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ORIGINAL

Mathematical modelling of thermal conductivity for nanofluid considering interfacial nano-layer

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Abstract Maxwell's classical model for predicting effective thermal conductivity of colloidal solution predicts the thermal conductivity of nanofluids quite satisfactorily. However, Maxwell's model does not consider the effect of interfacial layer, Brownian motion of nano-particle and nanoparticle aggregation. In this paper, the effect of interfacial layer on thermal conductivity is considered. A simple expression has been derived to determine thermal conductivity of nanofluid considering interfacial layer formed on the nano particles. The thermal conductivity of the interfacial layer has been precisely determined and results are found to be closer to the experimental values, hence, further improving the results of classical Maxwell model.

List of symbols

n	Particle shape factor
M_w	Molecular weight of liquid
N_A	Avogadro's constant
ρ	Density of the liquid
r_p	Radius of nanoparticle
t	Thickness of the interfacial nano-layer
υ	Particle volume concentration
k_p	Thermal conductivity of particle
k_m	Thermal conductivity of liquid medium
Q	Heat flow rate through interfacial layer
r	Radial distance from the centre of the particle
A	Surface area at a distance 'r' from the centre of nanoparticle
T	Temperature at a distance 'r' from the centre of nanoparticle
k_l	Thermal conductivity of interfacial nano-layer
k_c	Thermal conductivity of particle and interfacial nano-layer composite
k_{eff}	Effective thermal conductivity of nanofluid
EG	Ethylene glycol

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1 Introduction

The role of the fluid media cannot be ignored for development of energy efficient heat transfer equipment. Thermo-physical properties, particularly thermal conductivity, is the most important property that has to be taken into account for this purpose. Various techniques have been used to improve the heat transfer capability of a fluid by mixing milli or micro sized particles, with higher thermal conductivity, in the base fluid. But this also invites serious problems like poor suspension stability, channel clogging, pressure drop, pipeline erosion and many others. As a break through, Choi [1] introduced a new type of colloidal solution named 'nanofluid' in 1995 which showed better stability and rheological properties. Now it is expected that nanofluid may become the next generation heat transfer fluid [2].

It was observed that by mixing less than 6 % volume fraction of aluminium oxide and copper-oxide, nanoparticles or carbon nanotubes with an average diameter of 30 nm, the thermal conductivity of nanofluids could be enhanced by up to three times higher than that of the base fluids [3–5]. Maxwell [6] and Hamilton Crosser [7] have studied the effect of the volume fraction and thermal conductivity ratio between particle and base fluid.

Hamilton Crosser has also taken in account the effect of particle shape. Some models for thermal conductivity of nanofluid have been proposed by considering the brownian motion, interfacial layer and aggregation of particles [8–11]. According to some researchers, these effects are negligible [12]. Koo and Kleinstreuer [13] considered the significance of brownian motion in the transfer of energy. Role of interfacial effect was introduced by Jang and Choi [14].

Liquid around a nanoparticle takes a similar structure to the solid and consequently has different conductivity compared to the base fluid. Liquid molecules close to solid surface are known to form layered structures [15]. With these solid like layers, nanofluid structures consist of solid nanoparticles, shells (solid like liquid layer) and a bulk liquid. As the layered molecule are in an intermediate physical state between a solid and a bulk liquid [16], the shells would be expected to lead to a higher thermal conductivity than that of the bulk liquid. The thickness of these shells at the interface of particles plays an added role in heat transportation from solid to adjacent liquid. For particles of micro-meter size, the surface areas are small, e.g. for alumina powders with an average diameter of 10 μm, the SSA (Specific Surface Area) is only 0.15 $m^2\ g^{-1}$. Therefore, the effect of interfacial layer is negligible. However, nanoparticles have larger SSA, e.g. for alumina powders with an average diameter of 10 nm, the SSA is as large as 151 $m^2\ g^{-1}$, which is much larger as compared to micro-sized particle. Therefore, interfacial layer in nanofluid plays a significant role in heat transfer between nanoparticles and the base fluid. Thus, the solid like liquid layer, acts as a thermal bridge between the solid particle and the bulk liquid. Based on this assumption, Yu and Choi [17] have modified the Maxwell equation for the effective thermal conductivity of spherical particle-liquid suspensions to include the effect of this ordered liquid layer.

In this paper a mathematical model for determining the thermal conductivity of the nanofluid by considering the interfacial layer has been developed. Results obtained by using this model have been compared with the experimental data as well as Hamilton Crosser model.

