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A Parameter for Selection of Nano-dispersoids in Nanofluids for Thermal Applications

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Abstract. A model reported by the present investigators has earlier shown that the extent of heat pick up by a nanoparticle during its collision with the heat source in a given nanofluid would depend on the thermal conductivity (k_p, unit W/m.K), density (ρ, unit kg/m^3), elastic modulus (E, unit GPa) and Poisson's ratio (μ) of the nanoparticle and heat source. Considering the expression for collision period and thermal conductivity of nanoparticle, a factor $\chi = k_p(\rho/E)^{0.4}$ is proposed here and examined for the preliminary identification of the potential of a dispersoid in enhancing the thermal conductivity of a nanofluid. The χ-factor for Ag, Cu, CuO, Al_2O_3 and SiO_2 are 2960, 2247, 116, 14.1 and 5.5, respectively. The higher χ-factor of CuO compared to that of Al_2O_3 can explain why water and ethylene glycol (EG) based CuO-nanofluid is reported to show higher enhancement in the thermal conductivity, when compared to similar Al_2O_3-nanofluid. The χ for SiO_2 is much smaller than that for Ag, which also corroborates well with the marginal enhancement in thermal conductivity of water based nanofluid containing SiO_2 nano-particles. Therefore, a high value of χ of the nano-dispersoid can serve as a parameter for the design of nanofluids for heat transfer applications.

1. Introduction

Nanofluids are promising for advanced heat transfer applications since their thermal conductivities are often much greater than that of conventional heat transfer fluids. Diverse types of nanofluids have been produced and characterized since the last decade by different investigators [1-5]. The enhancement in thermal conductivity of nanofluids is found to depend on the type of nanoparticles and base fluid, volume fraction of nanoparticles, temperature of the liquid medium, size and shape of the nanoparticles, type of dispersant used for stabilization, etc.

Theoretical investigation on the thermal conductivity of nanofluids is limited. Although some discrete attempts have been made by some researchers to model the heat transfer of nanofluids [6-11], a universally accepted model still does not exist. The mechanism of heat transfer of nanofluids has not been established as yet. Conventional continuum models, such as Maxwell's model [12], Hamilton and Crosser's model [13], etc. underpredict the thermal conductivity enhancement of nanofluids to a great extent. Thus, designing the nanofluids for practical applications is still a real problem.

Recent simulations by Ghosh *et al.* [14] based on classical molecular dynamics (MD) have shown that during collision of a nanoparticle with a heat source a pulse-like heat transfer occurs. This phenomenon has, however, been overlooked in all other existing models of nanofluids. The nanoparticles inevitably move in the nanofluid by Brownian motion due to their small size and eventually collide with the heat source at a certain frequency depending on the Brownian motion parameters. The heat transfer due to this type of collision which is assisted by the Brownian motion leads to the enhancement in thermal conductivity of nanofluids. The model developed by Ghosh *et al.* [14] can be used to theoretically estimate the thermal conductivity of diverse types of nanofluids in order to design nanofluids for practical applications.

2. Brief Outline of the Model

The scheme of simulation as followed by Ghosh *et al.* [14] for estimating the thermal conductivity of a nanofluid has been outlined here. The detailed account can be found elsewhere [14]. Ghosh *et al.* [14] have considered a block-shaped Cu heat source in contact with a water based Cu (4 nm size)-nanofluid. The nanoparticles within the fluid are expected to move randomly by Brownian motion because of their small sizes. Furthermore, in course of their Brownian motion the nanoparticles will repeatedly collide with the heat source at a frequency, which depends on the Brownian motion parameters like temperature and viscosity of the base fluid, size of the nanoparticle, etc. During each collision the nanoparticle will acquire some heat from the heat source. Heat transfer during collision of the nanoparticles with the heat source is expected to be very fast due to direct solid-solid contact. Therefore, in a nanofluid in addition to normal conductive heat transfer through the base fluid itself (without nanoparticles) some amount of heat is carried by the nanoparticles due to their collision with the heat source. The extent of this additional heat transfer has been estimated in order to estimate the enhancement in thermal conductivity of the nanofluid.

The multiscale model developed by Ghosh *et al.* [14] suggests that the collision induced heat transfer depends on the thermal conductivity of the colliding particle as well as the period of collision of the nanoparticle with the heat source. The collision period (Δt_c) is given as [15]:

$$\Delta t_c = \frac{2.94}{V_{coll}} \zeta r_{np} \tag{1}$$

where

$$\zeta = [\frac{5}{2}\pi^2 \rho V_{coll}^2 \omega]^{2/5} \tag{2}$$

Here V_{coll} is the collision velocity, r_{np} is the radius of the nanoparticle, ρ is the density of the nanoparticle, ω is the elasticity parameter for the particle or heat source material. The elasticity parameter ω is defined by [15]:

$$\omega = \frac{1-\mu^2}{\pi E} \tag{3}$$

where, μ is the Poisson's ratio and E is the Young's modulus. Therefore, apart from size and collision velocity the elastic properties as well as the density of the nanoparticle influence the collision period.

