease by increasing both temperature and ethylene glycol volume fraction. The experimental data verify the obtained NEMD results.

The effect of the graphene oxide nanosheets on the density and viscosity of the nanofluids was examined with theoretical models and molecular dynamics simulation method. The nanofluids were simulated at three different volume ratios of water/ethylene glycol (75/25, 60/40 and 40/60) as the base fluids and three volume concentrations of graphene oxide nanoparticles (3%, 4%, and 5%) at several temperatures. The obtained results for the density of nanofluids by molecular dynamics and *Pak* and *Cho* [52] correlation were compared in Fig. 5.

As illustrated, the deviation in the predicted values of density decreases with increasing of the graphene oxide concentration. This concludes that the *Pak* and *Cho*

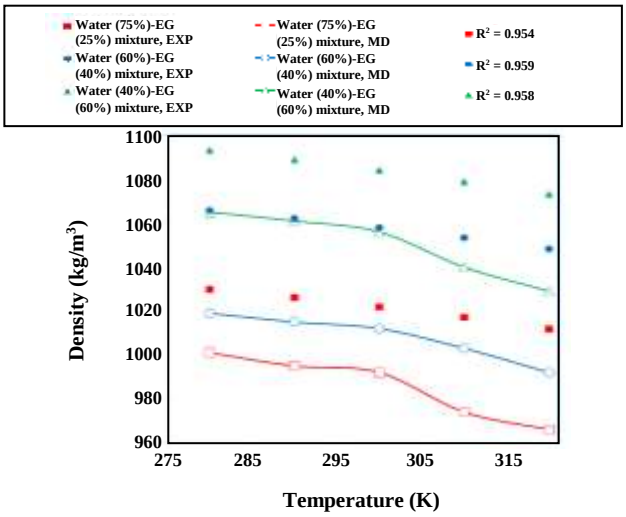

Fig. 3: Experimental and NEMD results for the density of water-ethylene glycol mixtures.

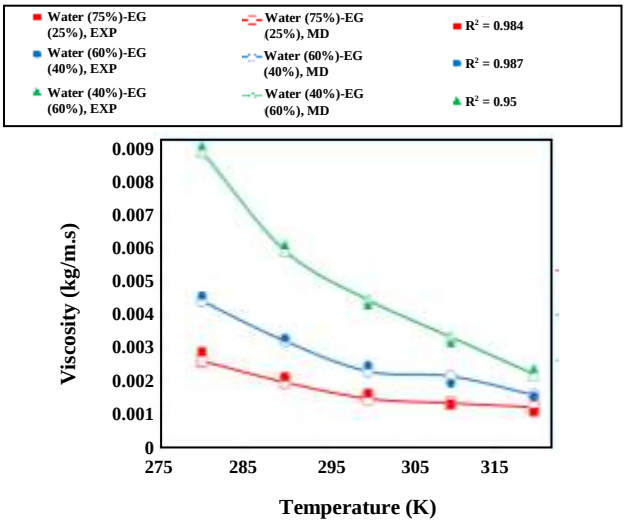

Fig. 4: Experimental and NEMD results for the viscosity of water-ethylene glycol mixtures.

correlation can predict the density of the nanofluids containing graphene oxide nanosheets [52]. The obtained results indicated that the density of nanofluids increases with increasing the concentration of GO nanosheets. The molecular dynamics simulations results show that the density of the nanofluids containing water (75%)-ethylene glycol (25%) as the base fluid increases by 1%, 1.7% and 2.2% for the volume fractions of 3%, 4% and 5% GO nanosheets, respectively at 289.85 K. Similarly, the density of the nanofluids containing water (60%)-ethylene glycol (40%) as the base fluid increases by 2.6%, 3.5% and 4.5% for the volume fractions of 3%, 4% and 5% GO nanosheets, respectively at 289.85 K. Also, at the same temperature, the density of the nanofluids containing water (40%)-ethylene glycol (60%) as the base fluid increases by 1.1%, 2.2% and 3.3% for the volume fractions of 3%, 4%, and 5% GO nanosheets, respectively. The density of nanofluids significantly decreases with increasing the temperature. Because the particles speed up and spread out due to adding heat to the fluid. Therefore, the fluid expands and the density decreases.

