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Nanofluids Transport Model Based on Fokker-Planck Equation and the Convection Heat Transfer Calculation

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Abstract: In current research about nanofluid convection heat transfer, random motion of nanoparticles in the liquid distribution problem mostly was not considered. In order to study on the distribution of nanoparticles in liquid, nanofluid transport model in pipe is established by using the continuity equation, momentum equation and Fokker-Planck equation. The velocity distribution and the nanoparticles distribution in liquid are obtained by numerical calculation, and the effect of particle size and particle volume fraction on convection heat transfer coefficient of nanofluids is analyzed. The result shows that in high volume fraction ($\phi = 0.8\%$), the velocity distribution of nanofluids characterizes as a "cork-shaped" structure, which is significantly different from viscous fluid with a parabolic distribution. The convection heat transfer coefficient increases while the particle size of nanoparticle in nanofluids decreases. And the convection heat transfer coefficient of nanofluids is in good agreement with the experimental result both in low ($\phi \leqslant 0.1\%$) and high ($\phi = 0.6\%$) volume fractions. In presented model, Brown motion, the effect of interactions between nanoparticles and fluid coupling, is also considered, but any phenomenological parameter is not introduced. Nanoparticles in liquid transport distribution can be quantitatively calculated by this model.

Key words: nanofluids, convection heat transfer, transport theory, Fokker-Planck equation

1 Introduction

Nanofluids, which are solid-liquid composite materials consisting of nanometer sized solid particles, fibers, suspended indifferent base fluids, have higher thermal conductivity[1–2] compared with the base fluid. They are the ideal heat transfer mediums and have broad application prospects in MEMS cooling, biotechnology and other fields. Therefore, thermal conductivity and the transport mechanism of nanofluids have been widely investigated.

In the convection heat transfer area of nanofluids，PAK and CHO[3] reported heat transfer data for turbulent flow of alumina-water and titania-water nanofluids in circular tubes. Their data show Nusselt numbers which are up to about 30% higher than pure fluid. The same results were also reported by XUAN and LI[4] for turbulent flow of copper water nanofluids. WEN and DING[5] reported heat-transfer enhancement due to the addition of γ-Al_2O_3 nanoparticles to de-ionized water flowing through a copper tube in the laminar flow regime. Their results indicate that the Nusselt number increases up to 47% when 1.6% volume fraction of γ-Al_2O_3 nanoparticles is added to water. HERIS, et al[6] reported experiments to study a laminar flow forced convection heat transfer of Al_2O_3-water nanofluid inside a circular tube with constant wall temperature. Moreover, various mechanisms and models have been proposed for explaining the enhancement of convective heat-transfer of nanofluids using various assumptions.

HEYHATA and KOWSARY[7] considered the effect of particle migration on flow and heat transfer of alumina-water nanofluids flowing through a circular pipe. Effects of slip between nanoparticles and liquid on the convection heat transfer performance of nanofluid was studied by BUONGIORNO[8] through establishing the theory model. The results show that, Brownian diffusion and thermophoresis are important factors to enhance convection heat transfer performance of nanofluid. KOO and KLEINSTREUER[9] considered the kinetic energy of the nanoparticles due to the Brownian movement and proposed a model for the effective thermal conductivity of nanofluids. PRASHER, et al[10], introduced a Brownian motion-based convective conductive model, which predicts the right trend regard to different parameters such as nanoparticle volume fraction, nanoparticle diameter, and temperature. HWANG, et al[11], researched convective heat-transfer coefficient of water-based Al_2O_3 nanofluids flowing through a uniformly heated circular tube in the fully developed laminar flow regime. They discussed the various parameter effects on remarkable enhancement of the convective heat-transfer coefficient and showed for the first time the flattened velocity profile due to particle migration induced by

