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Insight into the contribution of rotating Brownian motion of nonspherical particle to the thermal conductivity enhancement of nanofluid

Dongxing Song, Yang Yang, Dengwei Jing *

State Key Laboratory of Multiphase Flow in Power Engineering & International Research Center for Renewable Energy, Xi'an Jiaotong University, Xi'an 710049, China

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ABSTRACT

Up to now, most thermal conductivity models of nanofluid considering Brownian motion assumed that particles are spherical. It is obviously not the cases in the practical application. In our study, we successfully derived the equation of angular velocity of rotating Brownian motion ($\boldsymbol{\omega}$) as a function of particle size, mass and resistance coefficient and resistance moment coefficient etc. based on Langevin equation and energy equipartition theorem. By using a rotating Reynolds number Re_r, the effect of rotating Brownian motion of cubic particles was evaluated when the model is used to predict thermal conductivity of nanofluid. What' more, the thermal conductivity was chosen to experimentally verify the possible contribution of the rotating motion of nonspherical particles for the first time. Cubic nanoparticles of 30, 50 and 60 nm in sizes have been prepared and the thermal conductivities for their colloid suspensions were experimentally investigated. It was found that the prediction of the thermal conductivities for the cubic nanoparticle suspension "considering $\boldsymbol{\omega}$" is in very good agreement with the experimental values, while that for "without considering $\boldsymbol{\omega}$" case is much smaller than the experimental values. A decreasing and an increasing trend against cubic lengths were found for the two cases, respectively. When the cubic length is close to 1000 nm, the difference between the two cases is almost disappeared. The thermal conductivities become nearly constant with further increase of particle sizes. Our finding is rationalized by considering the competition between two key factors influencing the thermal conductivity, i.e., the interfacial thermal resistance and the *Re* induced by Brownian motion. The conclusion of our present work is expected to be especially valuable if the particle are of irregular shape and have the sizes below micrometers which are supposed to be the cases for many practical applications.

1. Introduction

Nanoparticle suspensions have been widely applied in many industrial processes such as in manufacturing polymers, ceramics, pharmaceutics, food, and paint. [1–3] and can also be widely found in the process of material preparation [4–6]. In particular, they have been investigated both experimentally [7–10] and theoretically [11–18], as nanofluid, for the enhancement of thermal conductivity and heat transfer. Although the underlying mechanism for the unusually improved thermal conductivity is not very clear, more investigation points the enhancement to the Brownian motion and the Brownian motion-induced microconvection [12,18–20]. It was found that Brownian motion of particles could affect the migration of particles and their distribution in fluid, which, in turn, gives rise to change in the heat transfer efficiency [21–22].

The Brownian motion of nanoparticles in nanofluid is complex and can be affected by size, shape and density of particle and also the properties of base fluid. Up to now, most thermal conductivity models considering Brownian motion assumed that particles are spherical [18,19]. For instance, in a very recent study, Shukla et al. [18] proposed a thermal conductivity model of spherical nanoparticle considering both Brownian motion and micro-convection. They extended their model to nonspherical nanofluids by using a simplified volume equivalent diameter $d_{ep} = (6V/\pi)^{1/3}$. In fact, many previous studies [23,24] have already found that the particle shape significantly affect the Brownian motion, especially on rotating Brownian motion, thus shape effects should not be overlooked in thermal conductivity model.

In fact, the Brownian motion of spherical and nonspherical particles and its induced phenomenon, such as diffusion, are subjects

* Corresponding author.
E-mail address: dwjing@mail.xjtu.edu.cn (D. Jing).

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Nomenclature

u	velocity vector, m/s
t	time, s
ρ	density of fluid, kg/m^3
p	pressure, Pa
ν	kinematic viscosity of fluid, m^2/s
f	volume force, N
Ns, *Re*	Stokes number and Reynolds Number
μ	dynamic viscosity, μ = νρ, Pa·s
F_r	resistance, N
R_{c_s}	resistance coefficient of spherical particle, N·s/m
r	radius of the particle, m
R_{c_c}	resistance coefficient of cube particle, N·s/m
U	velocity of particle, m/s
r	position vector with three components (x,y,z), m
L_O	momentum moment in the centroid of cube O, kg·m^2/s
M($\mathbf{F}_r$), M(**f**)	force moments of resistance $\mathbf{F}_r$ and volume force **f**, N·m
F_{B_c}	component of Random Brownian F_B, N
M_{xy}, M_{yz} and M_{zx}	components of Random Brownian F_B, N·m
ω	angular velocity, rad/s
J	momentum of inertia, kg·m^2
M($\mathbf{F}_r$)	force moments of resistance, N·m
R_{m_c}	resistance moment coefficient of cubic particle, N·m·s
$\mathbf{r}_{1-3}$	x, y, z
$\mathbf{F}_{B\_c,1-3}$	$\mathbf{F}_{B\_c}$ along x, y and z
m	mass of a particle, kg
k_B	Boltzmann constant, 1.38 × 10^{-23}, J/K
T	temperature, K
A (x,y,z)	application point of F_B,
O	the center of cubic particle
$\mathbf{M}_B$	momentum moment induced by F_B with three components M_{xy}, M_{xz} and M_y
C_1, C_2	correlation factors
α	a factor equal to $2R_bk_f/d$
Φ	volume fraction of solid phase
R_b	interfacial thermal resistance between liquid and solid phases, Km^2 W^{-1}
k_n, k_f and k_p	thermal conductivity of nanofluid, base fluid and nanoparticle, W/mK
d	the diameter (equivalent diameter) of nanoparticle, m
Pr	Prandtl number, equal to $c_p\mu/k$
Re_t, Re_r	Reynolds numbers induced by translation and rotating Brownian motion
k	constant coefficient or slope
2a	cubic length, m

