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Entropy generation analysis of particle suspension induced by Couette flow

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ABSTRACT

This paper describes the behavior of nanoparticle suspension under shear with non-equilibrium molecular dynamics (MD) approach. Couette flow with constant shear rate is applied to calculate its particle distribution and analyze its effect on velocity and viscosity. Also, analytical models are proposed to demonstrate the accuracy of the suspension viscosity evaluated by MD approach. Entropy generation plays the key role to estimate system irreversibilities due to fluid flow and heat transfer. So the entropy generation of the particle suspension is estimated in this paper. It presents that the particles tend to reside in the central part of fluid region with low shear rate, which restricts local entropy producing. And appropriate particle volume fraction and particle size may be helpful to reduce the entropy generation of the suspension. We also find that heat transfer would make much greater contribution to entropy generation when temperature gradient appears in the suspension.

1. Introduction

The suspension flow with solid nanoparticles, which can be widely applied in the fields of thermal management and energy storage, has been paid more and more attention since 90s of last century due to its high performance of heat transfer and large thermal capacity.

Currently, most of the work was focused on the study of thermal conductivity enhancements of nanoparticle suspension and also suspension's kinetic properties. Hong studied Fe nanofluids to find its high thermal enhancement performance [1–5]. Annop did the research work on rheological properties of alumina–water nanofluids with electrical double layer by experiments [6]. Keblinski [7] investigated the thermal properties of nanoparticle suspension and proposed a number of potential factors responsible for its anomalous increase in heat conduction.

Entropy generation is as critical as thermodynamic properties for thermal engineering system. Heat transfer performance of thermal management system needs to be maximized and its entropy generation also to be minimized to meets the requirement in system design and operation, since entropy generation plays a crucial role in the level of irreversibilities during the system operating process. Giangaspero [8] presented an application of the entropy generation minimization method to the pseudo-optimization of the configuration of the heat exchange surfaces in a Solar Rooftile with a commercial CFD code. Entropy generation in MHD porous channel with hydrodynamic slip and convective boundary conditions was also studied and found that entropy generation could be minimized via optimizing of geometrical and physical parameters of the system [9]. Singh [10] provided a theoretical investigation of the entropy generation analysis due to flow and heat transfer for convection in alumina-water nanofluids to find an optimum diameter at which the entropy generation is the minimum for the given nanofluid. Sohel [11] discussed different types of entropy generation in the circular microchannel and minichannel analytically using copper and alumina as the nanoparticles and water and ethylene glycol as the base fluids. A new whole field method was been done by Saffaripour [12] to measure the velocity and temperature distribution in the transition region between a 100 nm wide rectangular microchannel, which led to the frictional and thermal terms of entropy generation, and the results were beneficial to determine the highest thermal and hydraulic efficiencies. Heat transfer of fully-developed mixed convection nanofluid flow in vertical channel was studied by Chen [13] and entropy generation was numerically calculated and its relationship with viscous dissipation was tried to be studied. Mahian [14] reviewed the recent entropy generation studies due to flow and heat transfer of different nanofluids in various geometries and with different boundary conditions and found that appropriate channel size and

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particle volume fraction could be very beneficial in entropy generation decreasing. However, all the work about nanofluid has been subject to the continuum theory, and there's still lack of the study at molecular level to reveal the entropy generation mechanism.

As we all know, when at least one length scale of thermal system is less than 100 nm, the systems cannot be described by classical continuum theory since deviation from it might appear. In this communication, investigation of entropy generation of the thermal management system at molecular level is very necessary. However, based on the overview of the literature, this area is much less investigated and molecular dynamic study of entropy generation is not essentially addressed. So we focus on entropy generation of nanoparticle suspension subjected to shear Couette flow via molecular dynamics approach. Generally, entropy is produced by heat dissipation due to thermal conductivity and viscosity. Both local and global entropy generation are calculated in our article and we also explore the crucial factors including particle size, particle volume fraction, most primary, viscosity and temperature gradient. The relationship between non-uniform particle distribution and entropy generation is analyzed. This paper is organized as follow. In the next chapter we describe our model structures and simulation methodology. Section 3 presents the simulation results of kinetic and thermodynamic properties of nanoparticle suspension of Couette flow, and entropy generation evaluation is calculated and analyzed. Finally, Section 4 is a summary.

2. Model structures and simulation methodology

The structure used for Couette flow simulations is shown in Fig. 1. The initial crystalline structure is arranged as perfect FCC lattice with sizes $Lx = Ly = 30\sigma \times 30\sigma$ (in x and y in-layer directions) and 60σ in the normal to the in-layer (z) direction, where fluid atoms with saturated density of $0.8\sigma^3$, corresponding to the initial temperature, are confined between 6084 boundary atoms. Here, σ indicates the length scale parameter of the interatomic potential. In addition, the suspension is composed by the base fluid and randomly dispersed spherical particles. We mark solid wall atoms as green and liquid atoms shows grey. The colorful atoms indicate various nanoparticles. The finite size effect is limited by the application of periodic boundaries in x and y dimensions.