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Brownian diffusion and thermophoresis. Four possible mechanisms of enhanced convection heat transfer performance of nanofluid are presented by KEBLINSKI, et al[12] and EASTMAN et al[13]: (1) Brownian motion of the nanoparticles; (2) molecular-level layering of the liquid at the liquid-particle interface; (3) the nature of heat transport in the nanoparticles; (4) the effects of nanoparticle cluster. They postulated that the effect of Brownian motion could be ignored when contribution of thermal diffusion was much greater than Brownian diffusion. However, they only examined the cases of stationary nanofluids[14]. For non-stationary nanofluids, it showed that the Brownian motion of the nanoparticles at the molecular and nanoscale levels is a main mechanism controlling the convection heat-transfer enhancement of nanofluids[10, 15–16]. WANG, et al[17] and XIE, et al[18] considered that the convection heat-transfer enhancement of nanofluids should be dependent on the microscopic motion (Brownian motion and inter-particle forces) and particle structure. XUAN and LI[19] also considered two main reasons for the improved effective convection heat-transfer enhancement of nanofluids: (1) the increased surface area due to suspended nanoparticles; (2) the interaction and collision among particles. However, random motion characteristics of nanoparticles, Brownian motion effect of nanoparticles, particle collision effect and particle distribution are not considered in the present model[7, 9, 11–20].

In order to describe the random movement characteristics of nanoparticles, three models are mainly used at present: (1) Langevin equation model[21–22]; (2) Molecular dynamics[23–24] model; (3) Boltzman equation model[25–26]. But the number of particles simulated in Langevin equation and Molecular dynamics model is small, which will lead the simulation results to deviation from the actual situation. However, if particle number is more than enough, a very large number of kinematics equations will need to be solved and high performance computer is required. For Boltzmann transport model, most researchers used Lattice Boltzmann method[25–26] which the relaxation time was assumed to be constanta, but the actual nanoparticles in the liquid transport related to particle collision mechanism, and the relaxation time which depended on the distribution of nanoparticles was not constant. In addition, for high volume fraction of nanofluids, the collision effects between particles were one of the important factors affecting nanofluids heat transfer properties[17–19]. Therefore, the collision effect between the particles cannot be ignored. However, the collision effects were not considered in the above literature.

In this paper, based on Fokker-Planck equation, a convective heat transfer model of nanofluids in a circular tube is established. Nanoparticles are considered as random motion of the particles in the model. Particle collision effect, Brownian effect and viscous drag due to effect of nanoparticles and liquid caused by the slip are also considered in the model. The model does not introduce any phenomenological parameters, so it has better self-consistency and it is more in accord with the actual transport situation and well predicts the convection heat transfer coefficient of nanofluids. Consequently, distribution of random motion for nanoparticles in liquid can be described by this model.

2 Nanofluid Convection Heat Transfer Transport Model

As shown in Fig. 1, we assume that nanofluid flows in the fully developed pipe. Nanofluid is regarded as two-phase fluid which is composed of a liquid and nanoparticles. The liquid is regarded as a continuous medium which can be described by momentum equation and continuity equation. Nanoparticles are considered as discrete particles in random motion, and it is assumed that the particle distribution was isotropic and only be considered that distribution function changes along the r direction, then the microcosmic motion state of nanoparticles can be described by a distribution function $f(t, r, v)$. $f(t, r, v)\mathrm{d}r\mathrm{d}v$ indicates the number of particles in the infinitesimal domain of the phase space $\mathrm{d}r\mathrm{d}v$ which is centered on (r, v), and it satisfied Fokker-Planck equation. Nanoparticles are suspended in base fluid, because of slip in flow between the nanoparticles and the fluid, the viscous friction is produced, which is given by the Stokes formula:

$$F(r,v) = 6\pi\mu R(u - v)$$

where μ is the dynamic viscosity of the fluid and R is radius of nanoparticles. Accordingly, the sum of the viscosity frictions of a group of nanoparticles which equilibrium distributions are $f_{ea}(r,v)$ in the unit volume is given by

$$24\pi^2 \cdot \mu \cdot R \cdot \int_0^{\infty} (v-u)v^2 f_{eq}(r,v)\mathrm{d}v,$$

which can be seen as nanoparticles viscous friction statistical average in equilibrium state.

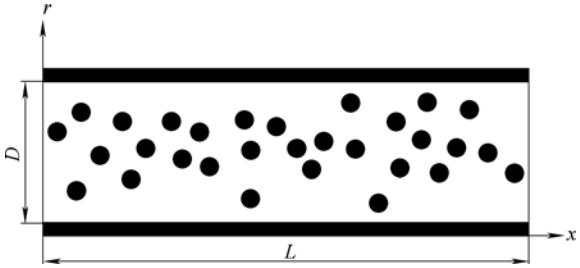

Fig. 1. Schematic diagram of nanofluids flow in the pipe

It is assumed that nanofluids flow along x in the pipe (length L and diameter D, $D/L \ll 1$), which is schematically shown in Fig. 1. The pressure gradient drives fluid (as Newtonian fluid) to flow along the x direction. With small Reynolds number, inertia effect in the momentum equations can be ignored, the velocity u is viewed as a function of r. It is assumed that the