2 Mathematical model

2.1 Mathematical models used earlier to predict thermal properties

Various models for thermal conductivity of nanofluid have been proposed. However, none of these models could successfully account for the observed enhancement of thermal conductivity of nanofluids. Following are some of the expressions of the conventional model of effective thermal conductivity of solid–liquid suspension:

$$\frac{k_{eff}}{k_m} = 1 + \frac{3(a-1)\upsilon}{(a+2)-(a-1)\upsilon}\ [6], \tag{1}$$

$$\frac{k_{eff}}{k_m} = \frac{a+(n-1)-(n-1)(1-a)\upsilon}{a+(n-1)+(1-a)\upsilon}\ [7], \tag{2}$$

$$\frac{k_{eff}}{k_m} = 1 + 3b\upsilon + \left[3b^2 + \frac{3b^2}{4} + \frac{9b^3(a+2)}{16(2a+3)} + \cdots\right]\upsilon^2\ [18], \tag{3}$$

$$\frac{k_{eff}}{k_m} = 1 + \frac{3(a-1)}{(a+2)-(a-1)\upsilon}\left[\upsilon + f(a)\upsilon^2 + O(\upsilon^3)\right]\ [19], \tag{4}$$

$$\frac{k_{eff}}{k_m} = 1 + a\upsilon + b\upsilon^2\ [20], \tag{5}$$

where,

$a = k_p/k_m$ and $b = (a-1)/(a+2)$.

2.2 Determination of thermal conductivity of interfacial nano-layer

In this model, It has been assumed that the variation of thermal conductivity of interfacial layer is linear along the thickness of layer. A suspension of mono-sized spherical particle is considered. Figure 1 shows a nanoparticle of radius (r_p) with thickness (t) of the interfacial layer and Fig. 2 shows the variation of thermal conductivity of interfacial layer along its thickness. Using the Langmuir formula of monolayer adsorption of molecules, Wang et al. [8] proposed the following relation for the thickness of the layer:

$$t = \frac{1}{\sqrt{3}}\left[\frac{4M_w}{\rho N_A}\right]^{1/3}. \tag{6}$$

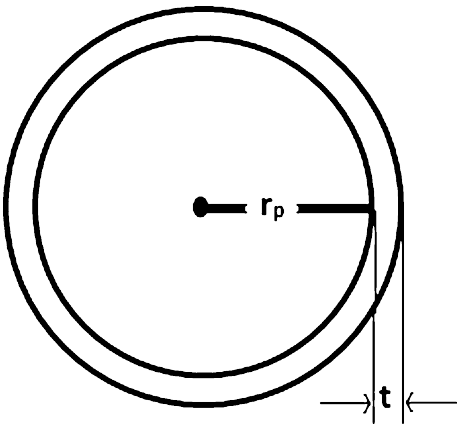

Fig. 1 Schematic model of nanoparticle with interfacial layer

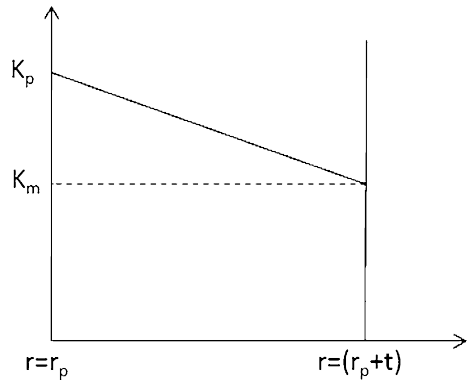

Fig. 2 Variation of thermal conductivity of interfacial along its thickness

The portion of interfacial layer just in contact with the particle has thermal conductivity (k_p) and the thermal conductivity goes on decreasing along the thickness of interfacial layer towards the base liquid medium and finally approaching the vale equal to 'k_m' just before it blends and behaves as liquid. Therefore, the equation for finding the thermal conductivity at a distance 'r' within the interfacial layer is:

$$k(r) = k_p - \left[\frac{k_p - k_m}{t}\right](r - r_p). \tag{7}$$

This can be rearranged as:

$$k(r) = (k_p + \lambda r_p) - \lambda r, \tag{8}$$

where $\lambda = (k_p - k_m)/t$.

