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Computational Analysis of Water/Cu Nano Fluid Dynamic Viscosity using Molecular Dynamic Simulations

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ABSTRACT

To enhance thermal management for micro-electric devices, nanofluids become promising working fluids for many thermo-fluid applications. Thermal characteristics of the working fluids can be improved by nano particles additives dispersed in the working fluid such as Cu-nanoparticles in water. The nanoparticle additives manage to alter thermal and dynamic properties of the working fluids such as the dynamic viscosity which plays an important role in specifying thermal and dynamic behaviour of the working media. In order to understand the effect of modifying the dynamic viscosity of the working media, the effective value of this property must be determined. The molecular dynamic (MD) simulation has been used to estimate the Cu/water nanofluid dynamic viscosity at partial volume fractions of φ=0.0125 % and φ= 0.02478 %, and at working temperatures 293 K, 303 K, 313 K, 323 K and 333 K. The used spherical shape nanoparticles are made up of numbers of 0.3-nm-diameter Cu-atoms. The MD simulation results have been compared to reliable experimental and analytical results. The estimated values of the dynamic viscosity using MD simulations converge very well to the experimental and analytical values of the dynamic viscosity, which reveals the advantages of using MD simulations to determine physical properties of nanofluid working medias and hence to design more efficient working fluids. The RDF shows good results for the SPCE model.

Keywords:
Cu/water nanofluid, Dynamic viscosity, Lammps software, Nanofluids, Molecular Dynamics.

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1 INTRODUCTION

Nanofluids are new working fluids which can be recognized as smart cooling/heating medium. Nanofluids fabricated by suspending of a number of nanoparticles inside one of the typical working fluid (water, ethylene glycol, transformer oil, engine oil, R113, oil etc.). There are plenty of nanofluids exist [1-5], which consist of various types of (around 1-100

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nm) nanoparticles (Cu, Al2O3, CuO, SiO2, TiO2, CNT, etc.), which are distributed uniformly in one of the base fluids (typical working fluids). Since base fluids have low thermal conductivity compared to the solid nanoparticles (metal or metal oxide) [6], adding nanoparticles to the base fluid improve heat transfer capacity of the working media [6,7]. Meanwhile, there will be an additional required pumping power to overcome pressure drop caused by the rise in dynamic viscosity associated with dispersing nanoparticles in the base fluid [8]. The MD simulation approach studies the effect of adding Cu nanoparticles in water on the dynamic viscosity. The term "Water/Cu" will be used to indicate nanofluids made out of copper nanoparticles suspended in water as a base fluid. Traditionally, Nanofluids performance could be studied either using the experimental approach which requires modern lab equipment with prohibitive price and operational costs, or using theoretical approach to solve cumbersome governing equations of such type of fluid flow problems. There are plenty of laboratory experiments in literature which investigate and evaluate nanofluid performances using high technological facilities with a prohibitive price and operational costs. Therefore, numerical methods [9-10] or Molecular dynamics approach [11] represent an ideal alternative approach to determine nanofluid's physical characteristics prior to the fabrication process. In the literature, there is an increase in the number of experimental studies compared to the Molecular Dynamics studies; these will be presented in the coming short literature reviews which include collection of most available experimental investigations made to measure the Cu/Water dynamic viscosity. Xinfang et al. [12] investigated the Cu/water nanofluid viscosity using capillary viscometers. They measured viscosity of Cu/Water nanofluid using capillary viscometers for mass fractions of copper nanoparticles between 0.04% and 0.16%, and for temperature range of 30-70 ^{o}C. The experimental results showed that the temperature and SDBS (Sodium Dodecylbenzene Sulfonate) concentration affect the viscosity of the Cu/Water nanofluid and that the mass fraction of Cu has small effect on dynamic viscosity. Some of the experiments investigated both viscosity and thermal enhancement associated with using nanofluids [13-14]. Mahbubul et al. [15] presented their literature review on the latest development on the viscosity of nanofluids, and concluded that nanofluids viscosity increases with the increase of partial volume fractions, and decreases with the increase of temperature but there are some contradictory results on the effects of temperature on viscosity, and remarkable effect of particle size on viscosity of nanofluids. Nguyen et al. [16] investigated experimentally the influence of both the temperature and the particle size on the dynamic viscosities of Al2O3-CuO/water hybrid nanofluid using a 'piston-type' calibrated viscometer. They concluded that particle size did not influence viscosity for particle volume fractions lower than 4%, but for higher particle volume fractions, particle size affected viscosity. They also observed that both temperature and particle volume fraction affect strongly dynamic viscosity. Wu et al. [17] performed an experimental investigations on Al2O3-H2O nanofluids with particle volume fractions of 0.0 % , 0.15% and 0.26% through the silicon-based trapezoidal micro channels and found that nanofluids with low particle volume fractions ($\phi \leq 0.26$ %) give rise to an obvious increase in the convective heat transfer coefficient and the Nusselt number, while it does not cause too much increase in the pressure drop and flow friction through silicon micro channels. Awais et al. [18] conducted comprehensive review to investigate the influence of size, concentration, type and shape of nanoparticles, working