interaction force between fluid and nanoparticles is only due to drag. When the viscous resistance between nanoparticles and fluid are considered, the fluid momentum equation will be simplified as

$$\mu\left(r\frac{\partial^2 u}{\partial r^2}+\frac{\partial u}{\partial r}\right)=\frac{\partial p}{\partial x}r-24\pi^2 R\mu r\int_0^{\infty}(v-u)v^2 f_{\mathrm{eq}}(r,v)\mathrm{d}v, \tag{1}$$

where p is the fluid pressure, and the particle distribution function satisfied Fokker-Planck equation:

$$\frac{\partial f}{\partial t}+v\frac{\partial f}{\partial r}+a\frac{\partial f}{\partial v}=-\frac{\partial}{\partial v}\left\{(A_1+A_2)f+\frac{1}{2}\frac{\partial^2}{\partial v^2}\left[(B_1+B_2)f\right]\right\}, \tag{2}$$

where a is the acceleration of particle,

$$A_1=\frac{9\mu(v-u)}{2R^2\rho_{\mathrm{p}}}$$

and

$$B_1=\frac{9\mu}{2R^2\rho_{\mathrm{p}}}\bullet\frac{k_{\mathrm{B}}T}{m_{\mathrm{p}}}$$

are the drift coefficient and the diffusion coefficient, m_{p} is the nanoparticle mass, ρ_{p} is the nanoparticle density, k_{B} is the Boltzmann constant, T is the temperature. A_2 and B_2 are the drift coefficient and the diffusion coefficient considering the effect of the interaction among particles. Eqs. (1), (2) corresponding to the initial and boundary conditions are expressed as follows:

$$f\big|_{t=0}=f^0, \tag{3}$$

where f^0 is the initial distribution,

$$f^0=n_0\left(\frac{m_{\mathrm{p}}}{2\pi k_{\mathrm{B}}T}\right)^{\frac{3}{2}}\exp\left(\frac{m_{\mathrm{p}}\mathrm{v}^2}{2k_{\mathrm{B}}T}\right),$$

it is Maxwell distribution, n_0 is nanoparticles average number density.

For liquid, the boundary conditions adopt nonslip condition:

$$u\big|_{r=D/2}=\big|u_{r=D/2}=0. \tag{4}$$

To nanoparticles, Maxwell boundary condition is adopted:

$$(A_1+A_2)f-\frac{1}{2}\frac{\partial}{\partial v}\left[(B_1+B_2)f\right]\Big|_{r=-D/2}=0, \tag{5}$$

$$(A_1+A_2)f-\frac{1}{2}\frac{\partial}{\partial v}\left[(B_1+B_2)f\right]\Big|_{r=D/2}=0. \tag{6}$$

The physical meaning of Eqs. (5) and (6) is when the nanoparticles on the upper and lower surfaces, they will be reflected back into the fluid.

The transport model of fluid in the tube can be described by Eqs. (1) – (6).

3 Drift and the Diffusion Coefficient Considering the Effect of the Collision Between Particles

In Eq. (2), A_2 and B_2 stand for the drift and the diffusion coefficient considered the effect of the collision between nanoparticles, A_2 and B_2 expression is related with the collision mechanism. Based on the transport theory, the collision among particles is regarded as the movement of a test particle in average potential field formed by a group of field particles. The elastic collisions occur between a test particle whose velocity is v and a group of field particles whose distribution is $f(v_1)$, the relative velocity before the collision is $\Delta u=v-v_1$, and becomes $\Delta u'=v'-v_1'$ after the collision, and $\Delta u=\Delta u'$. In spherical coordinates system, after the collision, velocity components are as follows:

$$\Delta u_{\mathrm{x}}'=\Delta u\bullet\sin\theta\bullet\cos\varphi,$$

$$\Delta u_{\mathrm{y}}'=\Delta u\bullet\sin\theta\bullet\sin\varphi,$$

$$\Delta u_{\mathrm{z}}'=\Delta u\bullet\cos\theta.$$

Based on the law of conservation of momentum, the test particle's speed difference between before and after the collision is

$$\Delta v=\left(\Delta u'-\Delta u\right)\bullet\left(\frac{m_1}{m+m_1}\right),$$

where m stands for the mass of the test particle and m_1 stands for the mass of the field particles.

