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A model of thermal conductivity of nanofluids with interfacial shells

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Abstract

We derive an expression for the effective thermal conductivity of nanofluids with interfacial shells. Comparing with conventional models, the expression is not only depended on the thermal conductivity of the solid and liquid and their relative volume fraction, but also depended on the particle size and interfacial properties. The theoretical results on the effective thermal conductivity of CuO/water and CuO/ethylene glycol nanofluids are in good agreement with the experimental data.

Keywords: Thermal conductivity; Nanofluid; Interfacial model

1. Introduction

Traditional heat transfer fluids, including oil, water, and ethylene glycol (EG) mixture are poor heat transfer fluids. Because the thermal conductivity of these fluids plays an important role in the development of energy-efficient heat transfer equipment, numerous methods have been taken to improve the thermal conductivity of these fluids. As we know, crystalline solids have thermal conductivities that are typically larger than those of fluids by two to three orders of magnitude. Therefore, fluids containing suspended solid particles can reasonably be expected to display significantly enhanced thermal conductivities relative to those of pure fluids. Until now numerous theoretical and experimental studies of the effective thermal conductivity of liquids containing suspended solid particles have been conducted. However, with very few exceptions, previous studies of the thermal conductivity of suspensions have been confined to those containing millimeter- or micrometer-sized particles.

In fact, the conventional coarse-grained particles used in heat transfer fluids are easily to settle and to clog mini- and micro-channels. Besides, because coarse-grained particles are relatively large, and thus have significant mass, they can abrade the surface that they contact. This results in shortened life-times of such components as water pumps and bearings [1]. However, nanoparticles appear to be ideally suited for applications in which fluids flow through small passages, because the nanoparticles are stable and small enough not to clog flow passages. And, nanoparticles with small sizes and masses would impart little kinetic energy in collisions with the component surfaces and thus would be expected to produce little or no damage [1]. So, nanofluids containing nanoparticles have been studied recently [2–4].

Nanofluids containing nanoparticles exhibit enhanced thermal conductivity. For example, a maximum increase in thermal conductivity of approximately 22% was observed in a CuO/EG nanofluid containing 4 vol.% CuO nanoparticles with the average diameter of 23.6 nm [1]. A similar behavior was observed in alumina/EG and Cu/EG nanofluids [3]. In other words, all the above experimental data are much larger than the theoretical predictions according to the existing models for the effective conductivity of a solid/liquid suspension. The expressions of the conventional models of the effective thermal conductivity of a solid/liquid suspension are as follows:

- Maxwell [5]:

$$\frac{k_{\mathrm{eff}}}{k_{\mathrm{m}}} = 1 + \frac{3(\alpha - 1)v}{(\alpha + 2) - (\alpha - 1)v}$$

- Hamilton and Crosser [6]:

$$\frac{k_{\mathrm{eff}}}{k_{\mathrm{m}}} = \frac{\alpha + (n-1) - (n-1)(1-\alpha)v}{\alpha + (n-1) + (1-\alpha)v}$$

- Jeffery [7]:

$$\frac{k_{\mathrm{eff}}}{k_{\mathrm{m}}} = 1 + 3\beta v + \left(3\beta^2 + \frac{3\beta^2}{4} + \frac{9\beta^3}{16}\,\frac{\alpha + 2}{2\alpha + 3} + \cdots\right) v^2$$

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- Davis [8]:

$$\frac{k_{\text{eff}}}{k_{\text{m}}} = 1 + \frac{3(\alpha - 1)}{(\alpha + 2) - (\alpha - 1)v}[v + f(\alpha)v^2 + 0(v^3)]$$

- Lu and Lin [9]:

$$\frac{k_{\text{eff}}}{k_{\text{m}}} = 1 + \alpha v + \text{b}v^2$$

- Bonnecaze and Brady [10,11]: numerical simulation

where k_{eff} is the effective thermal conductivity of solid/liquid suspensions, k_{m} and k_2 are the thermal conductivity of the base fluid and particle, respectively, n and v are the particle shape factor and particle volume fraction, respectively, and $\alpha = k_2/k_{\text{m}}, \beta = (\alpha - 1)/(\alpha + 2)$.All the existing theoretical models and theories are only depended on the thermal conductivity of the solid and liquid and their relative volume fraction, not on the particle size and interface between the particles and fluid. However, a recent experimental study has shown that molecules of normal liquids close to a solid surface organize into layered structures much like a solid [12]. Furthermore, there is evidence that such an organized solid-like structure of a liquid at the surface is a governing factor in the heat conduction from a solid wall to an adjacent liquid [13]. Therefore, Choi et al. [4] postulate that this organized solid/liquid interfacial shell makes the transport of energy across the interface effective. So, without considering the interfacial effect between the nanoparticles and fluid, we cannot interpret the enhanced thermal conductivity of nanofluids.