3. Results and Discussion

Computations based on MD simulation coupled with stochastic simulation have shown that the energy transfer mechanism proposed in the present model results in an appreciable enhancement in the thermal conductivity of the fluid, if agglomeration of nanoparticles is ignored [14]. The predicted enhancement in the thermal conductivity of the water based Cu (4 nm dia.) nanofluid as a function of the volume fraction of nanoparticles is plotted Fig. 1 on the basis of the proposed energy transfer mechanism alone. It is found that for a given volume percent of loading (≤0.3%), the theoretically estimated enhancement in thermal conductivity is much larger than those predicted by Maxwell's model [12], provided the nanoparticles are assumed to be free from directional (linear or fractal) agglomeration. It is also predicted that the enhancement in thermal conductivity of a water based nanofluid would increase linearly with the extent of Cu nanoparticles loading (≤0.3 vol.%) in the base fluid. The experimentally measured enhancement in the thermal conductivity of the water based Cu-nanofluid [14] as a function of the volume fraction of nanoparticles has also also been shown in Fig. 1. It is found that for a given volume percent of loading (≤0.3%), the theoretically estimated enhancement in thermal conductivity is about 25% more than the experimentally determined value for the present water based Cu-nanofluid. This deviation may be attributed to the smaller size of the nanoparticles (4 nm) considered in the present MD-stochastic model of nanofluid compared to the experimentally prevailing size of the Cu particles (6-100 nm). Thus, the experimental data for water based Cu-nanofluid [14] seems to be in reasonable agreement with the prediction of the present model. Moreover, the experimental data of water based Cu-nanofluids show a linear variation in the enhancement in thermal conductivity with the extent of Cu nanoparticles loading (≤0.3 vol.%) in the base fluid. This nature of variation is in conformity with the predictions of the present model (Fig. 1). The model developed by Ghosh *et al.* [14] thus gives a reliable prediction on the thermal conductivity of nanofluids.

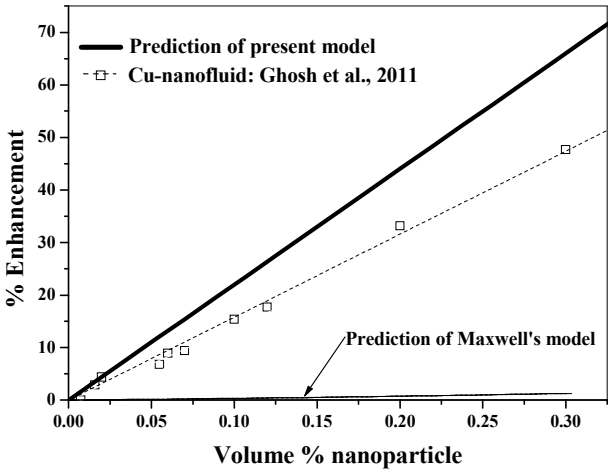

Fig. 1: Enhancement in thermal conductivity of nanofluid with volume fraction of nanoparticles of Cu in experimentally produced water based Cu-nanofluid (dashed line) [14] compared with the present theoretical prediction for the Cu+H_2O nanofluid (thick line) containing 4 nm size Cu particles. Here the straight dashed line represents linear regression through experimental data. The predictions of Maxwell's model for water based Cu-nanofluid depicts insignificant enhancement, as shown in the figure.

The variation of predicted thermal conductivity enhancement with volume% of Ag- or Zn-nanoparticle loading (<0.1 vol.%) has been compared in Fig. 2 with that of water based Cu-nanofluid. It is interesting to note that enhancement in thermal conductivity of water based Ag-nanofluid is 6.8 times that of water based Cu-nanofluid for the same volume of nanoparticle

loading, although Ag has only ~7% higher thermal conductivity than Cu. On the other hand, for a given volume of nanoparticle loading water based Zn-nanofluid would show merely 23% lower enhancement in thermal conductivity than water based Cu-nanofluid. The reason behind the markedly greater enhancement in thermal conductivity of Ag-nanofluid compared to that of Cu-nanofluid is mainly due to different interaction potential (manifested as different elastic modulus and collision period), which leads to much greater extent of heat absorption by the Ag nanoparticle compared to that by the Cu nanoparticle during the collision with heat source. Thus, the present simulation points out that Ag-nanofluid can be much more attractive than Cu-nanofluid for heat flux applications. On the other hand, the collision period of Zn nanoparticle (12.91 ps) is not significantly different from that of Cu nanoparticle (13.59 ps). Thus the difference is not so significant in the simulation results for Cu and Zn. The present model points out for the first time that the thermal as well as elastic and other physical properties of the suspended nanoparticles can have important influence on the thermal conductivity of nanofluids.