If $m=m_1$,

$$\Delta v=\frac{1}{2}(\Delta u'-\Delta u),$$

the drift and the diffusion coefficient are expressed as[27]

$$A_2=\int\Delta v f(v_1)\Delta u\bullet\sigma(\theta)\mathrm{d}v_1, \tag{7}$$

$$B_2=\int(\Delta v\bullet\Delta v)f(v_1)\Delta u\bullet\sigma(\theta)\mathrm{d}v_1, \tag{8}$$

where $\sigma(\theta)$ is collision differential cross section, particles are assumed spherically shaped, ϕ stands for a rigid spherical potential formed by flied particles, written as

$$\phi=\begin{cases}\infty, & r<d,\\ 0, & r>d,\end{cases}$$

where r is the distance between two centers of spheres, d is the diameter of the nanoparticles so

$$\sigma(\theta) = R^2 .$$

It is assumed that nanoparticles are isotropic in velocity space, Eqs. (7) and (8) are simplified as

$$A_2 = -2\pi R^2 \int_0^{\infty} (v - v_1)^2 v_1^2 f(v_1)\,\mathrm{d}v_1 , \tag{9}$$

$$B_2 = \frac{2(\pi+1)R^2}{9} \int_0^{\infty} (v - v_1)^3 v_1^2 f(v_1)\,\mathrm{d}v_1 . \tag{10}$$

It is shown from Eqs. (9) and (10) that the Fokker-Planck equation is a nonlinear partial differential equation. If the interaction among nanoparticles is considered, A_2 and B_2 depend on the distribution function of nanoparticles.

4 Numerical Calculation Method

4.1 Numerical methods

Introduce a Dimensionless system:

$$t^* = \frac{t}{t_0},\ v^* = \frac{v}{v_0},\ r^* = \frac{2r}{D},\ f^* = \frac{f}{f_0},\ u^* = \frac{u}{v_0},$$
$$t_0 = \frac{m_\mathrm{p}}{6\pi\mu R},\ v_0 = \sqrt{\frac{k_\mathrm{B}T}{m_\mathrm{p}}},\ f_0 = \frac{n_0}{v_0^3}.$$

The velocity u is only a function of r, when the distribution f and pressure have been known and the distribution f can be computed directly by integral. So, for solving the model, it is important to compute the equilibrium distribution f_{ea} firstly, then considering the effect of the collision, Eq. (2) is a nonlinear partial differential equation. The nonlinear equations of nanoparticles distribution function values of $F(x) = 0$ are obtained from the discretization of the phase space and velocity space, to solve $F(x) = 0$, we use the modified N point secant method, because it doesn't need to calculate the derivative of nonlinear equations. The time stepping method is used to calculate the nanoparticles distribution, when the distributions are approximately equal at the two adjacent time points, this distribution can be seen as the equilibrium f_{ea}.

4.2 Calculation of the drift and the diffusion coefficient A_2 and B_2

It can be seen from Eqs. (9) and (10), A_2 and B_2 are the integral of the unknown distribution function, in the iteration process, when calculate $f_j^{(K)}$ every time there must be an integration of v, it requires very large computation. So, we assume that the distribution function value f_j^K, which is a function value at the node j in velocity space, is the unvaried value in small interval $[v_j, v_j + \Delta v]$, A_2's and B_2's values at node i are given as follows:

$$(A_2)_i = \sum\nolimits_{j=1}^{n} C_{i,j} f_j^{(K)} , \tag{11}$$

$$(B_2)_i = \sum\nolimits_{j=1}^{n} D_{i,j} f_j^{(K)} , \tag{12}$$

where i and j are the values of discrete nodes in velocity space($i,\ \ j$=1, 2, $\cdots$, n),

$$C_{i,j} = -2\pi R^2 \int_{v_{j-\frac{1}{2}}}^{v_{j+\frac{1}{2}}} (v_\mathrm{i} - v_1)^2 v_1^2 \mathrm{d}v_1 ,$$

$$D_{i,j} = \frac{2(\pi+1)R^2}{9} \int_{v_{j-\frac{1}{2}}}^{v_{j+\frac{1}{2}}} (v_i - v_1)^3 v_1^2 \mathrm{d}v_1 .$$