Also, in the present study, the viscosity of nanofluids was obtained by both NEMD method and theoretical models at various GO concentrations and several shear rates. Figs. 6(a) and 6(b) show the obtained viscosity results versus temperature by theoretical models and NEMD method for the shear rate of 1 s^{-1}.

It is clear that the obtained viscosity of nanofluids by NEMD simulations are in agreement with the results of theoretical models. This implies that *Wang et al.* [31] and *Batchelor* [53] correlations are appropriate to predict the viscosity of the nanofluids containing GO nanosheets. The viscosity of nanofluids increases with increasing of the GO concentration and decreases with increasing of the temperature.

The molecular dynamics simulations results show that the viscosity of the nanofluids containing water (75%)-ethylene glycol (25%) as the base fluid increases by 33%, 43% and 56% for the volume fractions of 3%, 4%, and 5% GO nanosheets, respectively at 289.85 K. Similarly, the viscosity of the nanofluids containing water (60%)-ethylene glycol (40%) as the base fluid increases by 22%, 47% and 72% for the volume fractions of 3%, 4% and 5% GO nanosheets, respectively at 289.85 K. Also, at the same temperature, the viscosity of the nanofluids containing water (40%)-ethylene glycol (60%) as the base fluid increases by 24%, 53% and 81% for the volume fractions of 3%, 4%, and 5% GO nanosheets, respectively. As the GO nanosheets are well dispersed in the base fluids, the interfacial interactions are increased. Increasing the interfacial interactions in nanofluids due to the addition of the GO nanosheets leads to increasing the viscosity of nanofluids and the internal friction forces. The friction force in the mentioned fluid arises from the cohesion and momentum interchange between molecules. Furthermore, there are strong attractions between liquid and solid molecules which enhances the cohesion in the nanofluid. Also, the different velocities of nanoparticles

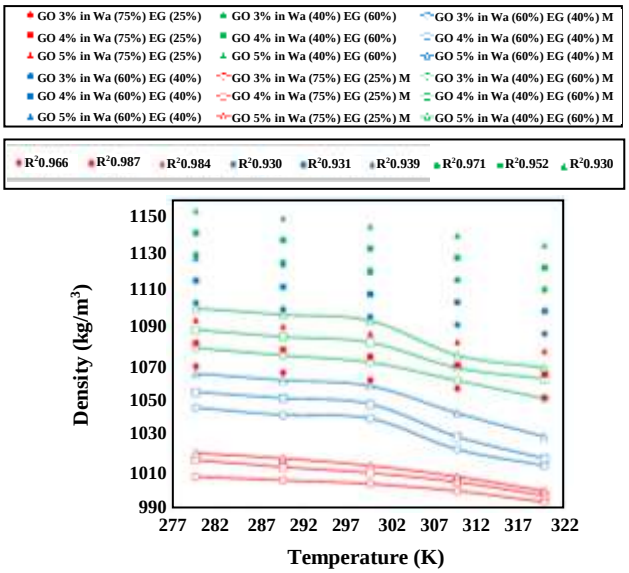

Fig. 5: The obtained density of water-ethylene glycol based GO nanofluids by Pak and Cho [52] equation and NEMD simulations.

and base fluid results in momentum exchange. The reason for increasing of the viscosity of nanofluids with increasing of GO concentration is related to the fact that nanofluids need to consume energy due to the molecular motion of nanoparticles in the base fluid. Therefore, more nanoparticles result in more internal energy consumption and viscosity increases. Moreover, as the temperature of nanofluid increases, the viscosity decreases. In other words, hot liquids have less viscosity than cold ones. Therefore, when energy is added to a liquid, the movements of molecules are intensified to slide past each other with greater ease. In a close meaning, as particles speed up and move apart, viscosity is negatively affected due to the easier movement of molecules. Increasing of the viscosity is desirable because of the enhancement in heat transfer capability. At the same time, this feature shows a great potential that can widely be applied to enhance thermal efficiency in industrial heat transfer fluids.

The molecular dynamics results for the viscosity of the nanofluids at shear rates of 0.5 and 0.05 s^{-1} were shown in Figs. 7 (a) and (b).

