

A New Theoretical Model for Predicting the Thermal Conductivity of Nanofluids

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Abstract

In this paper, a new theoretical model has been developed to predict the thermal conductivity of nanofluids. The new model combines the static mechanism considering the nanolayer effect and the dynamic mechanism considering the nanoparticle vibration effect. Comparison of the new model predictions with the experimental data available in literature shows good agreement at 0-2 vol% of nanoparticle volume fractions. The new model also gives better predictions compared to the Maxwell model.

Keywords: Theoretical Model, Thermal Conductivity, Nanofluids, Nanolayer, Nanoparticle Vibration

1 Introduction

Recently, the popularity of nanofluids as heat transfer fluids has increased significantly in research and industrial sectors. Nanofluids are solid nanoparticles with sizes < 100 nm that are suspended in base fluids such as water, oil, refrigerants, or ethylene glycol. Due to their enhanced thermal characteristics, nanofluids have a great potential to face several challenges in cooling technology, such as the application of ultra high heat fluxes and the trend of system miniaturization. The enhanced thermal conductivity is becoming one of the intense topic in nanofluids research due to its relationship with the heat transfer performance. Many efforts have been done to theoretically predict the thermal conductivity of nanofluids. However, there is no a model that is capable to predict a wide range of experimental data. It means that the heat transport mechanisms in nanofluids still remain poorly understood.

The classical models, such as Maxwell model, Bruggemen model, or Hamilton and Crosser model fail in predicting the thermal conductivity of nanofluids since those models were developed for predicting the thermal conductivity of suspensions containing mm or μm -sized solid particles. The classical models only considered a few parameters that contribute to the thermal conductivity of nanofluids, such as thermal conductivity of nanoparticles, thermal conductivity of base fluids, and concentration of nanoparticles. To consider other important parameters, i.e. temperature of nanofluids and size of nanoparticles, a number of theoretical models have proposed several factors or mechanisms that are possibly responsible for the enhanced thermal conductivity of nanofluids, such as interfacial layer and dynamic mechanisms.

The presence of liquid molecular layering at the solid-liquid interface has been observed experimentally by Yu et al. [1]. Several theoretical models [2-4] that consider the effect of interfacial layer between solid and liquid have been developed to predict the enhanced thermal conductivity of nanofluids. However, the interfacial layer models can not takes into account the temperature-dependent effect of the thermal conductivity of nanofluids.

The dynamic mechanisms of the conduction process in nanofluids consider the effects of nanoparticle and bulk fluid motions. Several dynamic mechanisms have been proposed, such as collision of nanoparticles due to the Brownian motion, nanoconvection, and micro-mixing. The collision between nanoparticles due to the translational Brownian motion enables solid-to-solid heat transfer process directly. However, a number of research have found that the translational Brownian motion of nanoparticle has no significant effect to the conduction process [5-8]. The Brownian motion of nanoparticle has indirect contribution to the thermal conductivity of nanofluids by causing nanoconvection and micro-mixing. Both mechanisms are suggested to have an important role in the thermal conductivity enhancement of nanofluids [6,9-11]. Kleinstreuer and Li [12] noted that the formula used by Jang and Choi [6] to calculate the liquid mean free path in their nanoconvection model is not applicable for liquid and only valid for ideal gas. Nie et al. [8] also analyzed that the possibility of micro-mixing in nano-

fluid is questionable. More experimental studies and molecular dynamic simulations are still needed to justify the physical correctness of nanoconvection and micro-mixing concepts.

Generally, theoretical models for the thermal conductivity of nanofluids rely on the empirical constants obtained only to fit the experimental data. So, the applicability of the models was limited. The unjustified assumptions used in the models also bring the controversy. In this study, we propose an alternative model for predicting the thermal conductivity of nanofluids. The model considers nanoparticle dynamic, especially vibration mechanism, and interfacial nanolayer effect. By combining the static model and the dynamic model, a new model is developed by no addition of the empirical constant. For validation, the new model is compared to the experimental data available in literature. This paper also provides an analytical calculation to examine that the contribution of translational Brownian motion to the thermal conductivity of nanofluids is negligible.

2 The Translational Brownian Motion Effect

The conduction process in fluid can be performed through the molecules collisions. In nanofluid, nanoparticle will transfer the heat to other nanoparticle when they collide to each other due to the translational Brownian motion. In this paper, we will provide an analytical formulation to support the conclusion that the contribution of the translational Brownian motion to the thermal conductivity of nanofluids is not significant.