temperature, formation of fouling on heat transfer surfaces, and magnetic field effect on heat transfer enhancement and pressure drop performance of nanofluids. They concluded that sedimentation and agglomeration of nanoparticles in nanofluids introduce fouling on heat transfer surfaces which yield higher pressure drop and hence greater pumping power when particle-size and concentration are increased. In this study, dynamic viscosity of the Cu/water nanofluid has been intensively investigated using Molecular Dynamics approach, in order to estimate the dynamic viscosity associated with two particle volume fractions (φ=0.0125 %, and φ=0.02478 %) at temperatures of 293, 313, 323 and 333 K. The Molecular Dynamics results compared with experimental and analytical results. The Molecular Dynamics results replicated very well the experimental and analytical results.

1.1 Basics of Molecular Dynamics

Different numerical methods can be used to simulate fluid flow based on the length and time scales of the system. As an example, at a millimeter length scale, fluid behaviours can be modelled using continuum level equations (e.g. Navier-Stokes equations, K-ϵ model, ...etc.), and at the discrete (nano-scale) level, fluid behaviours can be modelled using Molecular Mechanics arguments and Molecular Dynamics (MD) simulation. Figure 1 describes different time and length scales for simulating fluids using discrete and continuum models.

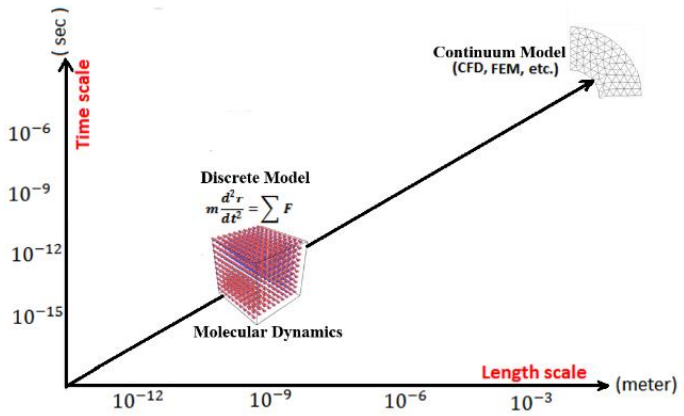

Figure 1. Length and time scales for discrete and continuum models created using (paint & office softwares)

Macroscale thermofluid problems can be modelled based on the Navier–Stokes and energy equations while Molecular Dynamics (MD) particle-based methods are mostly convenient to model thermofluid problems at the molecular level [19]. At the discrete (nano-scale) level; since fluid properties such as pressure changes with respect to space and time, their variations should depend on length and time dimensions in the order of the atomic scale. Therefore, the well-known continuum methods (CFD & FEM, etc.) [20-23] cannot be used to model these systems. In addition, nanofluid dynamic and thermal properties could be studied experimentally to perfectly predict macro scale properties of such fluids, but conducting such experiments requires expensive materials and operational costs. Taking advantage of the large computing capacity of modern computers, the Molecular dynamic approach provides an

effective tool to examine nanofluid thermal and dynamic properties before producing nanofluids in the lab. This can be done using MD simulation which can be run on an ordinary PC before buying lab equipment or materials. The process of preparing Molecular Dynamics simulation starts by defining initial positions and type of particles, that can be done either manually for simple systems or by using an advanced tool (e.g. Moltemplate software [24-25]) for more complex systems. The second step is to compute forces on each particle in the system based on the interaction potential between particles. The third step is to predict how particles move by integrating Newton's second law for an i-atoms system $F_i = \mathrm{m_i}\ \mathrm{dv_i}/\mathrm{dt}$, using a special algorithm (e.g. Verlet algorithm), as described by equations (1),(2)[26].