The value of 0.05 s^{-1} indicates the low shear rate and the viscosity at low shear rates is defined as the zero-shear viscosity. The zero-shear viscosity is an important scaling parameter; because, it is difficult to be measured. However, NEMD method has an easy procedure to calculate the mentioned value.

The effects of shear rates on the viscosity of the nanofluids were presented in Figs. 8(a)-(c) at low, medium and high temperatures.

The results show that the viscosity of nanofluids decreases with the increase of shear rate. Therefore, the water-ethylene glycol based GO nanofluid behaves as a non-Newtonian shear thinning fluid.

Shear thinning of well-dispersed suspensions can be related to the modifications in the structure and arrangement of interacting particles. Shearing may cause the orientation of particles in the direction of flow proportional to its gradient. This can break agglomerates and hence reduce the amount of solvent immobilized by the particles. The interaction forces may then decrease and change the flow resistance and the apparent viscosity of the system. This is the structural and molecular reason for non-Newtonian shear thinning behavior of the water-ethylene glycol based GO nanofluid.

CONCLUSIONS

The effect of adding graphene oxide nanosheets on the viscosity and density of the base fluid (water + ethylene glycol) with different volume, concentrations were investigated by molecular dynamics simulation method and some theoretical models. The obtained results demonstrated that the viscosity and density of nanofluids increases with increasing the volume concentration of GO nanosheets. Increasing the viscosity is related to improve the heat transfer capability. Therefore, it can be concluded that GO nanosheets have great potential to improve the thermal efficiency in industrial heat transfer fluids. Also, as the temperature increases, the viscosity, and density of the base fluid and nanofluid decreases. In order to validate the molecular dynamics results, the theoretical models were employed to calculate the density and viscosity of nanofluids. There was a good agreement between the obtained results by both NEMD method and theoretical models. According to the shear rate analysis, water-ethylene glycol based GO nanofluids behave as a non-Newtonian fluid. Also, the calculated errors in MD simulations were not more than 6% for density and 7% for the viscosity. Therefore, molecular dynamics method can play a constructive role in providing the cost effective and accurate solutions for investigators in the field of simulation of material properties due to its novel capabilities.