In this paper, we derive an expression for the effective thermal conductivity of nanofluids with interfacial shells. Comparing with conventional models, the expression is not only depended on the thermal conductivity of the solid and liquid and their relative volume fraction, but also depended on the particle size and interfacial properties. The theoretical results on effective thermal conductivity of water/CuO and ethylene glycol/CuO nanofluids with interfacial shells are in good agreement with the experimental data.

2. Model of the effective thermal conductivity of nanofluids with interfacial shells

Because interfacial shells are existing between the nanoparticles and liquid matrix, we can regard both the interfacial shell and the nanoparticle as a "complex nanoparticle". So, the nanofluid system should be regarded as complex nanoparticles dispersed in the fluid. Based on this consideration, we build up a new model for calculating the effective thermal conductivity of nanofluids. We assume that k_{eff} is the effective thermal conductivity of the nanofluid, and k_{c} and k_{m} are the thermal conductivity of the complex nanoparticles and the fluid, respectively.

Now let us discuss the thermal conductivity of the complex nanoparticles firstly. We assume that a complex

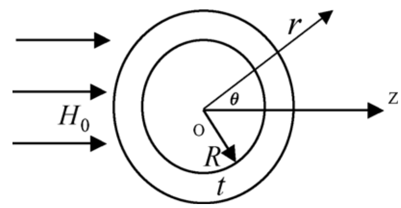

Fig. 1. The model of the complex nanoparticle.

nanoparticle is composed of a spherical nanoparticle of thermal conductivity k_1 with radii R and a spherical shell of thermal conductivity k_2 with a thickness t (as shown in Fig. 1).

Let the intensity $\vec{H}$ and heat flux q be respectively defined by

$$\vec{H} = -\nabla\phi \tag{1}$$

$$q = kH \tag{2}$$

where ϕ is the temperature distribution function and k is the thermal conductivity.

When applying the intensity, say H_0 on a nanofluid system along the z-axis (as shown in Fig. 1), we have the thermal conductivity equation and the boundary condition equations as follows:

$$\nabla^2\phi = \frac{\partial}{\partial r}\left(r^2\frac{\partial\phi}{\partial r}\right) + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\phi}{\partial\theta}\right) = 0 \tag{3}$$

$$\phi_1|_{r=0} = \text{constant}, \qquad \phi_3|_{r=\infty} = -H_0 r\cos\theta \tag{4}$$

$$\phi_1|_{r=R} = \phi_2|_{r=R}, \qquad \phi_2|_{r=R+t} = \phi_3|_{r=R+t} \tag{5}$$

$$k_1\left.\frac{\partial\phi_1}{\partial r}\right|_{r=R} = k_2\left.\frac{\partial\phi_2}{\partial r}\right|_{r=R}, \quad k_2\left.\frac{\partial\phi_2}{\partial r}\right|_{r=R+t} = k_3\left.\frac{\partial\phi_3}{\partial r}\right|_{r=R+t} \tag{6}$$

where ϕ_1, ϕ_2, and ϕ_3 are the temperature distribution function in the nanoparticle, interfacial shell, and outside the complex nanoparticle, respectively.

By the solution of the above equations, we get the temperature distribution functions

$$\phi_1 = -AH_0 r\cos\theta, \quad r < R \tag{7}$$

$$\phi_2 = -H_0(Br - Cr^{-2})\cos\theta, \quad R < r < R + t \tag{8}$$

where

$$A = \frac{9k_{\text{m}}k_2}{K}H_0 \tag{9}$$

$$B = \frac{3k_{\text{m}}(2k_2 + k_1)}{K}H_0 \tag{10}$$

$$C = \frac{3k_{\text{m}}(k_2 - k_1)r_0^3}{K}H_0 \tag{11}$$

$$K = (2k_{\text{m}} + k_2)(k_1 + 2k_2) - 2\alpha(k_2 - k_{\text{m}})(k_2 - k_1) \tag{12}$$