Now considering the condition of steady-state heat transfer across the interfacial layer with heat flow rate being constant and equal to Q, the following equation in spherical coordinates can be written as:

$$Q = -k(r)A\frac{dT}{dr}. \tag{9}$$

The surface area of an infinitesimally small interfacial layer at a distance r from the centre of particle, can be written as $A = \pi r^2$. Putting the value of A and k(r) in Eq. (9), rearranging and integrating it, the equation obtained as:

$$\frac{-4\pi\Delta T}{Q} = \int_{r_p}^{r_p+t} \frac{dr}{r^2\left[(k_p + \lambda r_p) - \lambda r\right]}. \tag{10}$$

Now considering the interfacial layer as a whole having equivalent thermal conductivity (k_l), the similar heat transfer equation for hollow sphere can be written as:

$$Q = -k_l 4\pi(r_p + t)r_p\frac{\Delta T}{t}. \tag{11}$$

$$\text{or } \frac{-4\pi\Delta T}{Q} = \frac{t}{r_p(r_p + t)k_l}. \tag{12}$$

Equating the right hand side of Eqs. (10) and (12) we obtain the value of equivalent thermal conductivity k_l as:

$$k_l = \frac{t}{r_p(r_p + t)\int_{r_p}^{r_p+t}\frac{dr}{r^2\left[(k_p+\lambda r_p)-\lambda r\right]}}. \tag{13}$$

On solving the integral:

$$k_l = \frac{t}{r_p(r_p + t)\left[A\ln\left(1 + \frac{t}{r_p}\right) + \frac{Bt}{r_p(r_p+t)} - \frac{C}{\lambda}\ln\left(1 - \frac{\lambda t}{k_p}\right)\right]}, \tag{14}$$

where $A = \lambda/(k_p + \lambda r_p)^2$, $B = 1/(k_p + \lambda r_p)$, and $C = \lambda^2/(k_p + \lambda r_p)^2$.

Equation (14), as obtained above, expresses the overall thermal conductivity of interfacial layer around nanoparticle in terms of the dimensions of the particle and the layer and the thermal conductivities of particle and the base fluid.

2.3 Determination of effective thermal conductivity of nanofluid

Xue and Xu [21] proposed the expression for determining the combined thermal conductivity of particle and interfacial layer and expressed as:

$$k_c = k_l\frac{2k_l + k_p + 2\tau(k_p - k_l)}{2k_l + k_p - \tau(k_p - k_l)}, \tag{15}$$

where $\tau = \left(\frac{r_p}{r_p + t}\right)^3$.

Now using Bruggeman's effective media theory [22] about two phase composites consisting of spherical particles, an equation for the effective thermal conductivity of the nanoparticle-fluid system (nanofluid) can be obtained as:

$$\left(1 - \frac{\upsilon}{\tau}\right)\frac{k_{eff} - k_m}{2k_{eff} + k_m} + \frac{\upsilon}{\tau}\frac{k_{eff} - k_c}{2k_{eff} + k_c} = 0. \tag{16}$$

Substituting the value of k_c in the above equation, the expression of the thermal conductivity of nanofluids with interfacial layer is:

$$\left(1 - \frac{\upsilon}{\tau}\right)\frac{k_{eff} - k_m}{2k_{eff} + k_m} + \frac{\upsilon}{\tau}\frac{(k_{eff} - k_l)(2k_l + k_p) - \tau(k_p - k_l)(2k_l + k_{eff})}{(2k_{eff} + k_l)(2k_l + k_p) + 2\tau(k_p - k_l)(k_l - k_{eff})} = 0. \tag{17}$$

The above expression, besides showing dependence on the thermal conductivity of the solid and liquid and their relative volume fraction, shows that the effective thermal

conductivity of nanofluids also depends on the particle size and interfacial properties.

3 Results and discussion

A novel model has been developed to analyse the value of effective thermal conductivity of nanofluid and compared it with the predictions of already existing model as well as with experimental data. The numerical model was used to find out the effective thermal conductivity of Al_2O_3–water, Al_2O_3–ethylene glycol, CuO–water and CuO–ethylene glycol nanofluids. The thermal conductivity of water and ethylene glycol was taken to be 0.604 and 0.258 W/mK [23] respectively and that of $Al_2O_3$and CuO was taken to be 46 W/mK [23] and 20 W/mK [24] respectively.

For Al_2O_3–water nanofluid the nanoparticle radius is taken as 30 nm and the thickness of interfacial layer is calculated as 0.2844 nm from Eq. (6). The present model shows the value of effective thermal conductivity of the interfacial layer as 10.53 W/mK. Figure 3 shows the comparison between the experimental findings [23], the present model and the Hamilton Crosser's model for Al_2O_3–water nanofluid.

For Al_2O_3–ethylene glycol nanofluid the nanoparticle radius is taken as 30 nm and the thickness of interfacial layer is calculated as 0.415 nm from Eq. (6). The present model shows the value of effective thermal conductivity of the interfacial layer as 8.9 W/mK. Figure 4 shows the comparison between the experimental findings [23], the present model and the Hamilton Crosser's model for Al_2O_3–ethylene glycol nanofluid.