$$r_{n+1} = r_n + \Delta t\ v_n - \frac{\Delta t^2}{2m}\ \frac{dU_n}{dr} \tag{1}$$

$$v_{n+1} = v_n - \frac{\Delta t}{2m}\ \left(\frac{dU_{n+1}}{dr} + \frac{dU_n}{dr}\right) \tag{2}$$

Where r_{n+1} and $v_{n+1}$are new position and velocity, respectively, Δt is the time step, m is the mass of the particle, U_n describes the interaction potential energy, which uses existing force field formula (Mathematical formula that describes interaction between particles), Example of such potential energy is as described in Figure 2, and takes the following general form (Eq. 3):

$$U(r) = \sum_{bonds} k_b\left(r - r_{eq}\right)^2 + \sum_{angles} k_a\left(\theta - \theta_{eq}\right)^2 + \sum_{dihedrals} k_t[1 + \cos(n\emptyset - \gamma)] + \sum_{non-bonded}\left[\frac{A_{ij}}{r_{ij}^{12}} - \frac{B_{ij}}{r_{ij}^{6}} + \frac{q_i q_j}{r_{ij}}\right] \tag{3}$$

In eq. 3 [26], the potential energy consists of all energy types such as bonds, angles, torsions, and inter- and intramolecular non-bonded interactions. The inter-atomic force is the derivative of this potential with respect to displacement. Parameters from the above equation are chosen to reproduce the experiment, k_b, r_0, k_a, k_t, n, γ, q_i, ε_{ij} and σ_{ij}

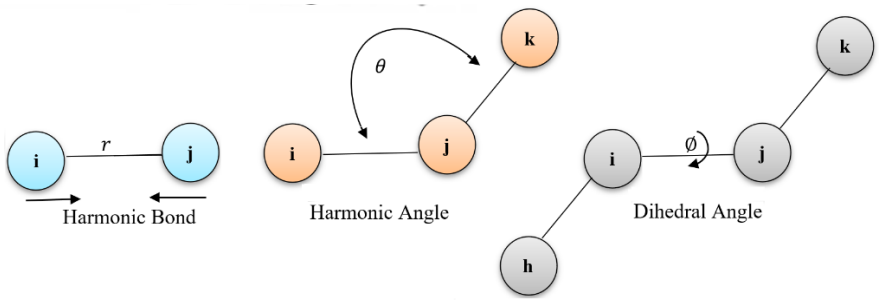

Figure 2. Interatomic forces, created using (paint & office softwares)

The values of dU_n/dr and dU_{n+1}/dr represent old and new interatomic forces. The new position and velocity of each particle can then be calculated based on the force exerted on each particle. After that, the fluid velocity and/or other flow parameters have to be adjusted to control the thermodynamic properties such as fluid temperature and pressure. Finally, repeat

this process until you get the desired number of steps. By repeating these steps, the trajectory of each particle in the simulation box can be calculated (see Figure 3), and viewed to examine how the studied system behaves under certain controlled condition (NPT, or NVT, NVE).

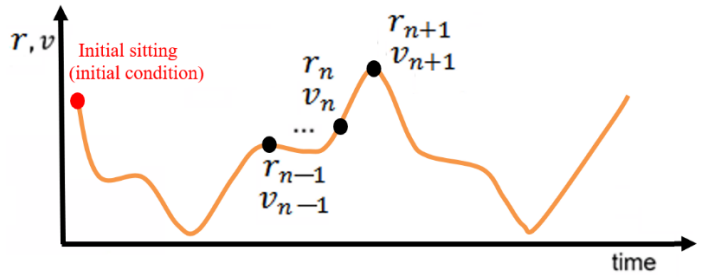

Figure 3. Describes the process of calculating the trajectory and velocity from Verlet algorithm, (paint & office softwares)

2 The Simulation Sitting of Cu/Water Molecular System

The simulation box is a cube of side length L = 3.10342 nm. As in figure 4, thousand H2O molecules organized in the simulation box using Moltemplate software [24-25], then 32 Cu-atoms of diameter = 0.3 nm, makes 2 Cu-particles (φ=0.0125%). The simulation boundary condition is taken as a periodic type. During calculation of the two physical properties, the three NPT, NVT and NVE ensembles were applied to each of the four Cu\water sitting. The running time was 3 ns. The Hydrogen atom is a blue ball, Oxygen is a red ball, Cu-atom is white ball