$$\alpha = \left(\frac{R}{R+t}\right)^3 \tag{13}$$

Substituting Eqs. (7) and (8) into Eq. (1), we can easily obtain the intensity ($\vec{H}_1$) the spherical nanoparticle and the intensity ($\vec{H}_2$) in the interfacial shell as follows:

$$\vec{H}_1 = A\vec{e}_z \tag{14}$$

$$\vec{H}_2 = B\vec{e}_z + \frac{C}{r^3}\vec{e}_z - \frac{3Cz}{r^4}\vec{e}_r \tag{15}$$

where $\vec{e}_z$ and $\vec{e}_r$ are the unit vectors along the axis and the vector radius, respectively. Due to $r > R$ approximately, we can have

$$\vec{H}_2 = B\vec{e}_z \tag{16}$$

We can introduce the effective thermal conductivity of the complex particle as follows:

$$\langle\vec{q}\rangle = k_c\langle\vec{H}\rangle \tag{17}$$

where $\langle\vec{q}\rangle$ and $\langle\vec{H}\rangle$ are the spatial average of the heat flux vector and the intensity respectively, i.e.,

$$\langle\vec{q}\rangle = \frac{1}{V}\int_v \vec{q}\,\mathrm{d}v \tag{18}$$

$$\langle\vec{H}\rangle = \frac{1}{V}\int_v \vec{H}\,\mathrm{d}v \tag{19}$$

Substituting Eqs. (14) and (15) into Eqs. (18) and (19) and, making use of the following relation

$$\langle\vec{q}_i\rangle = k_i\langle\vec{H}_i\rangle \quad (i = 1, 2) \tag{20}$$

we can obtain

$$\langle\vec{H}\rangle = [A\alpha + B(1-\alpha)]\vec{e}_z \tag{21}$$

$$\langle\vec{q}\rangle = [A\alpha k_1 + B(1-\alpha)k_2]\vec{e}_z \tag{22}$$

According to Eq. (17), we have the effective thermal conductivity of the complex particle

$$k_c = \frac{\langle\vec{q}\rangle}{\langle\vec{H}\rangle} = \frac{A\alpha k_1 + B(1-\alpha)k_2}{A\alpha + B(1-\alpha)} = k_2\frac{2k_2 + k_1 + 2\alpha(k_1 - k_2)}{2k_2 + k_1 - \alpha(k_1 - k_2)} \tag{23}$$

We turn now to discuss the thermal conductivity of the whole nanofluid. According to Bruggeman's effective media theory about two-phase composites consisting of spherical particles, we obtain an equation for the effective thermal conductivity of the nanoparticle-fluid system (nanofluid) [14]

$$\left(1 - \frac{v}{\alpha}\right)\frac{k_e - k_m}{2k_e + k_m} + \frac{v}{\alpha}\frac{k_e - k_c}{2k_e + k_c} = 0 \tag{24}$$

where v and v/α are the volume fraction of the nanoparticles and the complex nanoparticles, respectively. Substituting Eq. (23) into Eq. (24), we get an expression of the thermal conductivity of nanofluids with interfacial shells,

$$\left(1 - \frac{v}{\alpha}\right)\frac{k_e - k_m}{2k_e + k_m} + \frac{v}{\alpha}\frac{(k_e - k_2)(2k_2 + k_1) - \alpha(k_1 - k_2)(2k_2 + k_e)}{(2k_e + k_2)(2k_2 + k_1) + 2\alpha(k_1 - k_2)(k_2 - k_e)} = 0 \tag{25}$$

The above expression is not only depended on the thermal conductivity of the solid and liquid and their relative volume fraction, but also depended on the particle size and interfacial properties. In other words, it can interpret the size dependence of the thermal conductivity of nanofluids.

3. Application

Now we apply the novel model to analyze the size dependence of the thermal conductivity of Al_2O_3/water nanofluids. Based on Ref. [12], the thickness of the interfacial shell between the particles and fluid is several nm. We select $t = 3$ nm here. The thermal conductivities of Al_2O_3/water nanofluids with different-sized Al_2O_3 nanoparticles are shown in Fig. 2. We find that the thermal conductivity of the Al_2O_3/water nanofluid increases rapidly with decreasing nanoparticle size, in accord agree with the experimental phenomena [12]. In the calculation, the thermal conductivity of Al_2O_3 nanoparticles and water are taken as 46 and 0.604 $\mathrm{W\,m^{-1}\,K^{-1}}$, respectively [3], and that of the interfacial shell is estimated as 5 $\mathrm{W\,m^{-1}\,K^{-1}}$.