For CuO–water nanofluid the nanoparticle radius is taken as 12 nm and the thickness of interfacial layer is calculated as 0.2844 nm from Eq. (6). The present model shows the value of effective thermal conductivity of the interfacial layer as 5.628 W/mK. Figure 5 shows the comparison between the experimental findings [25], the present model and the Hamilton Crosser's model for CuO–water nanofluid.

For CuO–ethylene glycol nanofluid the nanoparticle radius is taken as 12 nm and the thickness of interfacial layer is calculated as 0.415 nm from Eq. (6). The present model shows the value of effective thermal conductivity of

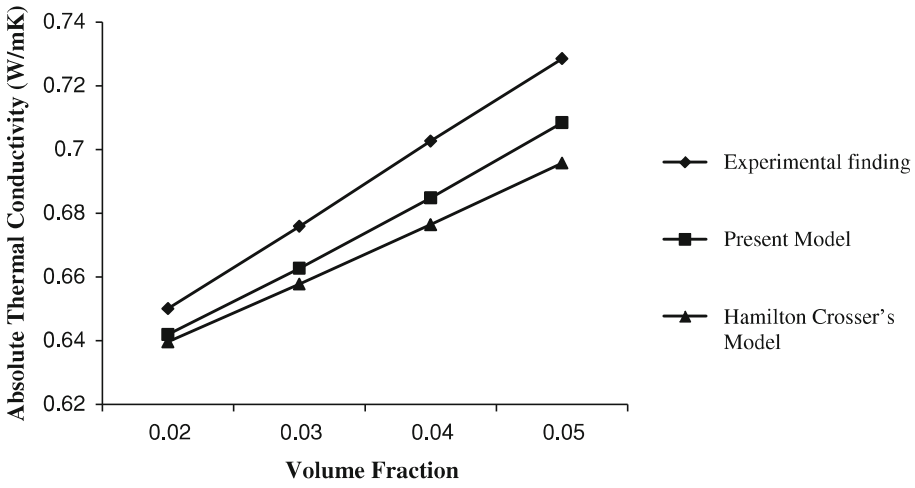

Fig. 3 Thermal conductivity variation for Al_2O_3–water nanofluid

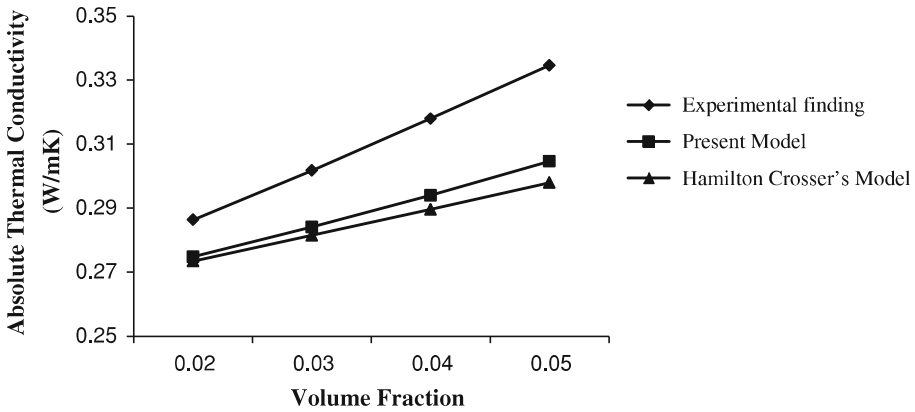

Fig. 4 Thermal conductivity variation for Al_2O_3–ethylene glycol nanofluid

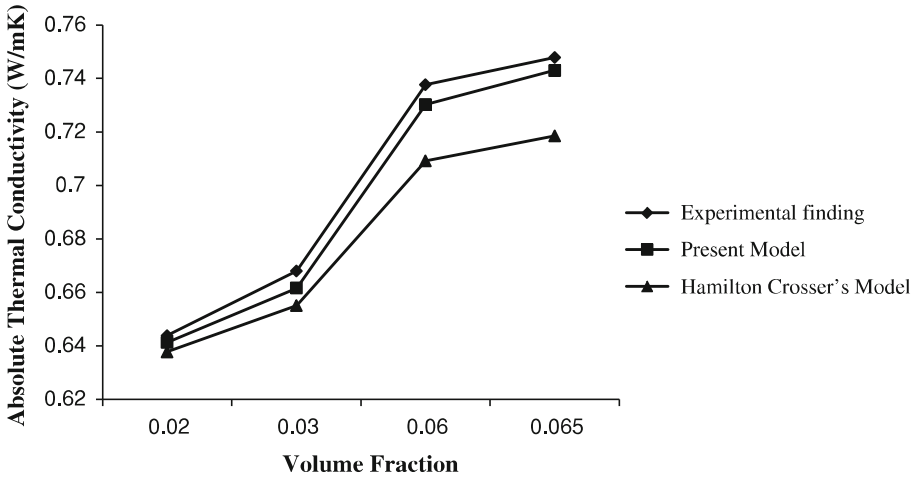

Fig. 5 Thermal conductivity variation for CuO–water nanofluid

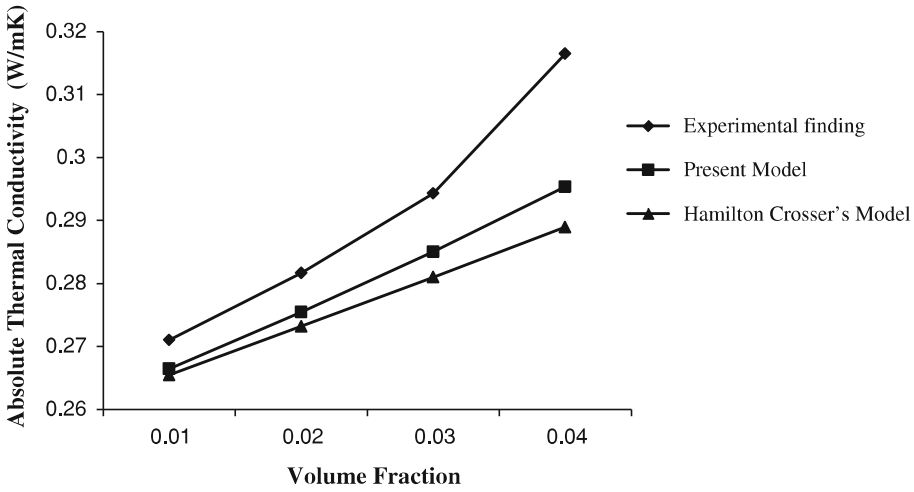

Fig. 6 Thermal conductivity variation for CuO–ethylene glycol nanofluid

Table 1 Percentage improvement of thermal conductivity in Al_2O_3–water, Al_2O_3–ethylene glycol

Volume fraction	Thermal conductivity (Al_2O_3–water nanofluid, W/mK)	Improvement in percentage	Thermal conductivity (Al_2O_3–EG nanofluid, W/mK)	Improvement in percentage
0.02	0.64197	77.65	0.27486	89.66
0.03	0.66274	72.53	0.28413	87.14
0.04	0.68486	68.00	0.29404	84.58
0.05	0.70845	61.34	0.30466	81.82

the interfacial layer as 4.626 W/mK. Figure 6 shows the comparison between the experimental findings [25], the present model and the Hamilton Crosser's model for CuO–water nanofluid.

