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Effect of chaotic movements of nanoparticles for nanofluid heat transfer augmentation by molecular dynamics simulation

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HIGHLIGHTS

- The orders of magnitude of translational and rotational motions for nanoparticles are given.
- The microscopic structure around a nanoparticle is proposed.
- Mechanisms of heat transfer enhancement in nanofluids are discussed.

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ABSTRACT

Through Molecular Dynamics simulation, the chaotic movements of nanoparticles in base fluid are investigated. Based on the simulated results of translational and rotational velocities of nanoparticles, the effect of nanoparticle movements for heat transfer in nanofluids is discussed. Furthermore, the influence of nanoparticle movements for the base fluid is studied. The fluid near a nanoparticle is divided into three levels: (1) absorption layer, (2) rotating fluid, and (3) spherical existential space, or called rotating fluid element. And the microscopic structure of nanofluid which is composed of countless rotating fluid elements is proposed.

1. Introduction

Nanofluids [1], the suspensions of nanometer sized particles in liquids, present fascinating features, including: anomalously high thermal conductivities at very low nanoparticle concentrations [2,3], and enormously enhanced heat transport performance [4,5]. Meanwhile nanofluids are more stable and have acceptable flow resistance increase. By using nanofluids as working fluid, heat transfer rate can be greatly increased with less pumping power expense. With the enhanced heat transfer properties, nanofluids have great potential as improved heat-management fluids which can be applied in developing highly compact and effective heat transfer equipment for many industrial applications, including automotive engineering, nuclear reactors, biomedicine, and electronics, etc [6].

Heat transfer experiments are indicating that thermal conductivity is not only the reason for heat transfer augmentation of nanofluids. Hence, proper detailed physical mechanism for nanofluid heat transfer augmentation still needs to be established [7]. Due to the very small size of nanoparticles, the chaotic movements of nanoparticles might be an important mechanism for explaining the nanofluid heat transfer augmentation. Xuan and Li experimentally demonstrated that the enhanced heat transfer by nanofluid results from two aspects: One is the increased thermal conductivity; and the other one is the chaotic movement of ultrafine particles accelerates energy exchange process in the fluid [8]. He et al. found that the enhanced heat transfer performance of nanofluid is better under turbulent flow [9]. The far more chaotic movements of nanoparticles under turbulent flow may account for their experimental results. Through scale analysis and numerical solutions, Hwang et al. proposed the flattened velocity profile due to particle migration induced by Brownian diffusion and thermophoresis as the possible mechanism of the convective heat transfer enhancement [10]. Cui et al. experimentally studied the flow characteristics of nanofluids in a wavy-walled tube. And the

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visualization experimental results showed: At the same Reynolds number the nanoparticles cause more homogeneous longitudinal mixing and enhance mass transferring of nanofluids, which indicates the micro-flow in nanofluids is enhanced [11]. Hence, we proposed the opinion that: besides increased thermal conductivity, heat transfer in nanofluids is further enhanced on the basis of changed flow characteristics and enhanced mass transfer.