The analytic solutions are as follows:

$$C_{ij} = 2\pi R^2 \left[\frac{(v_\mathrm{i} - x)^5}{5} - 2v_i \frac{(v_\mathrm{i} - x)^4}{4} + v_i^2 \frac{(v_\mathrm{i} - x)^3}{3} \right]_{v_1}^{v_2} ,$$

$$D_{ij} = -\frac{2(\pi+1)R^2}{9} \left[\frac{(v_\mathrm{i} - x)^6}{6} - 2v_i \frac{(v_\mathrm{i} - x)^5}{5} + v_i^2 \frac{(v_\mathrm{i} - x)^4}{4} \right]_{v_1}^{v_2} ,$$

$$v_2 = \frac{1}{2}(v_j + v_{j+1}) ,$$
$$v_1 = \frac{1}{2}(v_j + v_{j-1}) .$$

So, from Eqs. (11) and (12), it can be seen in the iteration process that the value $(A_2)_i^{(K+1)}$ and $(B_2)_i^{(K+1)}$ can be linearly superposed by f^K.

5 Calculation of Nanofluid Convection Heat Transfer Coefficient

The effective convection heat transfer coefficient α_{eff} of the nanofluid can be obtained by convection heat transfer coefficient α_f of the base fluid which uses the convection heat transfer coefficient of water, and convection heat transfer coefficient α_p due to the Brownian motion and collision of the nanoparticles, when nanoparticles are in equilibrium state, the α_p is given by Green Kubo equation[28]:

$$\alpha_\mathrm{p} = \frac{S}{3k_\mathrm{B}T^2} \int_0^{\infty} \big(q(0) \bullet q(t)\big) \bullet \mathrm{d}t,$$

where S is the area of the tube, $q(0)$ is the heat flux density at initial time, $q(t)$ is the heat flux density at any time, which is computed as

$$q(t) = 4\pi m_\mathrm{p} v_0^6 f_0 \int_0^1 \int_0^{\infty} v^{*5} r^* f^*(t^*, r^*, v^*) \mathrm{d}r^* \mathrm{d}v^*.$$

Dimensionless heat flux density:

$$q^*(t^*)=\frac{q(t)}{q_0}=\int_0^1\int_0^\infty v^{*5}r^*f^*\left(t^*,r^*,v^*\right)\mathrm{d}r^*\mathrm{d}v^*,$$

$$q_0=4\pi m_\mathrm{p}v_0^6f_0$$

We use the correlativity to compute the effective convection heat transfer coefficient[21], which in fully developed region, its dimensionless form is as follows:

$$\alpha_{\mathrm{eff}}^*=\phi\bullet\alpha_\mathrm{p}^*+(1-\phi),$$

$$\alpha_\mathrm{p}^*=\frac{\alpha_\mathrm{p}}{\alpha_\mathrm{f}},$$

where ϕ is the nanoparticle volume fraction.

6 Numerical Results and Discussion

We use this model to numerically simulate the convection heat transfer of nanofluids of Al_2O_3 and CuO particles.

Fig. 2(a) to Fig. 2(d) respectively show Al_2O_3 and CuO nanoparticles distribution function evolution with time. It can be seen from the figures that the particle distribution will deviate from the Maxwell equilibrium distribution at $T=300$ K, and evolve into a new equilibrium distribution, the peak of distribution gradually shifts to the right side, which indicates that the high-speed particles are few at the initial time, due to the collision, the energy of high-speed particles will be transferred to the low-speed particles as the result. Also, it can be seen that, at the same time point, the number of high-speed particles, at the situation of ignoring the effect of collisions, will be more than considering the effect of the collisions, because when the low-speed particles gain energy due to collisions, the high-speed particles will lose energy and become low-speed particles, however, the consolidated results of statistical average, it will lead to that, the number of high-speed particles is less at the situation of considering the effect of the collision than ignoring the effect of collision. This also shows that, when neglecting the effect of particle collisions, the nanoparticles as Brownian particles only transfer energy with the liquid molecules, leading to less energy consumption of nanoparticles than considering the effect of collisions, and the number of high-speed particles will increase with time, it is inconsistent with the actual nanoparticles transport situation, therefore, the collision effect cannot be ignored.