Table 1 shows the effective thermal conductivity of Al_2O_3–water nanofluid and Al_2O_3–ethylene glycol nanofluid obtained by the present model. It also gives the percentage improvement of thermal conductivity reported by current model. Percentage improvement is calculated as:

$$\text{Improvement in percentage} = \frac{\text{Experimental result} - \text{present model result}}{\text{Experimental result} - \text{Hamilton Crosser's model result}}$$

Similarly Table 2 shows the effective thermal conductivity of CuO–Water nanofluid and CuO–Ethylene Glycol nanofluid as well as the percentage improvement of thermal conductivity obtained by the present model.

Table 2 Percentage improvement of thermal conductivity in CuO–water, CuO–ethylene glycol

Volume fraction	Thermal conductivity (CuO–water nanofluid, W/mK)	Improvement in percentage	Thermal conductivity (CuO–EG nanofluid, W/mK)	Improvement in percentage
0.02	0.64130	42.29	0.26645	82.93
0.03	0.66160	49.72	0.27546	73.28
0.04	0.73028	25.93	0.28508	69.41
0.05	0.74301	16.54	0.29537	76.78

4 Conclusions

In this work, a new model for prediction of thermal conductivity has been proposed, considering the effect of interfacial layer formed around the nanoparticle. The results obtained were compared with Hamilton Crosser's model and the experimental data available. It has been found that the proposed model gives value of thermal conductivity of nanofluid more accurately than the Hamilton Crosser's model. As the effect of interfacial layer in case of nanofluid is significant; it is suggested that, it should also be taken into account for computing thermal conductivity of nanofluid.

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