FLOW AND HEAT TRANSFER BEHAVIORS OF WATER-BASED NANOFLUIDS CONFINED IN NANOCHANNEL BY MOLECULAR DYNAMICS SIMULATION

W. CUI^{a, b}, Z. SHEN^{a, b*}, J. YANG^{a*}, S. WU^b

^aSchool of Automotive Engineering, Harbin Institute of Technology, Weihai, China

^bSchool of Energy Science and Engineering, Harbin Institute of Technology, Harbin, China

The present work reports a molecular dynamics simulation on the flow and heat transfer behaviors of water-based nanofluids confined in a nanochannel. The Brownian motion of nanoparticles in the base fluid is analyzed. Rotational velocity of nanoparticle is found to be in the range of $1 \times 10^9 \sim 1 \times 10^{10}$ rad/s. Translational velocity of nanoparticles is calculated by MD simulation to be approximately 10m/s. By means of rotational and translational Peclet number the effect of nanoparticle movements for heat transfer augmentation with nanofluids near the fixed wall is evidently higher than that of base fluid, which indicates the velocity gradient and temperature gradient of nanofluids near the fixed wall is greater than those of single-phase base fluid. The change of nanofluid velocity and temperature profiles is attributed to the high-speed micro-motions of nanoparticles.

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1. Introduction

Nanofluids,^[1] produced by dispersing a small amount of solid particles with sizes on the order of nanometers (1-100nm) into traditional engineered fluid, are a new type of heat transfer fluids which attracts great interests of scientists for their significantly increased thermal conductivity and further improvement in convective heat transfer properties, and therefore it has been extensively studied in recent years. Eastman et al. have observed a 40% increase in thermal conductivity with 0.3 vol % copper nanoparticles of 10nm diameter.^[2] Das et al. reported thermal conductivity increase of up to 25% in water with 1-4 vol % alumina nanoparticles.^[3] Heris et al. reported that the Nusselt numbers of nanofluids are greater than that of water with the same Peclet number with Al₂O₃-H₂O and CuO-H₂O nanofluids, which demonstrates the adding of nanoparticles increases convective heat transfer properties of water.^[4] He et al. demonstrated experimentally that convective heat transfer of TiO₂-H₂O nanofluids is enhanced by 12% at Re=1500, while at Re=5900 the enhanced convective heat transfer effect has been increased by over 40%.^[5] Compared to conventional methods of enhanced heat transfer, nanofluids provide anomalously increased thermal properties and slightly increased flow resistance lost, which is extremely suitable for high-efficiency, compact, and high-heat-flux cooling applications. However, scientists still cannot confirm the microscopic mechanism hidden in the phenomenon of heat transfer enhancement with nanofluids, which is important for understanding energy transport process in nanofluids and further application of nanofluids.

^{*}Corresponding author: shenzj@hitwh.edu.cn

Some researchers proposed that Brownian motion of nanoparticles may be a key mechanism for explaining the abnormal increase in thermal properties of nanofluids. Koo et al. suggested that nanoparticles move randomly and thereby carry relatively large volume of surrounding liquid with them.^[6] As a result of Brownian motion nanofluids possess lower local temperature gradient compared with single-phase base fluid, and therefore the effective thermal conductivity of nanofluids is increased. Jang and Choi revealed that Brownian motion of nanoparticles at the molecular and nanoscale level is a key mechanism governing the thermal behavior of nanofluids and they proposed a theoretical model which connects the measured macroscale phenomena and molecular/nanoscale fluctuations.^[7] Hwang et al. revealed that the migration of nanoparticles due to Brownian motion and hot swimming movement is an important reason for convective heat transport enhancement in nanofluids.^[8] However, other researchers argued that Brownian motion has only minor effect on the heat transfer enhancement in nanofluids. Evans et al.^[9] reported that the hydrodynamics effects associated with Brownian motion have only a minor effect on the thermal conductivity of nanofluids. Buongiorno revealed by an order-of-magnitude estimation that energy transfer by nanoparticle dispersion is negligible.^[10] Brownian diffusion and thermophoresis have been identified as the two most important nanoparticle/base-fluid slip mechanisms. Therefore, more theoretical studies are still needed on the effect of nanoparticle motions for the heat transfer augmentation in nanofluids.

