Numerical simulation of nanoparticles coagulation process in a Cu/water nanofluids turbulent pipe flow

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Abstract. Numerical simulations of Cu/water nanofluid in a turbulent pipe flow are performed with considering the particle convection, diffusion, and coagulation. A general dynamic equation (GDE) of nanoparticles in a turbulent pipe flow has been derived with the Taylor Expansion Method of Moment (TEMOM) and the nanofluid flow in a horizontal circular tube has been simulated using the large eddy simulation (LES). The numerical results show the initial uniform distributions of particle volume concentration and size become non-uniform. The particle size increases with the development of coagulation process and the smaller diameter particles show more violent coagulation process inducing larger particle diameter growth rate. Because of the mixing of nanoparticles with short coagulation process and a paraboloid velocity distribution, the average size of particle at the tube center is smaller than that of near the wall.

1. Introduction

Enhancement of thermal conductivity of liquids is an extremely importance topic for the heat transfer system in industry development. Nanofluid is a suspension of nanoparticles (nominally 1–100nm in size) in conventional base fluids such as water, oils, or glycols. As a new type of efficient heat transfer medium with good heat transfer performance nanofluid has aroused the interest of many researchers [1-4]. A lot of studies found that the heat transfer performance of nanofluids compared to the base liquid increased obviously. It has become popular to use nanofluids to increase thermal performance in energy systems.

The physical mechanisms of nanoparticle transport and heat transfer enhancement are complex. Buongiorno[5] investigated slip mechanism between nanoparticles and base fluid and indicated that there were many slip mechanisms such as inertia, Brownian diffusion, diffusiophoresis, Magnus effect, fluid drainage, and gravity. Haddad et al.[6] and Michaelides[7] studied the thermophoresis and Brownian motion effect in nanofluid heat transfer enhancement, the result showed the enhancement in heat transfer was observed at any volume fraction of nanoparticles, as a result of thermophoresis and Brownian motion. The distribution of particle volume concentration is non-uniform because of thermophoresis force involves nanoparticle migration across the fluid in the opposite direction of the temperature gradient. The higher particle volume concentration, the higher nanofluid thermal conductivity is. Lam et al.[8] studied the movement of micrometer-sized dense phase particles in a circular tube and found that the highest radial particles’ density position was neither at the center position nor at the wall position during the motion, it was at $r/R = 0.8-0.9$ (close to the center); the
density of particles on the wall was the lowest and the highest density position increases with the distance from the wall, and the density gradually decreases towards the center. Abu-Nada[9] studied the effect of variable thermal conductivity and variable viscosity of nanofluid on heat transfer enhancement in Rayleigh-Bénard convection problem and found that the average Nusselt number was much more sensitive to the viscosity models than to the thermal conductivity models for Re>103. Masuda et al.[10] and Xie et al.[11] found that the rod-like SiC nanoparticles showed an enhancement of thermal conductivity over the spherical particles because a structure produced by the elongated particles that conducts heat through the fluid. In addition, turbulence eddies provide a strong energy source for the dispersion of nanoparticles in the fluid. Yang et al.[12] studied the mechanism of convective heat transfer enhancement in a turbulent flow of nanofluid by direct numerical simulation method and used field synergy principle to explicate the mechanism of heat transfer enhancement in a turbulent nanofluid flow. Jehad[13] numerical studied the forced convective heat transfer and friction factor of turbulent nanofluid flow through straight channels and the results showed that with an increase in the Reynolds number the Nusselt number increased and the friction factor decreased. After experimental and numerical investigation of turbulent nanofluid flow in helically coiled tubes, Bahremand[14] concluded that two-phase approach predicted much more accurate results than the homogeneous model. However, the nanoparticles did not affect the axial velocity and turbulent kinetic energy significantly, but the increase in nanoparticle diameter decreased the heat transfer coefficient.

Coagulation is the process that two particles collide each other and become a bigger one, which effect particles distribution and shape then change the heat transfer characteristic of nanofluid. Lin et al.[15-16] conducted a numerical simulation on flow and heat transfer characteristics of nanofluids with cylindrical and rod-like nanoparticles and firstly studied the nanoparticles orientation, coagulation and breakage effects on friction factor and Nusselt number in a pipe flow. The results showed the coagulation process changed the particle size and distribution and the rod-like nanoparticles strengthens heat transfer of nanofluids.

According to most of previous numerical studies, the distribution of particle volume concentration is usually assumed uniform without taking particle convection, diffusion, coagulation, and breakage into account. Turbulent effect on nanoparticle distribution has not been considered. Maintaining the constant particle size(<100nm), however, can be a challenge since particles frequently come into contact with each other—potentially leading to the formation of large particle agglomerates which can settle out of suspension[17]. Particle’s coagulation process changes the uniformity of the nanofluids, which in turn changes its physical properties. It is an important effect on the flow and heat transfer process. Therefore, the aim of this study focuses on the diffusion and coagulation process of particles in a turbulent flow of Cu/water nanofluids. It is necessary to clarify the phenomenon about coagulation and movement of nanoparticles in the flow field.