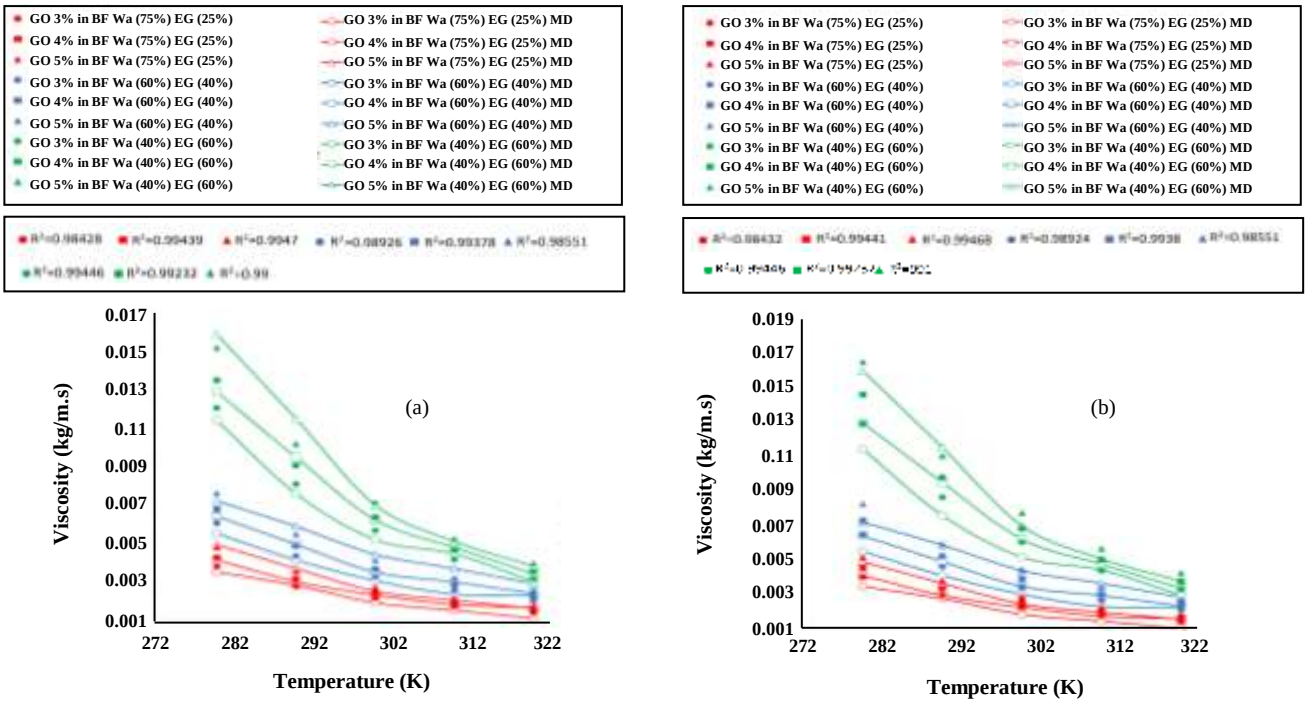

Fig. 6: a) The obtained viscosity of water-ethylene glycol based GO nanofluids by Wang et al. [31] equation and NEMD simulations for a shear rate of 1 s^{-1}. b) The obtained viscosity of water-ethylene glycol based GO nanofluids by Batchelor [53] equation and NEMD simulations for a shear rate of 1 s^{-1}.

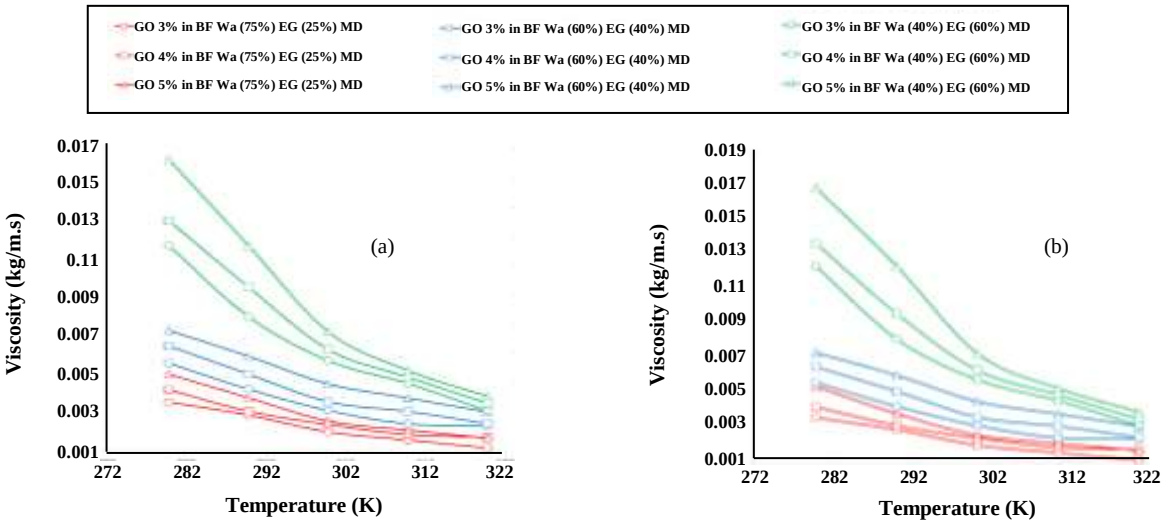

Fig. 7: a) The obtained viscosity of water-ethylene glycol based GO nanofluids by NEMD simulations for the shear rate of 0.5 s^{-1}. b) The obtained viscosity of water-ethylene glycol based GO nanofluids by NEMD simulations for the shear rate of 0.05 s^{-1}

Nomenclature

F	Force on the center of mass of molecule	r	Position of center of mass of the molecule
L	Angular momentum	T	Temperature, K
m	Mass of the molecule	V	Velocity, m/s
p	Translational momentum	μ	Viscosity, kg/m.s
		ρ	Density, kg/m^3