With statistical mechanics a molecular dynamics (MD) simulation is effective for giving most accurate nanoscale flow and transport phenomenon compared to any classical model based on continuum mechanics.^[11] This method provides a needed supplement to experimental measurements, which can be extremely difficult at such length scales. In this work, we have considered the flow and heat transfer of water-based nanofluids with MD simulation. The present work is intended to reveal the micro-motions of nanoparticles in a flow field, and obtain the microscopic flow and heat transfer behaviors of nanofluids. A simulation model of water-based nanofluids containing one Cu nanoparticle is established. The Brownian motion of nanoparticles is decomposed into rotation and migration and calculated by MD simulation. By means of rotational and translational Peclet number, the effect of nanoparticle Brownian motion for thermal conductivity enhancement of nanofluids is evaluated. Furthermore, velocity profile and temperature profile of nanofluid flow are obtained by MD simulation, and the difference of flow and heat transfer behaviors between nanofluids and single-phase fluid is investigated.

2. Simulation method and model

In the present work, a simulation system of nanofluids is created by the classical MD simulation code "Lammps".^[12] The simulation system is composed of water as the base fluid and one Cu nanoparticle installed in the centre of base fluid. The simulation system also contains a driving plate on the top for exerting shearing velocity and a fixed plate on the bottom. The size of simulation system is 6.51 nm×6.51 nm×14.3nm. And the height of fluid zone is 12.85 nm. The diameter of nanoparticle is 4nm. Based on previous literatures,^[11] it is found after several attempts that when the total quantity of simulated particle exceeds 10000 the influence of particle quantity for the simulation result is excluded. In the present work, the total particle quantity in the simulation system is 26421. Initially particle (Cu atom or H₂O molecule) distribution is arranged in accordance with Face Centered Cubic (FCC) lattice.

MD simulations employ empirical or semi-empirical potentials to describe interactions between atoms. Lennard-Jones (LJ) is a commonly used potential, which is used for describing interactions between gaseous or liquid atoms, which is written as:^[13]

$$u_{ij} = 4\varepsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right], \qquad (1)$$

where r_{ij} represents the distance between atom i and atom j ($r_{ij}=r_j-r_i$), ε is characteristics potential energy of interactions between molecules, σ is characteristics diameter of molecule. The first item

represents the repulsive force caused by overlap of the inner electrons or ions in an atom, and the second item represents the electrostatic attraction between dipoles.

During MD simulation, resultant force on each atom meets the Newton's law: ^[13]

$$m_i \frac{d^2 r_i}{dt^2} = \sum_{j \neq i} F_{ij} \quad , \tag{2}$$

where m_i and r_i represent the quality and location of atom i, and the interaction between atom i and atom j can be written as:

$$F_{ij} = -\frac{\partial u_{ij}}{\partial r_{ii}} , \qquad (3)$$

Substitute equation (1) to equation (3), the interactions between molecules can be written as:

$$F_{ij} = \frac{48\varepsilon}{\sigma^2} \left[\left(\frac{\sigma}{r_{ij}} \right)^{14} - \frac{1}{2} \left(\frac{\sigma}{r_{ij}} \right)^8 \right] \Gamma_{ij} , \qquad (4)$$

The model of nanofluid in the present work is composed of water molecules and copper nanoparticle. The LJ potential parameters that are suitable for governing interactions between Cu atoms and H_2O molecules can be calculated according to Lorentz-Berthelot mixing rule, which is written as^[13]:

$$\sigma_{sl} = \frac{\sigma_{ss} + \sigma_{ll}}{2} , \qquad (5)$$

$$\varepsilon_{sl} = \sqrt{\varepsilon_{ss} \Box \varepsilon_{ll}} \quad , \tag{6}$$