2. Numerical method

2.1. Governing equations of nanofluid

In this paper, the simulation is based on the unsteady, incompressible and fully developed turbulent flow field. The fluid flow was calculated based on the Euler approach and LES method has been used to simulate the flow field. The basic idea of LES is that the large-scale vortex in the flow field is obtained by solving the Navier-Stokes method directly, the small-scale vortex is simulated in the sub-grid mode. The filtered governing partial differential equations of mass, momentum, and energy, are as follows:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0
\]

\[
\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \mu \frac{\partial u_i}{\partial x_j} \right) + \frac{\partial \rho}{\partial x_j} \frac{\partial \tau_{ij}}{\partial x_j}
\]
Where \( \mathbf{u} \) is the filtered velocity, \( \rho \) is the fluid density, \( \mu \) is the kinematic viscosity of fluid, \( \mathbf{p} \) is the filtered pressure and \( \tau_{ij} \) is the sub-grid stress, which is the momentum transfer between filtered small-scale and resolvable-scale turbulent flow, and it is also the most important sub-scale term in large eddy simulation, which can be expressed as:

\[
\tau_{ij} = \overline{\mathbf{u}_i \mathbf{u}_j} - \overline{\mathbf{u}_i} \overline{\mathbf{u}_j}
\]

Smagorinsky eddy viscosity model is used as sub-grid mode, which can accurate and effective compute the flow. Assuming that the small-scale pulsation filtered by the isotropic filter is locally balanced. Then, the energy transfer from the solvable scale to the unsolvable scale equals the dissipation rate of the turbulent kinetic energy, the vortex-viscous form of the sub-grid Reynolds stress mode:

\[
\tau_{ij} = (C_s \Delta)^2 \overline{S_{ij}} (\overline{S_{ij}})^{1/2} - \frac{1}{3} \tau_{ii} \delta_{ij}
\]

Where \( \Delta \) is the filter size. This simple sub-grid stress model is called the Smagorinsky mode. The sub-grid vortex viscosity coefficient:

\[
v_i = (C_s \Delta)^2 (\overline{S_{ij}})^{1/2} \]

Where \( C_s \Delta \) is the mixing length, and the \( C_s \) is the Smagorinsky constant. \( \overline{S_{ij}} \) is the strain rate tensor for the solution scale and is defined as:

\[
\overline{S_{ij}} = \frac{1}{2} (\overline{\partial \mathbf{u}_i / \partial x_j} + \overline{\partial \mathbf{u}_j / \partial x_i})
\]

2.2. GDE for nanoparticles

The evolution of nanoparticles is related to the convection, diffusion, coagulation, and so on. The number of the particle per unit volume (number density) is expressed as a continuous function \( n = n(x, v, t) \) for the spatial position, the particle volume and time, then the general kinetic equation of particle number density can be expressed as:

\[
\frac{\partial n}{\partial t} + u \frac{\partial n}{\partial x} = D \frac{\partial^2 n}{\partial x^2} + \left( \frac{\partial n}{\partial t} \right)_{\text{coagulation}}
\]

Where, \( D \) is the particle diffusion coefficient defined as:

\[
D = k_B T \frac{k_B}{3 \pi \eta d}
\]

Where \( k_B \) is the Boltzmann constant, \( T \) is the temperature of the medium, \( C_c \) is the Cunningham slip correction factor,

\[
C_c = 1 + Kn[1.142 + 0.558 \exp(-0.999 / Kn)]
\]

Where \( d_p \) is the particle diameter, \( Kn \) is the Knudsen number \((Kn = \lambda / r_p, \text{where} \lambda \text{is the gas molecular mean free path,} r_p \text{is the particle radius})\). The physical meanings of the other variables in Eq. (8) are: \( u \) is the velocity of the flow field. The coagulation of particles in the fluid flow is governed by the GDE defined as:

\[
\left( \frac{\partial n}{\partial t} \right)_{\text{coagulation}} = \int_0^r \beta (v_1, v_2) n(v_1, t)n(v_2, t)dv_2 - \int_0^r \beta (v_1, v_2) n(v_1, t)n(v_2, t)dv_2
\]

Thus, substituting Eq. (11) into Eq. (9) we obtain:

\[
\frac{\partial n}{\partial t} + u \frac{\partial n}{\partial x} = \frac{\partial^2 n}{\partial x^2} + \left( \frac{1}{2} \int_0^r \beta (v_1, v_2) n(v_1, t)n(v_2, t)dv_2 \right)
\]

Where \( \beta \) is the collision coefficient of particles, the expression is:

\[
\beta = \frac{2k_B T}{\mu} \left( \frac{1}{v_1^{3/2}} + \frac{1}{v_2^{3/2}} \right)
\]
For equation (12), this paper uses the TEMOM to solve the equations, which was firstly proposed by Yu and Lin[18], and the detailed solving process in [19,20].