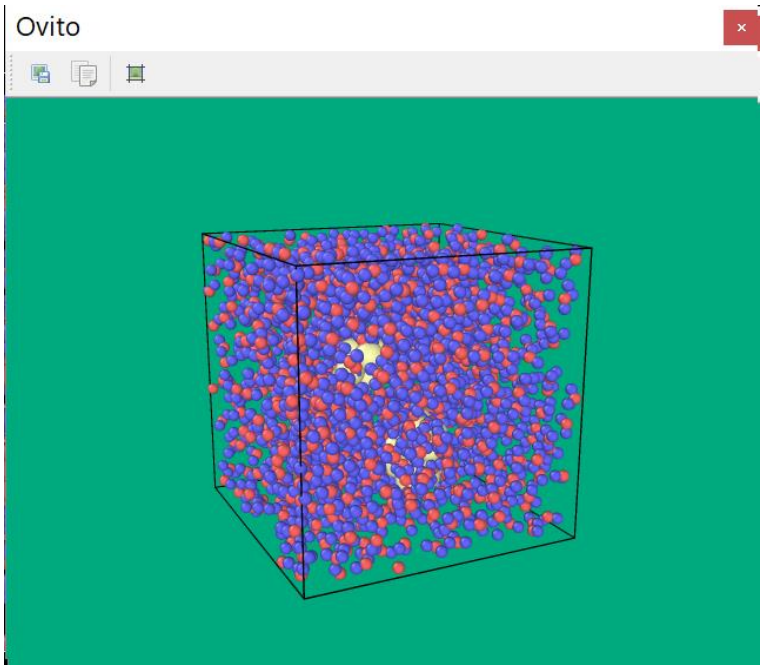

Figure 4. The simulated nanofluid with φ=0.0125% and temperature of 303 (generated in Moltemplate [24-25] and Lammps [27] softwares), displayed using Ovito software.

For the SPCE water model [11], the interatomic forces between molecules are described by the non-bonded terms from (Eq.4)

$$E_{ab} = \sum_{ij} \left[\frac{A_{ij}}{r_{ij}^{12}} - \frac{B_{ij}}{r_{ij}^{6}} + \frac{q_i q_j}{r(ij)} \right] \quad (4)$$

Where $A_{kk} = 4\varepsilon_k \sigma_k^{12}$ and $B_{kk} = 4\varepsilon_k \sigma_k^{6}$

The water interatomic forces are modelled using the SPCE water model, while those of the copper nanoparticles are computed from an inter-atomic energy model called (the EAM multi-body potentials). Table 1 describes parameters for the interatomic forces of the Cu/water.

Table 1. Pairwise force field coefficients for the Cu/water nanofluid [11, 28, 29, 30]

LJ parameters for non-bonding interactions between water molecules		
Molecules	ε (Kcal/mole)	σ(A)
H-H	0.04600	0.4000
H-O	0.08360	1.7753
O-O	0.15535	3.1570
The copper-copper (Cu-Cu) interatomic forces modelled using Cu_u3.eam		
LJ parameters for non-bonding interactions between copper molecules and both hydrogen and oxygen molecules		
Cu-H	0.65890	0.2117
Cu-O	1.19800	1.5870

Figure 5, presents (a) the size of two Cu-nanoparticles, (b) Cu-nanoparticles plus thousand SPCE water molecules. It is difficult to precisely predict the size of these two Cu-nanoparticles, but it is possible to approximate them.