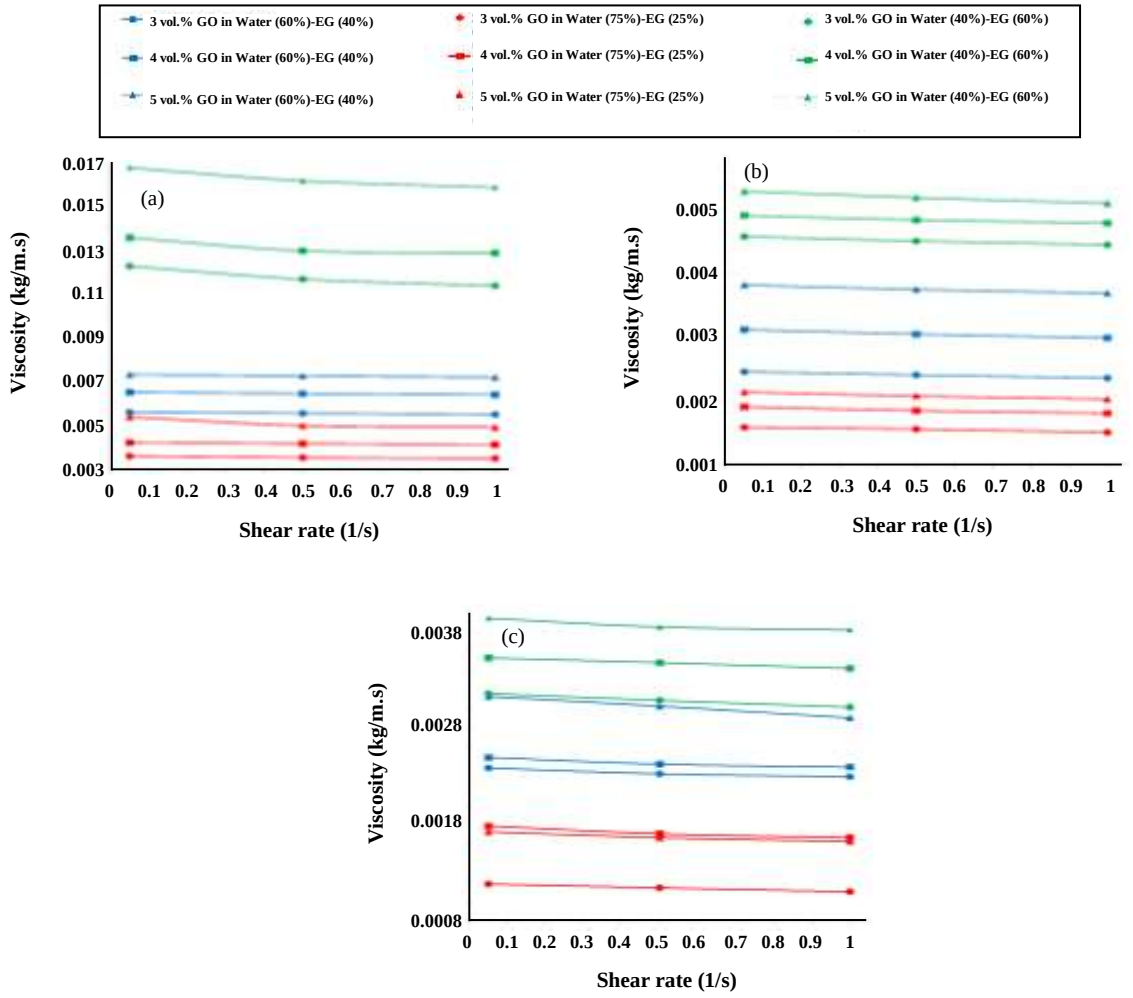

Fig. 8: a) The obtained viscosity of water-ethylene glycol based GO nanofluids as a function of shear-rate by NEMD simulations at a low temperature of 279.85 K. b) The obtained viscosity of water-ethylene glycol based GO nanofluids as a function of shear-rate by NEMD simulations at a medium temperature of 299.85 K. c) The obtained viscosity of water-ethylene glycol based GO nanofluids as a function of shear-rate by NEMD simulations at a high temperature of 319.85 K.

γ	Strain rate

Subscribes

bf	Base fluid
i	Space dimension
j	Space dimension
nf	Nanofluid
s	Solid

Received : Nov. 23, 2016 ; Accepted : Apr. 23, 2018

REFERENCES

[1] Namburu P.K., Kulkarni D.P., Misra D., Das D.K., Viscosity of Copper Oxide Nanoparticles Dispersed in Ethylene Glycol and Water Mixture, *Experimental Thermal and Fluid Science*, **32**: 397-402 (2007).