Fig. 3 shows the location distribution of particles with condition of the diameter. The results show that, when ignoring the collision effect, nanoparticles mainly distribute near the central tube. But when considering the collision effect, it will cause the nanoparticles to migrate near the tube wall, and the number of particles per unit volume will increase near the pipe wall. Nanoparticles along the pipe diameter approximate normal distribution.

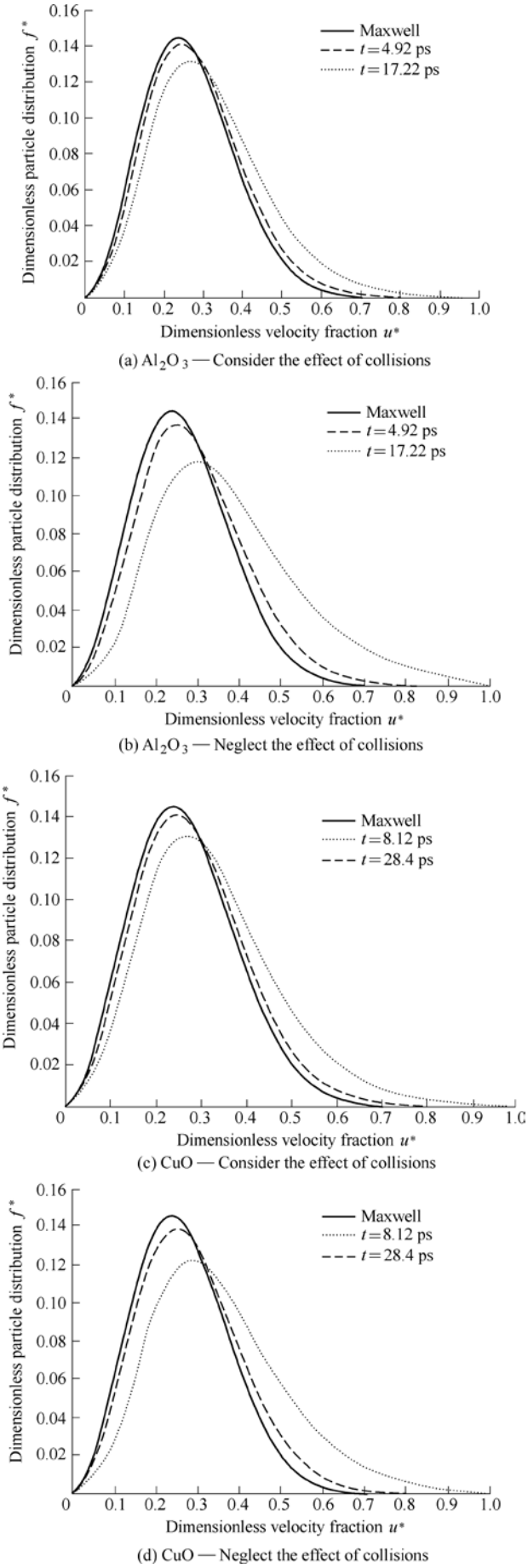

Fig. 2. Dimensionless particle distribution with condition of velocity (diameter of Al_2O_3 is 47 nm and that of CuO is 29 nm, volume fraction is 0.8%, initial temperature T=300 K)

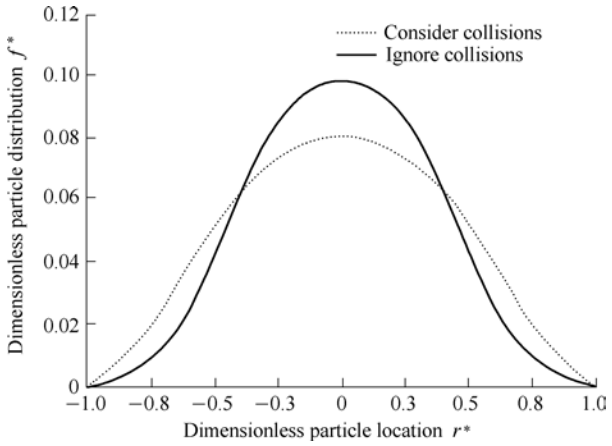

Fig. 3. Distribution of Al_2O_3 particles with condition of particle location

Figs. 4(a), (b) are fluid velocity of two materials with condition of the diameter of tube, the results shows that the fluid velocity considering the collision effect is less than the velocity neglecting the collision effect, because the particles collisions make viscous friction of fluid increase, leading to the fluid velocity decline. Comparing Fig. 4(a) with Fig. 4(b), it can be seen, velocity of CuO(CuO diameter of 29 nm) nanofluids is significantly greater than that of Al_2O_3(Al_2O_3 diameter of 47 nm).