The LJ potential parameters used in the present work are listed in Table 1. Currently there are several typical potential functions for describing interactions between water molecules, and SPCE potential is the most used one for describing interactions between water molecules,^[14] which is adopted in the present work. The potential parameters for SPCE potential could be found in literatures ^[14]. For the interactions between Cu atoms, embedded atom model (EAM) potential is employed. ^[15]

Table 1 LJ potential parameters for Cu-H₂O nanofluids

Atom 1	Atom 2	$\epsilon (g \text{ Å}^2/fs^2)$	σ (Å)
0	0	1.0568e-028	3.1506
Cu	Cu	6.5582e-027	2.338
Ο	Cu	8.3251e-028	2.7443

In the simulation, the cut-off radius is chosen to be $2.5\sigma_{oo}$. A mixed boundary condition is used: fixed wall boundary condition is applied along z-axis, while periodic boundary condition is used along x- and y- axis. NVE ensemble is used in the simulation. The time step length is 2fs. The length of relaxation time is 250ps and the snapshot of equalized simulation system after relaxation is shown in Fig.1. Fig.2 illustrates the internal energy of simulation system during the relaxation. It could be found in the figure that the simulation system is quickly becoming stable during the relaxation. After relaxation, a shearing velocity of 50m/s is applied to the driving plate. The simulation system is computed for 10000ps under different temperatures, including: 293K, 313K, 333K, and 353K. Firstly the movements of nanoparticle in nanofluids including rotation and migration are simulated by MD simulation. And the simulated results are analyzed by means of rotational and translational Peclet number to explore the effect of nanoparticle movements for heat transfer augmentation in nanofluids. Afterwards, the velocity profile and temperature profile are calculated by MD simulation and compared with those of single-phase base fluid to investigate the effect of nanoparticle movements for changing flow and heat transfer behaviors of nanofluids. Fig.3 illustrates the overall snapshots for the simulation system at different simulation time. It could be found in the figure that the nanoparticles are moving randomly in the base fluid.



Fig.1 Simulation system of nanofluids



Fig. 2. Internal energy of simulation system



Fig.3 Snapshot of simulation system at different simulation time

3. Results and discussion

3.1 Rotation of nanoparticles

The rotational speed of nanoparticle in base fluid is calculated through MD simulation. Fig.4-Fig.7 illustrate rotational speed of nanoparticles at temperatures of 293K, 313K, 333K, 353K, respectively. It could be found in the figures that the rotational velocity components of nanoparticles at 293K are in the range of -2×10^9 rad/s ~ 2×10^9 rad/s, with instantaneous maximum speed of 8×10^9 rad/s; The rotational velocity components of nanoparticles at 313K are in the range of -3×10^9 rad/s ~ 3×10^9 rad/s, with instantaneous maximum speed of 1×10^{10} rad/s; The rotational velocity components of nanoparticles at 333K are in the range of -4×10^9 rad/s ~ 4×10^9 rad/s, with instantaneous maximum speed of 8×10^9 rad/s; The rotational velocity components of nanoparticles at 353K are in the range of -6×10^9 rad/s ~ 6×10^9 rad/s, with instantaneous maximum speed of 1×10^{10} rad/s. Therefore, the nanoparticle is rotating at a quite fast speed in base fluid. The order of magnitude of angular velocity of nanoparticle is 10^9 . The rotary direction of nanoparticles is changing randomly. Rotation of nanoparticle is found to be influenced by temperature. Nanoparticle rotates faster at higher temperature. However, the influence of temperature does not induce qualitative change in angular velocity of nanoparticle, under the present investigation temperature range.