[2] Zafarani-Moattar M.T., Majdan-Cegincara R., Effect of Temperature on Volumetric and Transport Properties of Nanofluids Containing ZnO Nanoparticles Poly (ethylene glycol) and Water, *The Journal of Chemical Thermodynamics*, **54**: 55-67 (2012).

[3] Choi S.U.S., Eastman J.A., Enhancing Thermal Conductivity of Fluids with Nanoparticles, *ASME-Publications-Fed*, **231**: 99-106 (1995).

[4] Syam Sundar L., Venkata Ramana E., Singh M.K., Sousa A.C.M., Thermal Conductivity and Viscosity of Stabilized Ethylene Glycol and Water Mixture Al_2O_3 Nanofluids for Heat Transfer Applications: An Experimental Study, *International Communications in Heat and Mass Transfer*, **56**: 86-95 (2014).

[5] Murshed S., Leong K., Yang C., Enhanced Thermal Conductivity of TiO_2—Water Based Nanofluids, *International Journal of Thermal Sciences*, **44**: 367-73 (2005).

[6] Wasan D.T., Nikolov A.D., Spreading of Nanofluids on Solids, *Nature*, **423**: 156-159 (2003).

[7] Chaudhury M.K., Complex Fluids: Spread the Word About Nanofluids, *Nature*, **423**: 131-2 (2003).

[8] Lou Z., Yang M., Molecular Dynamics Simulations on the Shear Viscosity of Al_2O_3 Nanofluids, *Computers & Fluids*, **117**: 17-23 (2015).

[9] Sheremet M.A., Pop I., Free Convection in a Porous Horizontal Cylindrical Annulus with a Nanofluid Using Buongiorno's Model, *Computers & Fluids*, **118**: 182-190 (2015).

[10] Izadkhah M., Niya H.E., Moradkhani H., A Study on the Thermophysical Properties of Water/Ethylene Glycol Based Nanofluids Using Non-Equilibrium Molecular Dynamics and Computational Fluid Dynamics Methods. *Modares Mechanical Engineering*, **16**(7): 153-162 (2016) [in Persian].

[11] Mohebbi K., Rafee R., Talebi F., Effects of Rib Shapes on Heat Transfer Characteristics of Turbulent Flow of Al_2O_3-Water Nanofluid inside Ribbed Tubes, *Iranian Journal of Chemistry and Chemical Engineering (IJCCE)*, **34**: 61-77 (2015).

[12] Akram S., Nadeem S., Influence of Nanoparticles Phenomena on the Peristaltic Flow of Pseudoplastic Fluid in an Inclined Asymmetric Channel with Different Wave Forms, *Iranian Journal of Chemistry and Chemical Engineering (IJCCE)*, **36**(2): 107-125 (2017).

[13] Tao X., Jiazheng Z., Kang X., The Ball-Bearing Effect of Diamond Nanoparticles as an Oil Additive, *Journal of Physics D: Applied Physics*, **29**: 2932 (1996).

[14] Rapoport L., Leshchinsky V., Lapsker I., Volovik Y., Nepomnyashchy O, Lvovsky M, Ropovitz-Biro R., Feldman Y., Tenne R., Tribological Properties of WS 2 Nanoparticles under Mixed Lubrication, *Wear*, **255**: 785-793 (2003).

[15] Wu Y., Tsui W., Liu T., Experimental Analysis of Tribological Properties of Lubricating Oils with Nanoparticle Additives, *Wear*, **262**: 819-825 (2007).

[16] Jiao D., Zheng S., Wang Y., Guan R., Cao B., The Tribology Properties of Alumina/Silica Composite Nanoparticles as Lubricant Additives, *Applied Surface Science*, **257**: 5720-5725 (2011).

[17] Chandra Sekhara Reddy M., Vasudeva Rao V., Experimental Investigation of Heat Transfer Coefficient and Friction Factor of Ethylene Glycol Water Based TiO_2 Nanofluid in Double Pipe Heat Exchanger with and without Helical Coil Inserts, *International Communications in Heat and Mass Transfer*, **50**: 68-76 (2014).

