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# Molecular dynamics simulation on flow behaviors of nanofluids confined in nanochannel

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ABSTRACT

Nanofluids are new heat transfer liquids with remarkable heat transfer capability prepared by suspending nanoparticles in traditional heat transfer liquids (water, ethylene glycol and engine oil). The key reason for the enhanced heat transfer properties of nanofluids is not only their increased thermal conductivity but also the changed rheological behavior of base fluid due to the adding of nanoparticles. However, currently the investigation into influence of shear velocity on flow behaviors of nanofluids is still inadequate. In this paper molecular dynamics simulations are used to simulate flow behaviors of nanofluids confined in nanochannel under different shear velocities. Rotation and translation of nanoparticles and nonlinear velocity profiles of nanofluids are observed. The degree of nonlinearity, as well as the rotation and translation of nanoparticles, are enhanced with the shear velocity increasing. The existence of "solid-like" absorbed layers near the plates and around the nanoparticles is also demonstrated.


## 1. Introduction

Nanofluids were first proposed by Choi [1] from Argonne National Laboratory in 1995. Since then, many attentions are paid to experimental and theoretical studies on heat transfer and rheological behavior of nanofluids.

Abnormal heat transfer ability of nanofluids with a very low nanoparticle concentration has been demonstrated by experimental studies. Lee et al. [2] measured thermal conductivities of oxide nanofluids by a transient hot-wire method. For the copper oxide/ethylene glycol system, thermal conductivity can be enhanced by more than 20 percent at a volume fraction of 4%. Zhang et al. [3] have observed a 27% enhancement in thermal conductivity by adding only 0.5 wt% of carbon coated Cu nanoparticles in polyethylene glycol, and 49%, 40%, and 30% enhancement in thermal conductivity for carbon coated Cu, Al, and Fe nanoparticles loading of 1.5 wt%, respectively. Xuan and Li [4] experimentally investigated convective heat transfer and flow features of Cu-water nanofluids in a tube with a constant heat flux at wall. Their results showed that the nanofluids give remarkable enhancement of heat transfer rate compared to pure water. The same conclusion has also been demonstrated by Wen et al. [5] and Heris et al. [6] with CuO-water nanofluids and $Al_2O_3$-water nanofluids, respectively. Rheological behavior of fluid plays a significant role in heat transfer capability. A number of researchers have studied the rheological behaviors of nanofluids experimentally. Previous studies have demonstrated that some nanofluids are

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Newtonian fluids in nature, and the viscosity increases with the increase of concentration of nanoparticles [7–10]. However, other nanofluids have been observed to show non-Newtonian behavior (shear-thinning behavior) [11–14]. Nusselt number and convective heat transfer coefficient of nanofluids increase with nanoparticle concentration and Reynolds number. [15–17]

Currently, there are no theoretical formulas available to predict the anomalous thermal conductivity of nanofluids satisfactorily. Researchers are attempting to find more accurate theory to predict the thermal conductivity. Yu and Choi [18,19] proposed a modified Maxwell model to include the effect of ordered nanolayer around the nanoparticles and a modified Hamilton–Crosser model for suspensions of nonspherical nanoparticles to include the effect of a solid/liquid interface. Xuan et al. [20] and Koo and Kleinstreuer [21] proposed theoretical models to predict the thermal conductivity of nanofluids including the effect of the Brownian motion of the nanoparticles. Researchers have investigated the heat transfer capability of flowing nanofluids by numerical methods such as CFD. Akbari et al. [22] compared single-phase and two-phase CFD models for the predictions of laminar mixed convection of $Al_2O_3$-water nanofluids. They concluded that two-phase model is more accurate for the predictions of the convective heat transfer coefficient. Namburu [23] investigated the turbulent flow and heat transfer of nanofluids and proposed that Nusselt number increases by 35% for 6% CuO nanofluids over the base fluid at a constant Reynolds number. Dawood et al. [24] reported numerical simulation for three dimensional laminar mixed convective heat transfers at different nanofluids flow in an elliptic annulus with constant heat flux. The results revealed that $SiO_2$-Water nanofluid has the highest Nusselt number, followed by $Al_2O_3$-Water, ZnO-Water, CuO-Water, and lastly pure water. The Nusselt number increased as the nanoparticle volume fraction and Reynolds number increased; however, it decreased as the nanoparticle diameter increased. Shariat et al. [25] studied laminar mixed convection $Al_2O_3$-water nanofluid flow in elliptic ducts with constant heat flux boundary condition employing two phase mixture model. Results showed that in a given Reynolds number (Re) and Richardson number (Ri), increasing solid nanoparticles volume fraction increases the Nusselt number (Nu) while the skin friction factor decreases. Abdolbaqi et al. [26] numerically studied heat transfer enhancement of nanofluids under turbulent flow through a straight square channel under constant heat flux conditions at the upper and lower walls. The results showed that the heat transfer rates and wall shear stress increase with an increase of the nanofluids' volume concentration. Al-Shamani et al. [27] numerical studied heat transfer due to turbulent flow of nanofluids through rib-groove channel. Their results indicated that the Trapezoidal with increasing height in the flow direction rib-trapezoidal groove has the best heat transfer rate and high Nusselt number. It is also found that the $SiO_2$-nanofluid has the highest value of Nusselt number in comparison with the other type of nanofluids. The Nusselt number increases as the volume fraction increases and it decreases as the nanoparticle diameter increases.