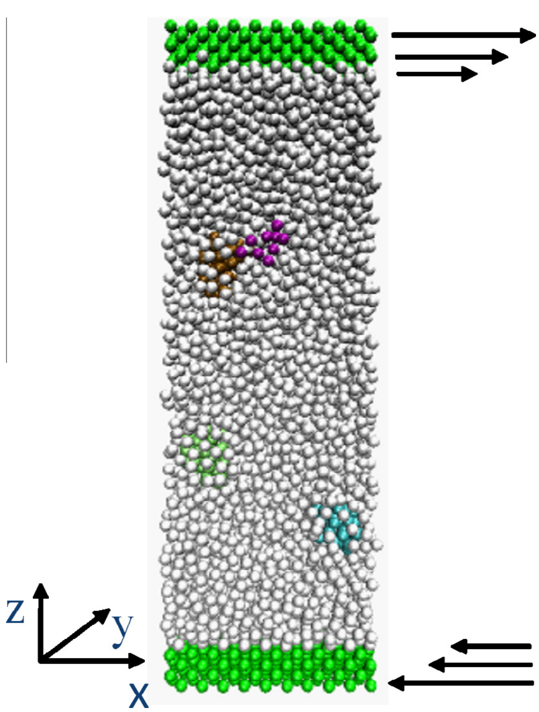

Fig. 1. The geometry and velocity sketch of Couette flow.

The truncated Lennard–Jones (L–J) potential is applied to describe the atom interaction:

$$V_{LJ}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \tag{1}$$

where, r is the interatomic spacing, while σ and ε are length and energy scale parameters, respectively. The cut off distance is chosen as 3.0σ. The strength of the interaction between solid atoms (including boundary atoms and nanoparticle atoms) ε_{ss} 4 times larger than that between liquid atoms ε_{ll}, and ε_{ll} is taken as reference energy scale parameter. The strength of interaction between solid and liquid atoms ε_{sl} is $2\varepsilon_{ll}$, obeying to the Lorentz–Berthelot combining rule [15].

$$\sigma_{1-2} = (\sigma_1 + \sigma_2)/2$$

$$\varepsilon_{1-2} = (\varepsilon_1 \cdot \varepsilon_2)^{1/2} \tag{2}$$

In the simulations, the initial structure is equilibrated at constant temperature and pressure (NPT) and the equilibrium state can be achieved when the velocity exhibits Maxwell distribution after 1,000,000 time steps. Then forces are added to the upper and lower boundaries with equal amount but opposite direction. Consequently, the energy of the total system is conserved. In this way, constant shear rate can be generated by boundaries' sliding to mimic Couette flow.

The boundaries are cooled at constant temperature in all simulations to remove the heat generated in the suspension by shearing and thus avoiding significant temperature increase. Another 35,000,000 time steps (20,000,000 time steps for pure fluid) "production runs" continues to get steady state to obtain mechanical properties and entropy generation. Equation of motions, governed by Newton's Law, is integrated by Verlet algorithm with a timestep of 0.05τ, where τ is the L–J time unit [16].

Entropy generation plays an important role in device performance analysis. Generally, fluid deformation, internal heat generation and absorption may contribute to viscous dissipation. All of these will result in entropy generation. Two approaches are applied to calculate entropy generation [14]. One method is to evaluate the local entropy generation of every point of the system at first and total generation can be obtained by integrating over the whole volume, which is very appropriate to study entropy generation at micro perspective. Another one is to make use of correlations for friction factor and Nusselt number to describe the system total entropy generation. Obviously, with MD method, Nusselt number has no definition and the correlations is also not available. So entropy generation here is described with first approach as following [17]:

$$S = \frac{k}{T^2}\left[\left(\frac{\partial T}{\partial x}\right)^2 + \left(\frac{\partial T}{\partial y}\right)^2 + \left(\frac{\partial T}{\partial z}\right)^2\right] + \frac{\eta}{T}\left\{2\left[\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial v}{\partial y}\right)^2 + \left(\frac{\partial w}{\partial z}\right)^2\right] + \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)^2 + \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right)^2 + \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right)^2\right\} \tag{3}$$

where, k, η indicate the effect thermal conductivity and effect viscosity of suspension, and u, v, w denote the x, y and z component of velocity. In our simulations, shear forces were added only along x direction and the gradient only occurred in z direction, so the formula can be simplified