[18] Syam Sundar L., Singh M.K., Sousa A., Thermal Conductivity of Ethylene Glycol and Water Mixture Based Fe_3O_4 Nanofluid, *International Communications in Heat and Mass Transfer*, **49**: 17-24 (2013).

[19] Reddy M.C.S., Rao V.V., Experimental Studies on Thermal Conductivity of Blends of Ethylene Glycol-Water-Based TiO_2 Nanofluids, *International Communications in Heat and Mass Transfer*, **46**: 31-36 (2013).

[20] Naddaf E., Abedi M.R., Zabihi M.S., Imani A., Electrocatalytic Oxidation of Ethanol and Ethylene Glycol onto Poly (o-Anisidine)-Nickel Composite Electrode, *Iranian Journal of Chemistry and Chemical Engineering (IJCCE)*, **36**: 59-70 (2017).

[21] Hajjar Z., Morad Rashidi A., Ghozatloo A., Enhanced Thermal Conductivities of Graphene Oxide Nanofluids, *International Communications in Heat and Mass Transfer*, **57**: 128-131 (2014).

[22] Wang G., Shen X., Wang B., Yao J., Park J., Synthesis and Characterisation of Hydrophilic and Organophilic Graphene Nanosheets, *Carbon*, **47**: 1359-136464 (2009).

[23] Kim J., Cote L.J., Kim F., Yuan W., Shull K.R., Huang J., Graphene Oxide Sheets at Interfaces, *Journal of the American Chemical Society*, **132**: 8180-81866 (2010).

[24] Shao G., Lu Y., Wu F., Yang C., Zeng F., Wu Q., Graphene Oxide: the Mechanisms of Oxidation and Exfoliation, *Journal of Materials Science*, **47**: 4400-4409 (2013).

[25] Rosas J.H., Gutiérrez R.R., Escobedo-Morales A., Anota E.C., First Principles Calculations of the Electronic and Chemical Properties of Graphene, Graphane, and Graphene Oxide, *Journal of Molecular Modeling*, **17**: 1133-1139 (2011).

[26] Shen X., Lin X., Yousefi N., Jia J., Kim J-K., Wrinkling in Graphene Sheets and Graphene Oxide Papers, *Carbon*, **66**: 84-92 (2014).

[27] Baby T.T., Ramaprabhu S., Enhanced Convective Heat Transfer Using Graphene Dispersed Nanofluids, *Nanoscale Research Letters*, **6**: 1-9 (2011).

[28] Yu W., Xie H., Li Y., Chen L., Wang Q., Experimental Investigation on the Thermal Transport Properties of Ethylene Glycol Based Nanofluids Containing Low Volume Concentration Diamond Nanoparticles, *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **380**: 1-5 (2011).

[29] Kumaresan V., Velraj R., Experimental Investigation of the Thermo-Physical Properties of Water–Ethylene Glycol Mixture Based CNT Nanofluids, *Thermochimica Acta*, **545**: 180-186 (2012).

[30] Suganthi K., Rajan K., A Formulation Strategy for Preparation of ZnO–Propylene Glycol–Water Nanofluids with Improved Transport Properties, *International Journal of Heat and Mass Transfe*, **71**: 653-663 (2014).

[31] Wang X., Xu X., S. Choi S.U., Thermal Conductivity of Nanoparticle-Fluid Mixture, *Journal of Thermophysics and Heat Transf*, **13**: 474-480 (1999).

[32] Mahbubul I., Saidur R., Amalina M., Latest Developments on the Viscosity of Nanofluids, *International Journal of Heat and Mass Transfer*, **55**: 874-885 (2012).

[33] Chen H., Ding Y., He Y., Tan C., Rheological Behaviour of Ethylene Glycol Based Titania Nanofluids, *Chemical Physics Letters*, **444**: 333-337 (2007).

[34] Allen M.P., Tildesley D.J., "Computer Simulation of Liquids", Oxford University Press; (1989).

[35] Hu C., Bai M., Lv J., Wang P., Li X., Molecular Dynamics Simulation on the Friction Properties of Nanofluids Confined by Idealized Surfaces, *Tribology International*, **8**: 152-159 (2014).