2.3. Numerical technique
The finite-volume method (FVM) has been used to solve the turbulent flow partial differential equations. The structured non-form grids have been performed to discretize the computational domain with finer grids close near the wall. The second order upwind scheme is used. The velocity and pressure fields are coupled utilizing the SIMPLE algorithm. The flow field is calculated by FLUENT software.

A moment method is used to transform GDE into an ordinary differential equation. The Taylor-Series expansion is adopted to close moment equations. Then the equations have been solved by Fourth-Order Runge-Kutta algorithm. The particle equations are dealt by FLUENT User-Defined Functions (UDF) module.

2.4. Computational parameters setting
The calculation geometric model is a three-dimensional horizontal straight tube shown in Figure 1. The simulation of the base fluid is water and the particles are Cu nanoparticles. The fluid containing nanoparticles flows from left to right. Pipe diameter \(D\) is 40mm, \(R\) for the radius, \(r\) for the radial position of the distance, \(L\) for the pipe length of 1000mm. The inlet condition is full developed velocity and no-slip wall condition in the pipe surface.

3. Results and discussion
3.1. Validation of simulation
A grid independency investigation is done both by considering the value of the particle volume concentration distribution and the mean Nusselt number to check for the independency of the results from the number of the used grids. Figure 2 shows the results of the nanofluid flow with Reynolds number 15 000 as the number of grid varies from 700 000 to 2200 000. According to the fluctuation of the particle volume concentration distribution in studied grids, the number of the grid was taken as 128000 considering the computing efficiency and accuracy.
The results of this study have been compared with the previous studies in order to validate the numerical method. Figure 3 shows the results for nanofluid flow under turbulent regime through a horizontal circular pipe with particle volume concentration at Reynold number 15000 and the present result is compared with that given by numerical result of Lin et al[17]. A satisfactory agreement among the results indicates that the numerical model is reasonable and reliable.

Figure 2. The results of the particle volume concentration at \( r/R=0.5 \) and \( x/D=20 \) of the pipe flow with \( Re=15000 \) to evaluate the grid independency.

Figure 3. Comparison between the present particle volume concentration distribution at \( Re=15000 \) and that of Ref.[17]

Figure 4. Particle size distribution changes with time at \( d_{p0}=1\text{nm}, Re=4367 \) and \( x=12.5D \)

Figure 5. Particle size distribution changes with time at \( d_{p0}=1\text{nm}, Re=8736 \) and \( x=12.5D \)

3.2. Nanoparticles size distribution evolution

Figure 4,5 show the nanoparticles size distribution evolution at \( x=12.5D \) and the initial particle size \( d_{p0} = 1\text{nm} \) with different flow Reynolds number as 4367 and 8736. The results show with the development of nanofluid flow in a turbulent pipe, nanoparticle size changes from uniform distribution to non-uniform distribution because of particle diffusion, collision and coagulation processes. The particle size becomes larger with time. The particle size growth rate is different in the pipe. In the different flow Reynold number, the particle diameter size changes differently with time. But at last the particle size distribution reaches a stable curve shape. At the pipe center particle size is smaller than that of near the wall because of the flow velocity distribution and particle diffusion.
3.3. Effect of particle initial size on coagulation

Figure 6 and Figure 7 show the dimensionless particle size distribution with different particle initial size at \( Re = 109194 \) and \( t=60s \). \( \delta = \frac{dp}{dp_0} \) is the particle diameter growth rate. The result shows that the nanoparticles diameter growth rate with different primary particle sizes is different. The larger initial particle size, the weaker coagulation effect is. The particle size grows quickly with small initial size. Because of the coagulation and mixture, the smaller the initial particle size, the faster the particle growth happens. It can be known from the particle collision frequency theory that the collision frequency of the particles is inversely proportional to the inertia of the particles, so the particles are less opportunity to collide and coagulate with larger particle sizes. The smaller the initial particle size, the more vigorous Brownian motion happens, which is one of the factors that enhance the coagulation process. From the position of \( x = 2.5D \) to \( x = 12.5D \), particles size continued grows because of the coagulation process.

![Figure 6](image-url)

**Figure 6.** Particle size distribution with different initial particle sizes with \( Re=109194 \), \( x = 2.5D \) and \( t=60s \)

![Figure 7](image-url)

**Figure 7.** Particle size distribution with different initial particle sizes with \( Re=109194 \), \( x = 12.5D \) and \( t=60s \)

4. Conclusions

Numerical simulations of Cu/water nanofluid in a turbulent pipe flow are performed with LES and TEMOM. FVM has been used to discrete the turbulent flow. The nanoparticle size distribution evolution has been studied considering the effects of flow turbulence and initial particle diameter. According to the results the main findings are as follows.

1. With the development of nanofluid flow in a pipe, nanoparticle size changes from uniform distribution to non-uniform distribution because of particle diffusion, collision and coagulation processes.

2. Nanoparticle size distribution changes with the flow time, Reynold number and initial particle diameter. The coagulation process enhances with the increasing of the turbulent strengthen and decreasing of the particle size.

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