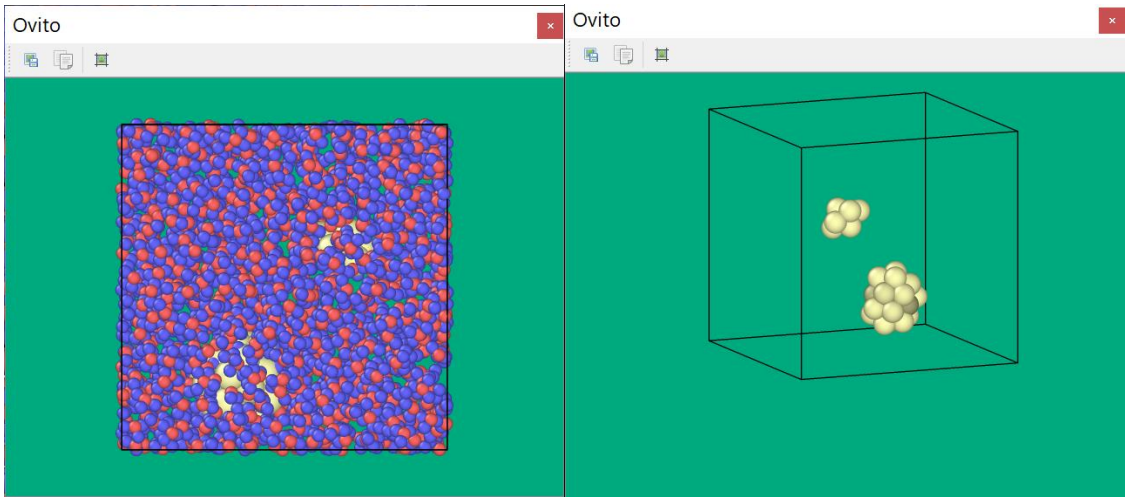

Figure 5. (a) The two nanoparticles generated from 32 Cu-atoms (diameter of one atom = 0.3 nm) (b) thousand H2O water molecules plus two Cu-nanoparticles, after 1 ns NPT ensemble (generated in Moltemplate [24-25] and Lammps [27] softwares), displayed using Ovito software.

The RDF is an important parameter to chick the convergency of the model. Water molecules shows good behaviours since the convergence toward one is guaranteed, see figure 6.

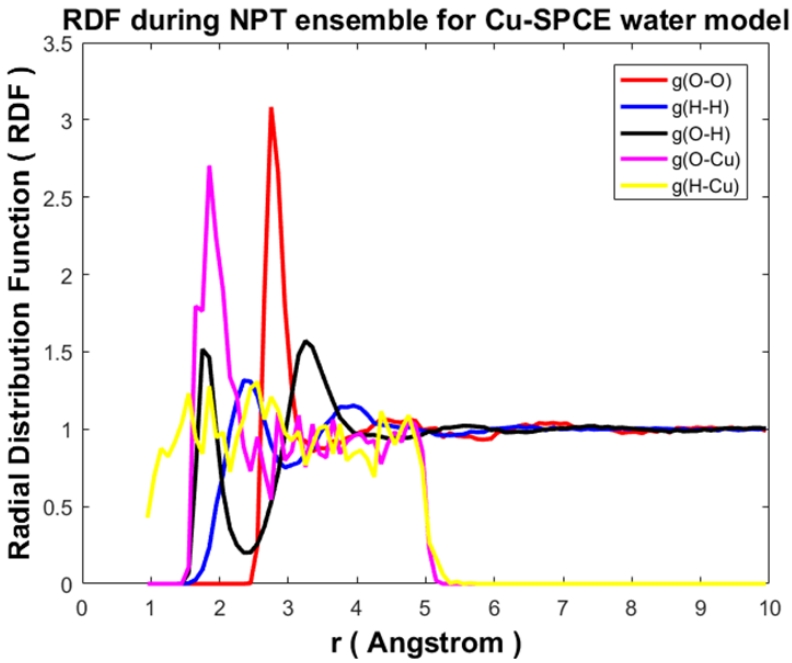

Figure 6. The RDF of the Cu/water nanofluid.

3 Green Kubo Formula

The Green Kubo formula relates microscopic fluxes to thermal conductivity or dynamic viscosity during the three ensembles (NPT, NVT, or NVE), where the G-K method can be

used to calculate the transport properties when the simulated system equilibrated for enough time [11,28-29], see (Eq. 5)

$$q = \left[\sum_{j=1}^{M} v_j E_j - \sum_{\propto=1}^{M} H_N \sum_{j=1}^{M} v_{Nj}\right] + \frac{1}{2}\left[\sum_{i=1}^{M}\sum_{j=1,j\neq i}^{M} r_{ij}(v_j . F_{ij})\right] \quad (5)$$

Where the total energy per atom is Ej, the displacement and the interatomic forces are rij and Fij, respectively. The particle speed is vj, and the number of particles is M. The averaged partial enthalpy H_N defined as in (Eq. 6)

$$\eta = \frac{shear\ stress}{strain\ rate} = -\frac{\tau}{dv/dy} \quad (6)$$

4 Dynamic Viscosity

The dynamic viscosity can be defined as the ratio between shear stress to the strain rate, which is given by [11], see (Eq. 7)

$$H_N = \frac{1}{M}\sum_{j=1}^{M}\left(E_j + r_j . F_j\right) \quad (7)$$

Where the shear stress (τ) is proportional to the velocity gradient (dv/dy). Dynamic viscosity can be calculated using the Green-Kubo formula [11], as in (Eq. 8)

$$\eta_{xy} = \frac{V}{k_B T}\int_0^{\infty} < \delta_{xy}(0)\delta_{xy}(t) > dt \quad (8)$$