of long-standing interest [23–31]. Brenner [25,26] investigated translational and rotational Brownian motion of non-spherical particles and their diffusion coefficients by a macroscopic hydrodynamic model based on a generalized Fick's law. By relating the diffusion and hydrodynamic resistance matrixes, they finally discussed the generalization of the Stokes-Einstein equations. They are good theoretical work investigating the rotating and translational Brownian motion of non-spherical particles. However, there was no experimental work was conducted to verify the validity of their theoretical results. Hernández-Contreras et al. [23,27] investigated the tracer-diffusion properties of nonspherical colloidal particles. In their study, homogeneity approximation and decoupling approximation is introduced to describe the translational and rotational Brownian motion of a nonspherical tracer particle [23]. Branka et al. [24] investigated the Brownian dynamics of suspensions of rod-like particles by the Brownian dynamics simulation method. They calculated both the long-time translational self-diffusion coefficient and the rotational self-diffusion coefficient of the particle. It was found that single-particle diffusion matrix does affect both the rotational and translational diffusion properties. Mulhollanda et al. [32] studied the effect of particle rotation on the drift velocity for nonspherical aerosol particles by theoretical analysis. In their study, a 1D model considering particle acceleration and an orientation dependent friction coefficient is proposed and discussed. Butenko et al. [33] investigated the Brownian motion of a fixed helically shaped bacterium by a real-time three-dimensional confocal microscopy. The translational and the rotational diffusion coefficients of the bacteria were measured. It was proposed that the spiral shape of bacteria could increase their ability of passive Brownian diffusion.

Although it has been well agreed that the rotating Brownian motion of nonspherical particles could significantly affect the particle diffusion and the properties of suspension, rare study has been conducted considering its effect on thermal conductivity. In our study, as a case study, cubic shape will be considered and the contribution of rotating Brownian motion of nonspherical particle to the thermal conductivity enhancement of nanofluid was investigated both experimentally theoretically for the first time. For the mathematical model, the controlling equations of particles motion in fluid are simplified based on the dimensional analysis to find the crucial parameters affecting the resistance coefficient of small particle of arbitrary shape. Then Langevin equation was employed to derive the expressions of root-mean-square velocity and angular velocity of Brownian motion of cubic particles. By introducing rotating *Re*, we proposed a new thermal conductivity model considering rotating Brownian motion. To validate this model, experimental work has also been conducted by employing Ag nanofluid with cubic Ag nanoparticles of various sizes side lengths. In the last part, comparisons of our theoretical prediction with the experimental results are made and theoretical findings were then discussed in detail.

2. Model and experimental validation

2.1. Model description

2.1.1. Controlling equations for a cubic nanoparticle in fluid

The motion of a particle in fluid can be described by the Navier-Stokes equation,

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} = -\frac{1}{\rho}\nabla p + \nu\nabla^2\boldsymbol{u} + \boldsymbol{f}, \tag{1}$$

where **u** is velocity, m/s, t is time, s, ρ is density of fluid, kg/m^3, p is the pressure, Pa, ν is kinematic viscosity of fluid, m^2/s, and **f** is volume force, m/s^2. The first two terms from the left-hand side describe the inertia effects induced by the unsteady and uneven flow field, corresponding to "unsteady" term and "convective" term, respectively. For nanoparticles, some reasonable simplifications can be made. Here, by introducing characteristic time t_0, length L, and velocity U of flow field, we have [34]:

$$\frac{\frac{\partial \boldsymbol{u}}{\partial t}}{\nu\nabla^2\boldsymbol{u}} = \frac{\frac{U}{t_0}\frac{\partial \boldsymbol{u}^*}{\partial t^*}}{\frac{\nu U}{L^2}\nabla^{*2}\boldsymbol{u}^*} \propto \frac{L^2}{\nu t_0} = Ns, \tag{2-1}$$