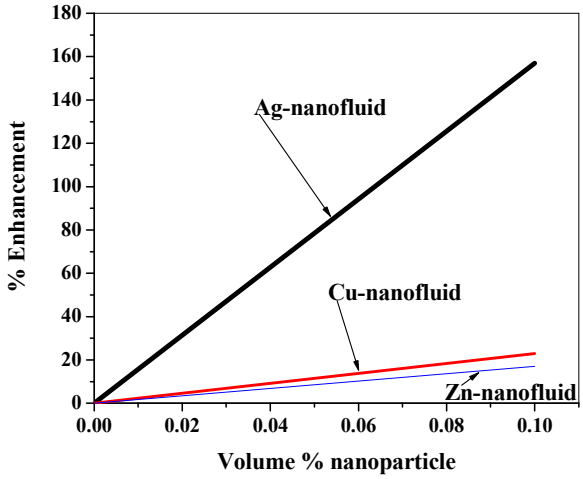

Fig. 2: The enhancement in thermal conductivity of water based Ag-, Cu- and Zn- nanofluid, predicted by present MD-stochastic model as a function of volume of nanoparticle loading. All nanoparticles are assumed to be spheres of 4 nm diameter.

It is to be noted here that Eapen *et al.* [16] have reported a limited enhancement in thermal conductivity in well dispersed nanofluid suspensions of silica and perfluorinated particles (MFA) in water, which they found to be in agreement with Maxwell's mean-field theory. Their results are also in contrast with most of the experimental data of thermal conductivity enhancement in nanofluids reported in the literature [1-4]. This apparent controversy can be potentially explained on the basis of the present model which, for the first time, has highlighted the importance of heat exchange during impact of nanoparticles with the heat source. The thermal conductivity of a nanofluid should enhance with the increase in thermal conductivity of the nanoparticles, as well as, with the duration of collision of nanoparticles with the heat source. Considering the expression of collision period (Eq. 1) and thermal conductivity of nanoparticle, a factor

$$\chi = k_p (\rho/E)^{2/5} \tag{4}$$

can be intuitively proposed for preliminary identification of the potential of a dispersoid in enhancing the thermal conductivity of a nanofluid. Table 1 presents the thermal conductivity (k_p), density (ρ), elastic modulus (E) from which the χ-factor for different nano-dispersoids have been calculated. Simplification of the unit for χ has not been done in this Table to avoid its fractional expression. The high value of χ for Ag (2960) may indicate its high effectiveness as a nano-

dispersoid in a fluid for heat transfer applications. Table 1 shows that χ for Ag (say, χ_{Ag}) > χ_{Cu} > χ_{Zn}. Indeed detailed simulation has shown that the predicted thermal conductivity of water based Ag-nanofluid > Cu-nanofluid > Zn-nanofluid (Fig. 2). The χ_{SiO_2} (5.46) is much smaller than χ_{Ag} (2960) (Table 1), which corroborated well with the experimental results of Eapen *et al.* [16] displaying marginal enhancement in thermal conductivity of water based nanofluid containing SiO_2 particles. The elastic modulus of MFA is not known, but its thermal conductivity (0.2 W/mK) is even less than water. So the rate of heat transfer through MFA particle during the collision is expected to be less than that through water medium. This can account for the experimental results of Eapen *et al.* manifesting a decrease in thermal conductivity of water based nanofluids containing MFA particles compared that in water medium [16]. Table 1 also shows that CuO particle has greater thermal conductivity and χ-factor as compared to Al_2O_3 particles. This may qualitatively explain, why water and ethylene glycol based CuO-nanofluid show higher enhancement in the thermal conductivity, when compared to similar Al_2O_3-nanofluid [5]. Thus, the MD-stochastic model proposed earlier seems to have a good potential in designing nanofluids for advanced heat transfer applications.

Table 1: Properties of some materials of nanoparticles used in nanofluids.

Material	Thermal conductivity [W/m.K]	Density [kg/m^3]	Elastic modulus [GPa]	χ-factor [(W/mK)(kg/m^3.GPa)$^{2/5}$]
Ag	429	10500	83	2960
Cu	401	8920	120	2247
Zn	113	7140	108	604
CuO	20	6570	81.6	116
Al_2O_3	5.43	3690	353	14.12
SiO_2	1.4	2200	71.7	5.46
MFA	0.2	2140	-	-

4. Conclusion

Simulation of thermal conductivity of nanofluids by a MD-stochastic model proposed earlier by present investigators [14] has predicted that thermal conductivity of water based Ag-nanofluid > Cu-nanofluid > Zn-nanofluid. Based on these results a factor χ is proposed here and examined to identify the effectiveness of various nanodispersoids in contributing to the anomalous thermal conductivity of the nanofluids.

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