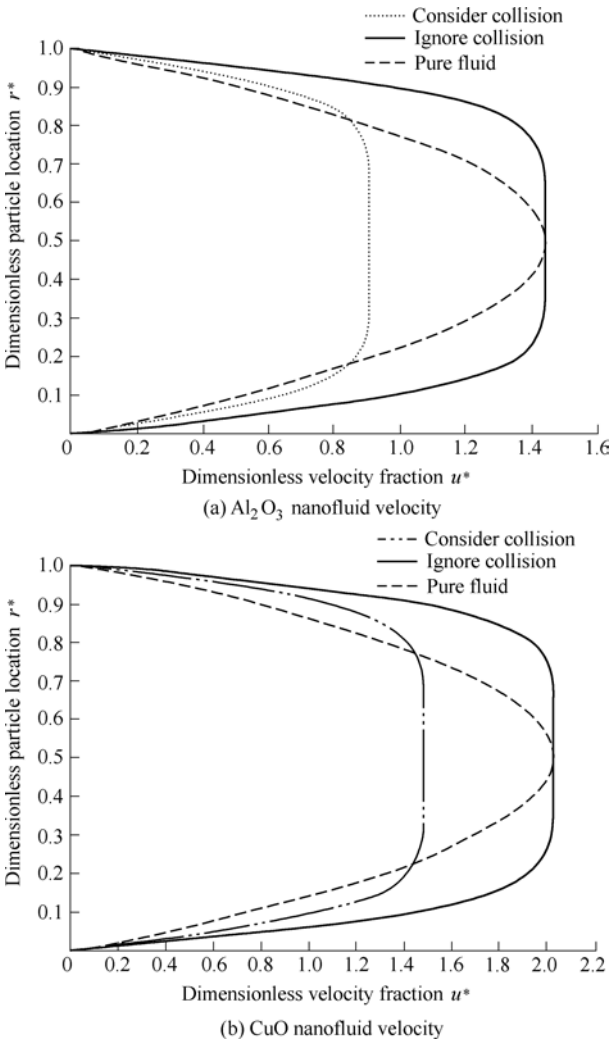

Fig. 4. Nanofluid velocity with condition of dimensionless location(diameter of CuO is 29 nm, volume fraction is 0.8%, initial temperature T=300 K)

The factors affecting the velocity of nanofluids are in many aspects: the model ignores other factors; the model only takes into account the influence of particle size and concentration of particles. The formula of Stokes is used to approximate simulation the viscous force between particles and fluid. Moreover, the viscous resistance between particles and fluid is proportional to the particle diameter. Viscous resistance of large size particles of fluid is larger than that of the small particles, which leads to a decrease in the large size particle nanofluid velocity. In addition, the velocity distribution of nanofluids is "cork-shaped", which is significantly different with parabolic profile of the single-phase liquid. It can be seen from Fig. 3, because particle migration with particle Brownian motion effect and the effect of the collision between particles, most of the nanoparticle concentration in the central tube lead to nanofluids equivalent viscosity increasing in the central tube, viscous resistance increasing, velocity difference between adjacent nanofluids layer decreasing in the central tube. What results in nanofluid velocity distribution is flat in the central tube. It is the same as those of Ref. [11].