Much effort has been paid on the mechanisms of the excellent heat transfer ability by using nanofluids. Sarkar and Selvam [28] demonstrated that the thermal transport enhancement of nanofluids is mostly due to the increased movement of liquid atoms in the presence of nanoparticles and transport process for mass and heat is similar. Eapen et al. [29] showed that the thermal conductivity enhancement arises from a strong short-ranged attraction between nanoparticle and liquid. They also demonstrated that the Brownian motion of the clusters have only an insignificant role in the enhancement, which is consistent with Evans' achievement [30]. However, other researchers [31–33] reported that the Brownian motion of nanoparticles constitutes a key mechanism of the thermal conductivity enhancement. Li et al. [34] and Sachdeva and Kumar [35] showed that liquid layers around the nanoparticles lead to the more significant enhancement of the thermal conductivity of the nanofluids. But Xue et al.[36] reported that the enhancement of thermal conductivity of nanofluids cannot be explained by altered thermal transport properties of the layered simple liquid. Nie et al. [37] suggested that the thermal conductivity enhancement of nanofluids is due to the high thermal conductivity of nanoparticles themselves, but the fluid molecules make no evident contribution to the enhancement of thermal conductivity attributable to the presence of the nanoparticles at volume fractions less than 5%. Keblinski et al. [38] showed that the key factors in understanding thermal properties of nanofluids are the ballistic, rather than diffusive, nature of heat transport in the nanoparticles, combined with direct or fluid-mediated clustering effects that provide paths for rapid heat transport.

Molecular dynamics (MD) method is a computational method that solves atomic classical equations of motion with known interatomic potentials, and the physical properties can be calculated with statistical mechanics. Mohebbi conducted prediction of specific heat and thermal conductivity of nanofluids by a combined equilibrium and non-equilibrium MD simulation [39]. The results showed that the thermal conductivity increases with increasing the loadings and decreasing the temperature. They proposed that the thermal transport enhancement in nanofluid was mostly due to the increased movement of surrounding liquid phase atoms in the presence of non-metallic nanoparticle. Loulijat et al. examined the influence of solid–solid inter-atomic potential type on thermal conductivity of nanofluids by MD simulations [40]. They suggested that the thermal conductivity of (Ar–Cu) nanofluid is influenced by the type of potential used in the simulation. Sun et al. [41] focused on nanofluid's effective thermal conductivity in high-shear-rate Couette flow. It was the first attempt to calculate the thermal conductivity of shearing fluid in equilibrium molecular dynamics (EMD) method, in which transport properties are calculated by Green–Kubo formula. The nanoparticle in the nanofluid in shear field is found to rotate under the action of the velocity gradient. They have proposed that the rotation induces enhanced “microconvection” effect which is the main reason for the linear increase in the effective thermal conductivity of the shearing nanofluid with the shear rate increasing. They have also found that the increase is more sharply with lower volume fraction of nanoparticle than with higher volume fraction, because the “microconvection” effect is weakened in the nanofluid with higher volume fraction of nanoparticle resulted by the slower nanoparticle rotation speed.

The present work is designed based on the following basic understanding: the key reasons for the enhanced heat transfer