Based on the thermal conductivity theory for monoatomic gas derived by Bird et al. [13], the contribution of nanoparticles collisions due to the translational Brownian motion to the thermal conductivity of nanofluids (k_{BM}) is expressed as

$$k_{BM} = \frac{1}{3} \phi \rho_p c_p \bar{v} \lambda \quad (1)$$

where ϕ , ρ_p , c_p , \bar{v} , and λ are volume fraction, density, specific heat at constant pressure, average velocity, and mean free path of nanoparticles, respectively. In contrast to several research that used the kinetic theory of gas formulation ($\bar{v} = \sqrt{(18k_B T)/(\rho \pi d_p^3)}$) [6,7,9,10] to calculate the nanoparticle velocity, this study uses the diffusion approximation [14] in order to be more realistic for nanofluid system. The mean free path of nanoparticles is approximated by $\lambda = \sqrt{2D_{eff}t}$ [14] and the characteristic time ($t = \rho_p d_p^2 / (18\mu_f)$) is derived from the solution of Langevin equation of stochastic process [7], where d_p is nanoparticle diameter and μ_f is dynamic viscosity of base fluid. The effective diffusion coefficient for a suspension of spheres having finite particle volume fraction is calculated by Eq. (2) [15]

$$D_{eff} = D(1 - 1.5\phi) \quad (2)$$

where the diffusion coefficient is determined by Einstein-Stokes Equation ($D = k_B T / (3\pi\mu_f d_p)$) which is suitable for liquid system. Then, by using $\bar{v} = \lambda/t$, Eq. (1) is re-written as

$$k_{BM} = (\phi - 1.5\phi^2) \frac{2\rho_p c_p k_B T}{9\pi\mu_f d_p} \quad (3)$$

Fig. 1 shows us the ratio between the thermal conductivity of nanofluids due to the translational Brownian motion of nanoparticles (Eq. (3)) and the thermal conductivity of base fluids for Al₂O₃-water nanofluid and ZrO₂-water nanofluid.

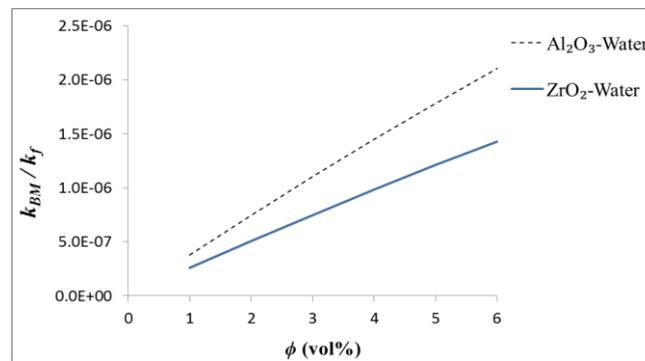


Fig. 1. The contribution of the translational Brownian motion to the thermal conductivity of nanofluids as the function of nanoparticle volume fractions

It is found that the nanoparticles collisions due to the translational Brownian motion gives no significant effect to the thermal conductivity of nanofluids.

3 Modelling the Thermal Conductivity of Nanofluids

The new model developed here consists of static model and dynamic model. The model also considers the interfacial nanolayer effect.

3.1 Static Model

The static part of the model is obtained from the Maxwell model [2] (see Eq. (4)) that is modified by Yu and Choi [2] to incorporate the effect of interfacial nanolayer (see Eq. (5) and (6))

$$k_{Maxwell} = \frac{k_p + 2k_f + 2\phi(k_p - k_f)}{k_p + 2k_f - \phi(k_p - k_f)} k_f \quad (4)$$

$$k_{Yu-Choi} = \frac{k_{pe} + 2k_f + 2\phi(k_{pe} - k_f)(1 + \beta)^3}{k_{pe} + 2k_f - \phi(k_{pe} - k_f)(1 + \beta)^3} k_f \quad (5)$$

$$k_{pe} = \frac{2(1-\gamma) + (1+\beta)^3(1+2\gamma)\gamma}{-(1-\gamma) + (1+\beta)^3(1+2\gamma)} k_p \tag{6}$$

where $\beta=2h/d_p$ and $\gamma=k_{lr}/k_p$. h is the thickness of nanolayer, k_p , k_f and k_{lr} are the thermal conductivity of nanoparticle, base fluid and nanolayer, respectively.

Since the molecular structure of interfacial layer is more ordered than that of bulk of liquid, the thermal conductivity of layer is assumed to be higher than that of bulk of liquid but is still lower than that of nanoparticle. Based on several studies [1,16], nanolayer thickness is predicted to be in the range of 1-2 nm. In this paper, the thermal conductivity and the thickness of nanolayer are set at $2k_f$ and 1 nm, respectively.