Furthermore, we compare the model with the experimental data of CuO/EG and CuO/water nanofluids. We find that the theoretical results given by the novel model are in good agreement with the experimental data. It is somewhat nonlinear with the nanoparticles' volume fraction, whereas those theoretical results given by the existing models are smaller than the experimental data and linear with the nanoparticles' volume fraction (shown in Figs. 3 and 4). In the calculation, the thermal conductivity of CuO nanoparticles, EG and

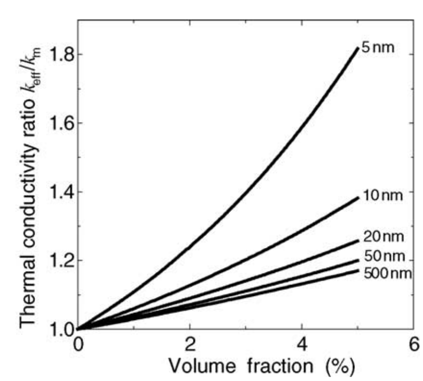

Fig. 2. The relation between the Al_2O_3 volume fraction and effective thermal conductivity of Al_2O_3/water nanofluids with different-sized Al_2O_3 nanoparticles.

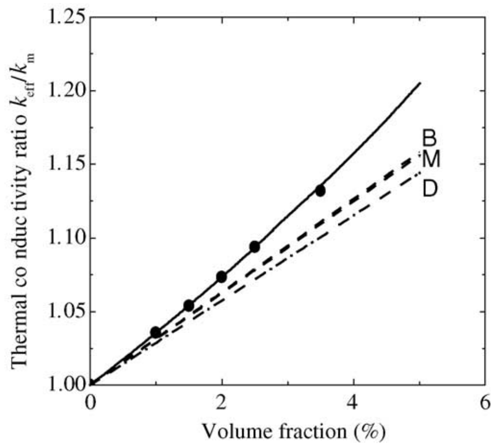

Fig. 3. Comparison between the measured data for a CuO/water nanofluid (solid circles) and those predicted by the novel model (solid line) and existing models. Because all calculated values given by the conventional model are almost identical at low volume fractions, some of the calculated values are shown as dashed lines: B = Bonnecaze and Brady; M = Maxwell; D = Davis.

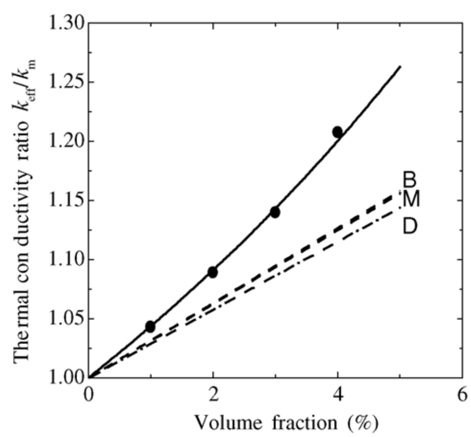

Fig. 4. Comparison between the measured data for a CuO/water nanofluid (solid circles) and those predicted by the novel model (solid line) and existing models. Because all calculated values given by the conventional model are almost identical at low volume fractions, some of the calculated values are shown as dashed lines: B = Bonnecaze and Brady; M = Maxwell; D = Davis.

water are taken as 69, 0.258 and 0.604 $W\,m^{-1}\,K^{-1}$, respectively [3], and those of the interfacial shells in CuO/EG and CuO/water nanofluids are fitted as 10 and 1.2 $W\,m^{-1}\,K^{-1}$, respectively.

4. Conclusions

In summary, we derive an expression for the effective thermal conductivity of nanofluids with interfacial shells. Comparing with conventional models, the new expression is not only depended on the thermal conductivity of the solid and liquid and their relative volume fraction, but also depended on the particle size and interfacial properties. Using the model, we can easily understand the mechanism of the particle size dependence of the thermal conductivity of nanofluids. The theoretical results on the effective thermal conductivity of CuO/water and CuO/EG nanofluids with interfacial shells are in good agreement with the experimental data.

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