Where η is the dynamic viscosity and the stress tensor δ_{xy} is given by (Eq. 9)

$$\delta_{xy} = \sum_{i=1}^{M}\frac{\delta_{x_i}\delta_{y_i}}{m_i} \pm \sum_{i>j}^{M}\left(x_i - x_j\right)\frac{\partial U_{ij}(y)}{\partial y_j} \quad (9)$$

The potential energy is U_{ij} describes the interatomic forces between two particles and it is the derivative of the potential energy with respect to y.

5 Analytical Dynamic Viscosity

Both particle volume fraction and particle shape and also temperature degree can affect dynamic viscosity. The analytical dynamic viscosity (Eq.10) [31]:

$$\mu_{nf} = \mu_{bf}\left(1 + \frac{\varphi}{100}\right)^{11.3}\left(1 + \frac{T_{nf}}{70}\right)^{-0.038}\left(1 + \frac{dp}{170}\right)^{-0.061} \quad (10)$$

Where μ_{bf}, μ_{nf} are the base fluid and the analytical nanofluid dynamic viscosity respectively. The particle volume fraction of the nanoparticles is denoted by the term "φ", dp is particle diameter (nm), T_{nf} is nanofluid temperature (C^o).

6 RESULTS AND DISCUSSIONS

Figure 7 illustrates dynamic viscosity of the Cu/water nanofluid from Molecular Dynamic simulation compared to the selected sets of experimental dynamic viscosity [32] and analytical results [31], at temperatures 293 K, 303 K, 313 K, 323 K and 323 K. The triangular symbols, blue curve, represent current MD dynamic viscosity results at partial volume fraction of (φ=0.0125%) , the circular symbols, green curve, represent analytical results]31] at partial volume fraction of (φ=0.0125%), and the star symbols, black curve, represent experimental values given by reference [32] at (φ=0.011%). The experimental values of pure water dynamic viscosity reported by reference [32] were plotted as x symbols, red curve. By inspecting these results, current MD simulation gave results which are generally in acceptable agreement with the experimental and analytical results. At temperatures less than 313 K, current MD simulation results show higher values of the dynamic viscosity as compared to the corresponding values given by experiments, but converge towards experimental values for higher temperatures. The reported discrepancy at lower temperatures can be justified by the slightly different partial volume fractions between the two cases. Another explanation for this deviation is that the accuracy of the current results may be contaminated by numerical errors associated to the SPCE model used to predict interatomic forces between molecules [11, 28, 29]. The results from the experimental work made by Wilk et al. [32] show for (φ=0.011%) almost the same dynamic viscosity of pure water, but dispersing Cu nanoparticle must increase dynamic viscosity, therefore, MD and analytical results seem to be more accurate.