[36] Lu W.-Q., Fan Q.-M., Study for the Particle's Scale Effect on Some Thermophysical Properties of Nanofluids by a Simplified Molecular Dynamics Method, *Engineering Analysis with Boundary Elements*, **32**: 282-289 (2008).

[37] Frenkel D., Smit B., "Understanding Molecular Simulation: from Algorithms to Applications", Academic Press; (2001).

[38] Maruyama S., Molecular Dynamics Method for Microscale Heat Transfer, *Advances in Mumerical Heat Transfer*, **2**: 189-226 (2000).

[39] Eapen J., Li J., Yip S., "Probing Transport Mechanisms in Nanofluids by Molecular Dynamics Simulations", *Proceeding of the 18th National and 7th ISHMT–ASME Heat and Mass Transfer Conference, IIT Guwahati*, India; (2006).

[40] Plimpton S., Fast Parallel Algorithms for Short-Range Molecular Dynamics, *Journal of Computational Physics*, **117**: 1-19 (1995).

[41] Erfan-Niya H., Izadkhah S., Molecular insights into Structural Properties Around the Threshold of Gas Hydrate Formation, *Petroleum Science and Technology*, **34**:1964-71 (2016).

[42] Gharebeiglou M., Erfan-Niya H., Izadkhah S., Molecular Dynamics Simulation Study on the Structure II Clathrate-Hydrates of Methane+ Cyclic Organic Compounds, *Petroleum Science and Technology*, **34**: 1226-1232 (2016).

[43] Dauber-Osguthorpe P., Roberts V.A., Osguthorpe D.J., Wolff J., Genest M., Hagler A.T., Structure and Energetics of Ligand Binding to Proteins: Escherichia Coli Dihydrofolate Reductase-Trimethoprim, A Drug-Receptor System, *Proteins: Structure, Function, and Bioinformatics*, **4**: 31-47 (1998).

[44] Sadus R.J., "Molecular Simulation of Fluids", *Amsterdam:* Elsevier Science; (2002).

[45] Chang J, Kim H., Molecular Dynamic Simulation and Equation of State of Lennard-Jones Chain Fluids, *Korean Journal of Chemical Engineering*, **15**: 544-51 (1998).

[46] NOSÉ S.I., A Molecular Dynamics Method for Simulations in the Canonical Ensemble, *Molecular Physics*, **100**: 191-8 (2002).

[47] Berendsen H.J., Postma J.P.M., van Gunsteren W.F., DiNola A., Haak J., Molecular Dynamics with Coupling to an External Bath, *The Journal of Chemical Physics*, **81**: 3684-3690 (1984).

[48] Simmsons A., Cummings P., Non-Equilibrium Molecular Dynamics Simulation of Dense Fluid Methane, *Chemical Physics Letters*, **129**: 92-98 (1986).

[49] Wang B., Cummings P., Non-Equilibrium Molecular Dynamics Calculation of the Shear Viscosity of Carbon Dioxide/Ethane Mixtures, *Molecular Simulation*, **10**: 1-11 (1993).

[50] Lees A., Edwards S., The Computer Study of Transport Processes under Extreme Conditions, *Journal of Physics C*: *Solid State Physics*, **5**: 1921 (1972).

[51] Sun C., Lu W.-Q., Liu J., Bai B., Molecular Dynamics Simulation of Nanofluid's Effective Thermal Conductivity in High-Shear-Rate Couette Flow, *International Journal of Heat and Mass Transfer*, **54**: 2560-2567 (2011).

[52] Pak B.C., Cho Y.I., Hydrodynamic and Heat Transfer Study of Dispersed Fluids with Submicron Metallic Oxide Particles, *Experimental Heat Transfer an International Journal*, **11**: 151-170 (1998).

[53] Batchelor G.K., "An Introduction to Fluid Dynamics", Cambridge University Press; (2000).

[54] Bagri A., Mattevi C., Acik M., Chabal Y.J., Chhowalla M., Shenoy V.B., Structural Evolution During the Reduction of Chemically Derived Graphene Oxide, *Nature Chemistry*, **2**: 581-587 (2010).

[55] "Handbook A.F.", American Society of Heating, Refrigerating and Air-Conditioning Engineers, Inc: Atlanta, GA, USA. (2009).