Researchers have conducted numerical analysis on the thermal properties of nanofluids and the mechanisms of heat transfer enhancement. Jang et al. numerically investigated the cooling performance of a microchannel heat sink with nanofluids, and they have found that nanofluids reduce both the thermal resistance and the temperature difference between the heated microchannel wall and the coolant [12]. The cooling performance of a microchannel heat sink with water-based nanofluids containing diamond is enhanced by about 10% compared with that of a microchannel heat sink with water. Bianco et al. numerically investigated the developed laminar forced convection flow of a water-Al_2O_3 nanofluid in a circular tube, submitted to a constant and uniform heat flux at the wall. The maximum difference in the average heat transfer coefficient between single- and two-phase models results is about 11%. Convective heat transfer coefficient for nanofluids is found to be greater than that of the base liquid. Heat transfer enhancement is found to be influenced by the particle volume concentration, wall shear stress values, and Reynolds number [13]. Ellahi et al. examined the non-Newtonian nanofluid flow with heat transfer and variable viscosity by means of the homotopy analysis method [14–16]. Explicit analytical expressions for the velocity field, the temperature distribution and nanoconcentration have been derived analytically. And the effects of various physical parameters on velocity, temperature, and nanoconcentration are discussed by using graphical approach. Azmi et al. developed a numerical model for turbulent flow of nanofluids in a tube with twisted tape inserts [17]. The model is based on the assumption that van Driest eddy diffusivity equation can be applied by considering the coefficient and the Prandtl index in momentum and heat respectively as a variable. The coefficient and the Prandtl index in the eddy diffusivity equation of momentum and heat is obtained from the numerical values as a function of Reynolds number, concentration and twist ratio. An enhancement of 94.1% in heat transfer coefficient and 160% higher friction factor at Reynolds number Re = 19,046 is observed at a twist ratio of five with 3.0% volumetric concentration when compared to flow of water in a tube. Palm et al. numerically investigated the heat transfer enhancement capabilities of coolants with suspended metallic nanoparticles inside typical radial flow cooling systems [18]. Their results clearly indicated considerable heat transfer benefits with the use of fluid/solid particle mixtures. It was also found that the use of temperature-dependent properties make for greater heat transfer predictions with corresponding decreases in wall shear stresses when compared to predictions using constant properties. Hassan et al. presents three-dimensional transient model for vapor chamber (flat heat pipe) and the effect of nanofluids on its performance [19]. Their results show that the nanoparticles added to the working fluid decrease vapor chamber temperature, liquid velocity and liquid pressure and increase mass evaporated. They also showed that Cu nanofluid has the greatest effect on the vapor chamber temperature compared with CuO and Al_2O_3 nanofluids. Zeeshan et al. developed the analytic and numerical solutions for the steady flow of viscous nanofluid between the concentric cylinders [20]. Expressions of velocity, temperature, concentration and nanoparticle fraction are derived. Numerical values for Dufour and thermophoresis parameters are tabulated by optimization method. Hasan et al. numerically examined the effect of using nanofluid in micro pin fin heat sink [21]. And the result indicated that, using of nanofluid instead of pure fluid as a coolant leads to enhanced heat transfer performance by increasing the amount of heat dissipated but it also leads to increased pressure drop for all fins shapes and nanofluids studied. Delavari et al. numerically simulated turbulent and laminar flow heat transfer in nanofluids passing through a flat tube in 3D using computational fluid dynamics for single and two-phase approaches [22]. A small difference in the friction factors of the tube was observed between the two approaches and the Nusselt number for the two-phase model was markedly different from that for the single-phase model; however, the volumetric flow for the same heat transfer rate decreased and less pumping power was required for the nanofluids. Sheikholeslami et al. numerically examined the magnetohydrodynamic effect on convection heat transfer of nanofluid [23–26]. The results indicated that Nusselt number is an increasing function of nanoparticle volume fraction, Rayleigh numbers and inclination angle while it is a decreasing function of Hartmann number. And it could also be found that increasing Rayleigh number leads to decrease heat transfer enhancement while opposite trend is observed with augment of Hartmann number. In computational fluid dynamics, there are commonly four popular approaches for the numerical simulation of two-phase flow, including: the single-phase model, the mixture multiphase model, the Eulerian–Eulerian multiphase model, and the Euler–Lagrange multiphase model. Among these models the Eulerian–Eulerian [27–30] and the Euler-Lagrange multiphase models [13,31–33] are more appropriate for numerically simulating the flow of nanofluids. Hussein et al. reviewed the computational simulation of nanofluids and found that most of the numerical works are in agreement with the results of experimental work [6]. The suspensions of solid nanoparticles significantly enhance heat transfer and the heat transfer coefficient of nanofluids is found to be larger than that of its base fluid at the same Reynolds number. Additionally, increasing the volume fraction of solid nanoparticles increases the heat transfer of nanofluids. The authors have concluded that the enhancement of the heat transfer of the nanofluids may be caused by the suspended nanoparticles increasing the thermal conductivity of fluids, and the chaotic movement of ultrafine particles increases fluctuation and turbulence of the fluids, accelerating the energy exchange process. Kakac et al. summarized the important research works on the enhancement of the forced convection heat transfer with nanofluids [34]. They have pointed out that more experimental results and the theoretical understanding of the mechanisms of the particle movements are needed to understand heat transfer and fluid flow behavior of nanofluids. Sarkar et al. reviewed the natural and forced convective heat transfer and pressure drop correlations for both laminar as well as turbulent flows of nanofluid [35]. Large deviation of *Nu* has been observed between proposed correlations both for laminar and turbulent flow. The authors pointed out that one reason for this phenomenon may be due to the lack of common understanding on basic mechanism of nanofluid flow.

Molecular dynamics (MD) is a computer simulation method of physical movements of atoms and molecules in the context of N-body simulation [36]. The trajectories of atoms and molecules are determined by numerically solving the Newton's equations of motion for a system of interacting particles, where forces between the particles and potential energy are defined by molecular mechanics force fields. As this method starts with the Newton's equations of motion, the simulation results is infinitely close to the real situation which means, in theory, that the simulated results is as accurate as experiment. MD simulation is able to solve the small region and obtain the microcosmic mechanism, and may be the unique accurate method for simulating micro flow at present [37]. To investigate the mechanism of chaotic movements of nanoparticles for nanofluid heat transfer, MD method is much more suitable, compared to conventional experimental or numerical simulation method. Currently much work by MD simulations has