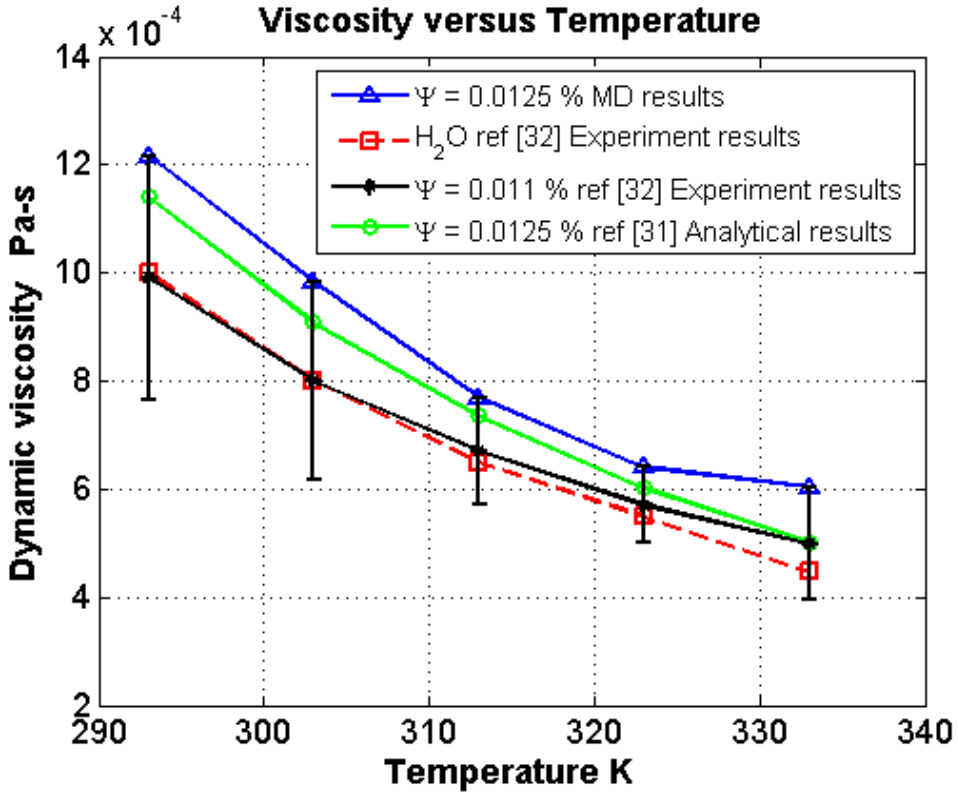

Figure 7. Molecular Dynamics, and experimental dynamic viscosities Cu/Water nanofluid versus temperatures between 293 K to 333 K.

To examine the effect of partial volume fraction variations on the dynamic viscosity, another extra MD simulation have been carried out. The partial volume fractions used are φ=0.0125 %, and φ= 0.02478 %, at temperatures 293 K, 303 K, 313 K, 323 K, and 333 K. Figure 8 represents the MD results compared to the analytical results [31], both modules showed slight increments in dynamic viscosity as partial volume fraction increases. As depicted from Figure 8, as nanofluid temperature increases dynamic viscosity decreases. However, the SPCE water model start to affect viscosity results as temperature increases above 313 K. In general, the effect of varying particle volume fractions on the dynamic viscosity is less than the effect of temperature changes for the studied range of temperatures and partial volume fractions.

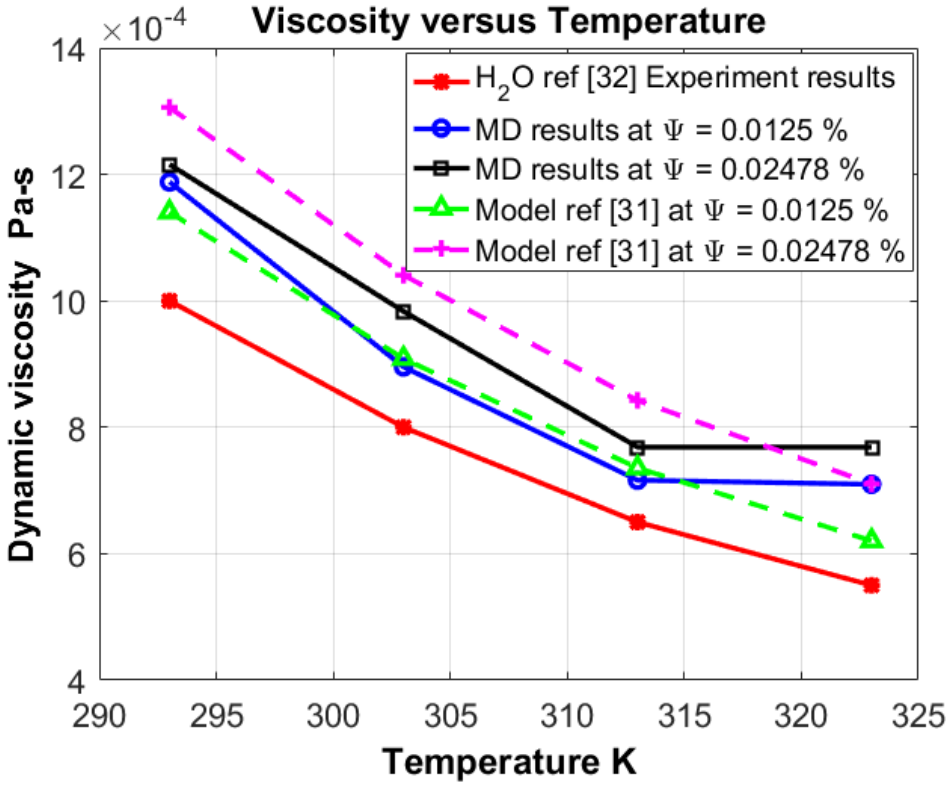

Figure 8. Cu/Water nanofluid MD and analytical viscosity results for temperatures (293 K to 333 K) and partial volume fractions (φ=0.0125 %, and φ=0.02478 %).