3.2 Dynamic Model

In liquid, the conduction process can be related to the molecular vibration activity. In this study, the development of dynamic model for the thermal conductivity of nanofluids is based on the contribution of nanoparticles vibration to the heat conduction. According to the Bridgman theory of energy transport in pure liquid [13], the liquid molecules are assumed to be arranged in a cubic lattice and energy is transferred from a lattice plane to the next one by vibration mechanism at the sonic velocity (v_s) of the given fluid. Then, by reinterpreting the thermal conductivity equation for monoatomic gases at low density [13], the contribution of nanoparticle vibration to the thermal conductivity of nanofluid is modelled as follow

$$k_{vib} = \phi \rho_p c_p v_s \bar{x}_p \tag{7}$$

where \bar{x}_p is root-mean-square displacement of nanoparticle.

Referring to the Meibodi et al. model [17], the sonic velocity of energy transfer at the nanoparticles vibration is assumed to be similar to that at the base fluid molecules vibration. The analytical work of Nie et. al. [8] has shown that the speed of phonon transport will not be affected due to the insertion of nanoparticles in the low volume fraction. The sonic velocity at the base fluid molecules can be determined from the thermal conductivity formula of liquid (Bridgman Equation) [13] as given below

$$k_f = 2.80(N_A/V)^{2/3} k_B v_s \tag{8}$$

where N_A is Avogadro number and V is molar volume. Then, the sonic velocity of nanoparticle vibration in Eq. (7) is determined from Eq. (8). The root-mean-square displacement of nanoparticle (\bar{x}_p) is approximated by using the Einstein theory on diffusion for Brownian particles ($\bar{x}_p = \sqrt{2D_{eff}t}$). So, the thermal conductivity of nanofluid that comes from the contribution of nanoparticle vibration takes the following form

$$k_{vib} = \phi \rho_p c_p \left[\frac{k_f}{2.80(N_A/V)^{2/3} k_B} \right] \bar{x}_p \quad (9)$$

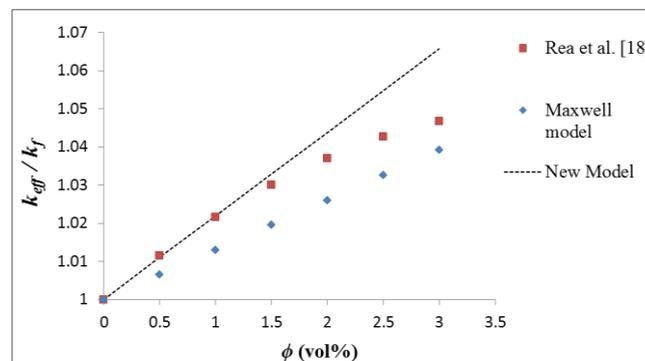
Finally, the effective thermal conductivity of nanofluid is obtained by adding the static model and the dynamic model as shown in Eq. (10).

$$k_{eff} = k_{static} + k_{vib} \quad (10)$$

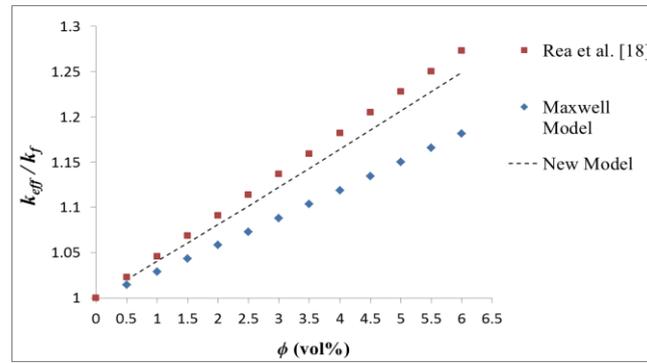
4 Results and Discussion

For validation, the new model predictions are compared to several experimental data available in literature as well as the Maxwell model predictions, as shown in Fig. 2. As shown in Fig. 2a, the thermal conductivity of ZrO₂-water nanofluid predicted by the new model agrees well with the experimental data for nanoparticle concentrations ranging from 0 to 2 vol%. After 2 vol%, the increase of the experimental thermal conductivity tends to be nonlinear. The agglomeration of nanoparticles when the concentration goes up from 2 vol% may become one of the possible reasons for this characteristic. The effect of agglomeration to the thermal conductivity of nanofluid is strongly related to the size and configuration of nanoparticle cluster. Both parameters depend on many factors, such as time, nanofluids concentration, and solid particle type. However, when nanoparticle cluster reaches over a certain size limit, it will experience the sedimentation due to the gravitational force effect. The sedimentation process causes the reduction of nanoparticle concentration in nanofluid and hence decreases the thermal conductivity of nanofluids.