Fig.4 Angular velocity of nanoparticle at 293K



Fig.5 Angular velocity of nanoparticle at 313K







Fig.7 Angular velocity of nanoparticle at 353K

The effect of nanoparticle rotation for heat transfer augmentation in nanofluids could be analyzed by means of defining the rotational Peclet number, Pe_r : ^[10, 16]

$$Pe_{r} = \frac{\nu l}{\alpha} = \left(\tau_{w}/\mu\right) \cdot \left(d_{p}^{2}/\alpha\right) = \omega \cdot \left(d_{p}^{2}/\alpha\right), \tag{7}$$

where v is the velocity, l is the characteristic length, τ_w is the shear stress at the wall, μ is the fluid viscosity, d_p is the particle diameter, ω is angular velocity of nanoparticle, and $\alpha = k/\rho c$ is the fluid thermal diffusivity. In Eq.(7) the term (dp^2/α) represents the time constant for conduction heat transfer, while the term (τ_{ω}/μ) represents the angular velocity of the particle. Therefore, if the angular velocity of the particle ω is large enough, then Pe_r is large, and heat transfer enhancement by particle rotation is possible.

In the present work, the rotation speed of nanoparticle in water is demonstrated to be in the range of $1 \times 10^9 \sim 1 \times 10^{10}$ rad/s. The thermal conductivity k, density ρ , and heat capacity c_p of liquid water at 273K~373K is about 0.6W/m·K, 1×10^3 kg/m³, and 4kJ/kg·K. Then the thermal diffusion coefficient of water is calculated to be about 1.5×10^{-7} m²/s. Hence the rotational Peclet number, Pe_r , is approximately 1. The rotation of nanoparticle is proved to be effective for heat transfer enhancement in nanofluids.

3.2 Migration of nanoparticles

The translational speed of nanoparticle in base fluid is also calculated by MD simulation. Fig.8-Fig.11 illustrate translational speed of nanoparticles at temperatures of 293K, 313K, 333K, 353K, respectively. It could be found in the figures that the translational velocity components of nanoparticles along non-shearing directions at 293K are in the range of $-3m/s \sim 3m/s$, with instantaneous maximum speed of 7m/s; The translational velocity components of nanoparticles along non-shearing directions at 313K are in the range of $-4m/s \sim 4m/s$, with instantaneous maximum speed of 9m/s; The translational velocity components of nanoparticles along non-shearing directions at 313K are in the range of $-4m/s \sim 4m/s$, with instantaneous maximum speed of 9m/s; The translational velocity components of nanoparticles along non-shearing directions at 313K are in the range of $-5m/s \sim 5m/s$, with instantaneous maximum speed

of 9m/s; The translational velocity components of nanoparticles along non-shearing directions at 353K are in the range of $-7m/s \sim 7m/s$, with instantaneous maximum speed of 12m/s. Hence, the nanoparticle is migrating at a quite fast speed in base fluid. The order of magnitude of translational velocity of nanoparticle is 10. The translational direction of nanoparticles is changing randomly. Migration of nanoparticle is found to be influenced by temperature. Nanoparticle migrates faster at higher temperature. However, the influence of temperature also does not induce qualitative change in translational velocity of nanoparticle, under the present investigation temperature range.



Fig.8 Translational velocity of nanoparticle at 293K



Fig.9 Translational velocity of nanoparticle at 313K



Fig.11 Translational velocity of nanoparticle at 353K

The migration of nanoparticle may also be effective for heat transfer enhancement in nanofluids. The definition of translational Peclet number, Pe_t is given by:

$$Pe_{t} = \frac{vl}{\alpha} = \left(v/d_{p}\right) \cdot \left(d_{p}^{2}/\alpha\right), \tag{8}$$

The time period of migration of the nanoparticle is $\tau = d_p / v$ (sec). The time heat takes in diffusing a characteristic distance of one particle diameter d_p (4nm) in a fluid of thermal diffusivity α_f (cm²/sec), is $t \sim d_p^2 / \alpha_f$ (sec). The augmentation is expected if τ is of the same order of magnitude as t or larger, which can be written as,

$$d_p^2/\alpha_f \sim d_p/\nu, \qquad (9)$$

The thermal diffusion coefficient of water is calculated to be about $1.5 \times 10^{-7} \text{m}^2/\text{s}$. In the present work, the translational velocity of nanoparticles is calculated by MD simulation to be approximately 10m/s. Hence, one can easily calculate the order of magnitude of τ is of the same order of *t*. Therefore the migration of nanoparticle is also proved to be effective for heat transfer enhancement in nanofluids.