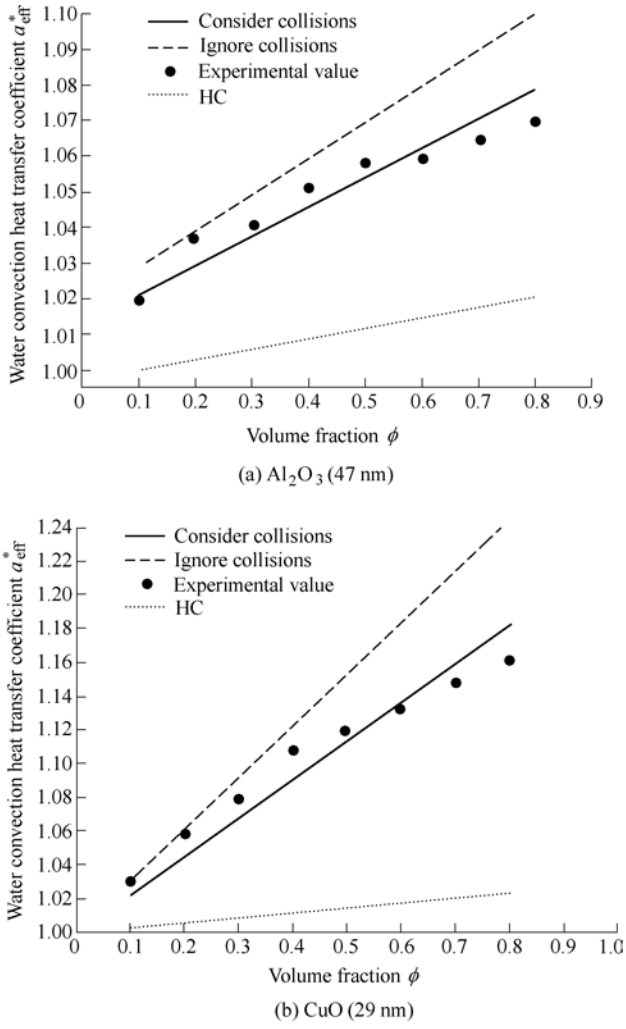

Fig. 5. Water convection heat transfer coefficient with condition of the volume fraction(Reynolds number Re=800, initial temperature T=300 K)

The simulation results of Figs. 5 (a), (b) show that, the convection heat transfer coefficient considering the collision effect is in better agreement with the experimental value than without considering the collision effect, and the error increases with the particle volume fraction increases, indicating that the interaction between nanoparticles is an important factor in increasing nanofluid convection heat transfer coefficient, especially for large volume fraction of particles the collision effect cannot be ignored. It also can be seen that, the CuO nanofluids have higher increase in convection heat transfer coefficient than the Al_2O_3 nanofluids.

As shown in Fig. 6, it can be seen, with the increase of the size of nanoparticle, nanofluid Convection heat transfer coefficient decrease gradually, because the suspension performance of particles decreases with nanoparticles size increase, particle precipitation makes the properties of nanofluids return to base fluid, as a result, the Convection heat transfer coefficient will decrease. It can be seen from the figure that, the prediction values obtained by this model considering the effect of particles interactions are in good agreement with the experimental values, while the prediction error of ignoring the effect of particles interactions is significantly larger.

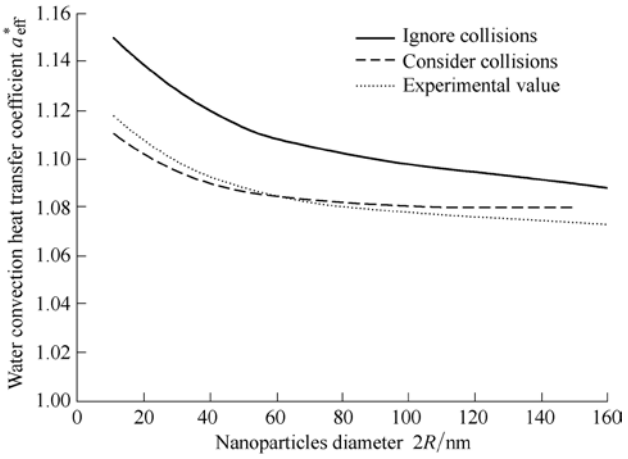

Fig. 6. Al /water convection heat transfer coefficient with condition of diameter of nanoparticles(Volume fraction is 3%, Reynolds number Re =800, initial temperature T=300 K)

7 Conclusions

(1) Compared with the current phenomenological experience models, the model established does not introduce any phenomenological parameters, so it has better self-consistency.

(2) Distribution of nanoparticles in the fluid is obtained, and the results show that，nanoparticles distribution along the pipe diameter is not uniform, approximate normal distribution. In high volume fraction, particle collision effect cannot be ignored; velocity of nanofluids in the pipe in the middle is “flat” distribution, which is significantly different from single-phase viscous fluid with a parabolic distribution.

(3) The variation of thermal conductivity of nanofluids with condition of nanoparticles volume fraction is in good agreement with the experimental result within the range of 0.1%(low volume fraction) to 0.8%(high volume fraction). When the particle size is smaller, the thermal conductivity is better, magnitude of improving the heat transfer coefficient of nanofluids is larger.

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