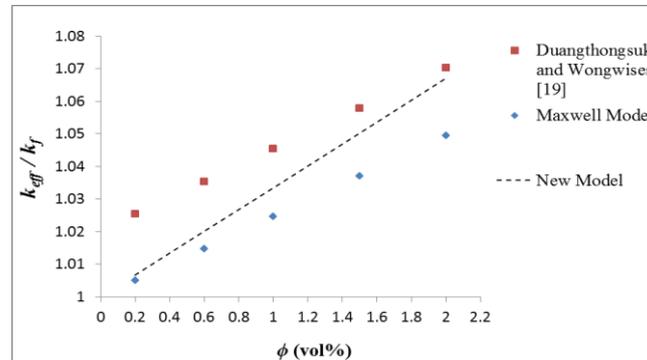
Fig. 2a shows that the deviation of the new model predictions from the experimental data is 0-2.13% over 0-3 vol% of concentrations range. It is noted that the concentration range of 0-2 vol% gives the maximum deviation limit of 1%. It is also found that the prediction of the Maxwell model is much lower than the experimental data, especially for higher nanoparticle volume fractions.



(a)



(b)



(c)

Fig. 2. Comparison of the new model predictions with the Maxwell model prediction and the experimental data for (a) ZrO₂-water nanofluid, (b) Al₂O₃-water nanofluid, and (c) TiO₂-water nanofluid

Similar to ZrO₂-water nanofluid, the prediction by the new model for Al₂O₃-water nanofluid has a good agreement with the experimental data in the concentration range of 0-2 vol% as shown in Fig. 2b. In that concentration range, the deviation of the new model predictions from the experimental data is below 1%. Over 0-6 vol%, the deviation goes from 0 to 1.86%. The prediction of the new model is absolutely better than that of the Maxwell model. In contrast to ZrO₂-water nanofluid case, the experimental thermal conductivity shows the linear enhancement when the nanoparticle concentration increases from 2 to 6 vol%. It means that Al₂O₃-water nanofluid has less possibility to experience the agglomeration at higher concentration compared to ZrO₂-water nanofluid. It is because the density of ZrO₂-water nanofluid is higher than that of Al₂O₃-water nanofluid. It can be also seen in Fig. 2b that the new model prediction is still lower than the experimental data because the value of nanolayer thermal conductivity is set only at $2k_f$. For ZrO₂-water nanofluid, the range of value between the thermal conductivity of nanoparticle and that of base fluid is not wide enough, so it is reasonable to set the thermal conductivity of nanolayer at $2k_f$. For Al₂O₃-water nanofluid, the range of value between the thermal conductivity of

nanoparticle and that of base fluid is so wide enough that the thermal conductivity of nanolayer could be higher than $2k_f$. The higher the thermal conductivity of nanolayer, the closer the new model prediction to the experimental data of Al_2O_3 -water nanofluid.

Fig. 2c shows the predicted thermal conductivity of TiO_2 -water nanofluid compared to the experimental data and the Maxwell model prediction. It can be seen that the new model prediction gets closer to the experimental data with increasing nanoparticle volume fraction from 0.2 to 2 vol%. The new model gives better prediction than the Maxwell model which is consistently much lower than the experimental data over all the observed nanofluid concentrations. The deviation of the new model prediction from the experimental data ranges from 0.29 to 1.83% at the concentration range of 0.2-2 vol%.

All the above comparisons confirm that although the new model predictions show good agreement with the experimental data obtained from literature at very low nanoparticle volume fractions, it is still better than the predictions of Maxwell model. This is because the new model considers nanoparticle size and temperature effects that are ignored by the Maxwell model. As predicted before, the Maxwell model underpredicts all the experimental data of the thermal conductivity of nanofluids. The maximum deviation of the new model predictions from the experimental data is found to be 2.13%. Generally, the deviation of less than 1% takes place when the nanofluid concentration is below 2 vol%.

Conclusion

In summary, we propose a new theoretical model for predicting the thermal conductivity of nanofluids by combining the static mechanism including nanolayer effect and the dynamic mechanism of nanoparticle vibration. Comparing to the Maxwell model, the new model shows better agreement with the experimental data available in literature. The new model matches well with the experimental data at a certain range of nanofluids concentration. We have also given another analytical calculation to prove that the contribution of translational Brownian motion to the thermal conductivity of nanofluids is negligible.

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