7 CONCLUSIONS

Our Molecular Dynamics viscosity results have been confirmed with reliable available experiments. This study concludes that the MD results converges to the analytical results [31]. It is also noticeable, that both the MD and the analytical results mimic the experiments viscosities at the studied range of partial volume fractions and temperatures. The dynamic viscosity increases by increasing the partial volume fraction of the dispersed nanoparticles. However, increasing nanofluid temperature decreases viscosity. A thermal enhancement could

be achieved by using Cu/water nanofluid but there will be an extra pumping power required to overcome friction between nanoparticles themselves and the friction force developed between the nanofluid and the pipe walls. Current MD simulation results agreed very well with experiments and analytical results. Both analytical results and MD simulation results showed an increase in the dynamic viscosity values as particle volume fraction increases. MD simulation, analytical and experimental results indicate that the Dynamic viscosities decrease as the working temperature increase. The dynamic viscosity results from the current MD simulations showed small deviation from the experimental and analytical results, but it is in the acceptable range. To the best of our knowledge, shear stress and rigid water models do not accurately predict dynamic viscosity when vapour is generated at higher temperature in the simulated box. This reasoning can be examined by lowering working temperature levels and /or increasing simulation time or using more accurate models to predict interatomic forces. Although another water model might simulate more accurately the dynamic viscosity of water such as the TIP4-2005. We conclude that the MD results are in an acceptable accuracy for engineering applications and that MD simulation reduce the cost and complexity associated with experiments and allow engineers to design new mono or hybrid nanofluids as an efficient working fluid, before buying an expensive lab equipments or materials.

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التحليل الحسابي للزوجة الديناميكية للمائع النانوي (ماء+ نحاس) باستخدام المحاكاة لديناميكية الجزيئات

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الملخص

لتعزيز الأستفادة المثلي من الطاقة الحرارية للأجهزة الكهربائية الدقيقة ، غدت الموائع النانوية (nanofluids) تستخدم كبديل لموائع التبريد المعتادة في العديد من التطبيقات الهيدروحرارية (thermofluid). فيمكن تحسين الخصائص الحرارية لموائع التشغيل عن طريق إضافة جزيئات نانوية في مائع التشغيل (مثل إضافة جزيئات النحاس النانوية في الماء). تسهم إضافة الجسيمات النانوية في تغيير الخصائص الحرارية والديناميكية لموائع التشغيل مثل اللزوجة الديناميكية التي تلعب دورًا مهمًا في تحديد السلوك الحراري والديناميكي لموائع التشغيل. لفهم تأثير التغيرات باللزوجة الديناميكية لمائع التشغيل ، يجب تحديد القيمة الفعالة لهذه الخاصية. تم استخدام المحاكاة لديناميكية الجزيئات (Molecular Dynamic Simulation) لتقدير اللزوجة الديناميكية للمائع النانوي المنشاء من نثر جزيئات النحاس في الماء (Cu/water) بكسور حجم جزئية ϕ= 0.0125% و ϕ= 0.0247% ،وعند درجات حرارة 293 كلفن، 303 كلفن، 313 كلفن، 323 كلفن،و 333 كلفن. تتكون الجسيمات النانوية المستخدمة(nanoparticles) ذات الشكل الكروي من ذرات (atoms) نحاس قطرها 0.3 نانومتر. تمت مقارنة نتائج المحاكاة مع نتائج تجريبية (experiments) وتحليلية (analytic) موثوقة. نتائج المحاكاة تقاربت بشكل جيد جدًا مع القيم التجريبية والتحليلية للزوجة الديناميكية ، وذلك يبين مزايا استخدام المحاكاة لديناميكية الجزيئات (MD) لتحديد الخصائص الفيزيائية لموائع التشغيل النانوية وبالتالي لتصميم موائع تشغيل أكثر كفاءة. بدراسة لدالة التوزيع الشعاعي RDF نجد أن نموذج الماء المستخدم SPCE يعطي نتائج مقبولة لعدد جزيئات الماء المستخدمة.

الكلمات الدالة:
المائع النانوي (نحاس + ماء).
اللزوجة الديناميكية.
برنامج المحاكاة لامب.
الموائع النانوية.
دراسة ديناميكاالجزيئية.

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