3.3 Velocity profile

Velocity profiles of nanofluids at 293K, 313K, 333K, and 353K are calculated by MD simulation and shown in Fig.12. The velocity profile of single-phase base fluid is also calculated and shown with solid line in the figure for comparison. It could be found in the figure that the local velocity of nanofluids near the fixed wall is evidently higher than that of base fluid. That is, the velocity gradient of nanofluids near the fixed wall is greater than that of single-phase base fluid. As for the influence of temperature, despite all the velocity profiles of nanofluids at different temperatures differ from that of single-phase fluid, the velocity profiles of nanofluids at different temperatures do not shown qualitative difference, under the present investigation temperature range. In the previous sections the micro-motions of nanofluid velocity profile compared to single-phase base fluid to be of high speed. The change of nanofluid velocity profile compared to single-phase base fluid is attributed to the high-speed micro-motions of nanoparticles.



Fig.12 Velocity profile of nanofluids with different temperatures



Fig.13 Temperature profile of nanofluids at different simulation time

3.4 Temperature profile

By applying temperature difference on the fluid confined within plates, temperature profile of nanofluids can be obtained. In this case, the shearing velocity on driving plate remains 50m/s, meanwhile the temperatures applied on driving plate and fixed plate are 293K and 343K, respectively. The temperature of fluid area is not controlled after relaxation of 600ps.

In the previous section, the velocity profile has been found to be different from that of base fluid. The changed fluid field will directly affect the temperature field. Fig.13 shows the temperature profile of nanofluids at different temperatures. In the figure the temperature profile of single-phase base fluid is also calculated and shown with solid line for comparison. It could be found in the figure that the temperature profile of nanofluids near the fixed wall is evidently higher than that of base fluid. That is, the velocity gradient of nanofluids near the fixed wall is greater than that of single-phase base fluid. Furthermore, the temperature profiles of nanofluids at different simulation time are different, which indicates the influence of nanoparticle movements for the temperature profile of nanofluids is pulsing.

4. Conclusions

In this paper, flow and heat transfer behaviors of water-based nanofluids confined in nano channel is studied by MD simulation. The orders of magnitude of nanoparticle rotation and migration have been obtained and the effect of nanoparticle movements has been verified by means of rotational and translational Peclet number. Velocity profile and temperature profile of nanofluids confined in nanochannel are calculated and the difference of flow and heat transfer behaviors between nanofluids and single-phase base fluid is obtained. The following conclusions have been drawn:

1. Rotational velocity of nanoparticle is found to be in the range of $1 \times 10^9 \sim 1 \times 10^{10}$ rad/s through MD simulation. The rotational Peclet number, Pe_r , is calculated to be approximately 1. Translational velocity of nanoparticles is calculated to be approximately 10m/s by MD simulation. The time period of nanoparticle migration τ is found to be of the same order of time heat takes in diffusing a characteristic distance t. The rotation and migration of nanoparticle are proved to be effective for heat transfer enhancement in nanofluids.

2. Velocity profile and temperature profile of nanofluids confined in nanochannel are obtained. It is found that the local velocity and temperature of nanofluids near the fixed wall is evidently higher than that of base fluid. That is, the velocity gradient and temperature gradient of nanofluids near the fixed wall is greater than those of single-phase base fluid. The change of nanofluid velocity and temperature profiles compared to single-phase base fluid is attributed to the high-speed micro-motions of nanoparticles.

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