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Modeling Effective Thermal Conductivity of Al_2O_3 Nanoparticles in Water and Ethylene Glycol Based on Shape Factor

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***Abstract*—In this study, a new model of predicting effective thermal conductivity for Al_2O_3 nanoparticles dispersed in ethylene glycol (EG) and water regarding the shape factor and volume fraction of nanoparticles, is developed. It has been proved that considering Al_2O_3 particles as spherical molecules is not acceptable assumption. Starting from Brailsford and Major general equation for multi-component materials, an equation has been derived that is based on shape factor of nanoparticle. Also, the according to morphology of Al_2O_3, a new shape factor for these nanoparticles witch is more realistic, is given which TEM images confirm this. Finally, theoretical results have been compared with experimental data. It is shown that shape factor value applied for Al_2O_3 / Water system cannot be used for Al_2O_3 / EG system and EG molecules cover Al_2O_3 nanoparticles differently that must be considered in equations.**

***Index Terms*—Shape factor, Effective Thermal Conductivity, Al_2O_3 nanoparticle, suspensions.**

I. Introduction

Nanofluids are dilute liquid suspensions of nanoparticles with dimensions smaller than 100nm.

It has been more than 100 years that the thermal conductivity enhancement of conventional fluids by the suspension of solid particles, in size of millimeter and micrometer, has been well known [1].

Much attention has been paid in the past decade to this new type of fluids due to their enhanced properties and behavior associated with heat transfer. The enhanced thermal behavior of nanofluids could provide a basis for an enormous innovation for heat transfer intensification, which is of major importance to a number of industrial sectors including transportation, power generation, micro-manufacturing, thermal therapy for cancer treatment, chemical and metallurgical sectors, as well as heating, cooling, ventilation and air-conditioning [2].

It has been demonstrated that nanofluids consisting of CuO or Al2O3 nanoparticles in water or ethylene glycol exhibit enhanced thermal conductivity [3]. For 4 vol% CuO nanoparticles with average diameter 35 nm dispersed in ethylene glycol, approximately 20% enhancement in thermal conductivity was observed and similar behavior has been reported for Al2O3/ethylene glycol nanofluid [4]. Furthermore, the effective thermal conductivity has shown to be increased by up to 40% for the nanofluid consisting of ethylene glycol containing approximately 0.3 vol% Cu nanoparticles of mean diameter < 10 nm [5].

Lee et al. formulated water based nanofuids containing Al2O3 nanoparticles without any chemical dispersants and performed experiments to show that the Al2O3–water nanofuids they formulated have good suspension and dispersion characteristics and high thermal conductivities at the concentrations from 1 to 5 vol. % [1]. This work started new experimental investigations [4, 6, 7] for the effective thermal conductivity of Al2O3 nanoparticles suspended in water or ethylene glycol. In addition, Patel et al. showed that the enhancement of the effective thermal conductivity of toluene-based nanofluids containing Au is significant (by as much as 14%) at very low concentration of Au nanoparticles in the 0.005– 0.011 vol. % range [8].

Q. Xue, considered an interfacial shell between the nanoparticles and liquid matrix and regarded both the interfacial shell and the nanoparticle as a complex nanoparticle [9].

In order to predict thermal conductivity of fluids with suspension particles have been introduced. Most of these models are based on Maxwell [10] pioneer works. Later, Hamilton and Crosser [11], Jeffery [12], Davis [13], Lu and Lin [14], Bonnecaze and Brady [15] presented new models to describe thermal conductivity behavior of solid/liquid systems.

Table 1 presents conventional models of effective thermal conductivity of suspensions. Where k_{eff} is the effective thermal conductivity of the suspension, n is a shape factor of nanoparticle, v is nanoparticle volume fraction. k_m and k_c are the thermal conductivity of the suspending medium and solid particle, respectively. Also, α and β are empirical fitting parameters which are defined as (k_c/k_m) and $(\alpha-1)$ / $(\alpha+2)$, respectively.

In this article, using experimental data provided by Lee et al [3] and H.Q. Xie [4], it has been shown that shape factor value can be affected by based fluid molecules. Also, new correlation for predicting thermal conductivity of Al_2O_3/ Water and Al_2O_3/ EG systems has been introduced.

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TABLE 1 CONVENTIONAL MODELS FOR EFFECTIVE THERMAL CONDUCTIVITY ESTIMATION OF NANOFLUIDS

Model	Mathematical Expression	Comments
Maxwell [10]	$\frac{k_{eff}}{k_m} = 1 + \frac{3(\alpha-1)v}{(\alpha+2)-(\alpha-1)v}$	Developed for spherical nanoparticles
Hamilton-Crosser [11]	$\frac{k_{eff}}{k_m} = \frac{\alpha+(n-1)-(n-1)(1-\alpha)v}{\alpha+(n-1)-(1-\alpha)v}$	For cylindrical particles n=6 and spherical particles n=3
Jeffery [12]	$\frac{k_{eff}}{k_m} = 1 + 3\beta + \left(3\beta^2 + \frac{3\beta^2}{4} + \frac{9\beta^2(\alpha+2)}{16(2\alpha+3)} + \cdots\right)v^2$	Includes pair interaction of spherical particles
Davis [13]	$\frac{k_{eff}}{k_m} = 1 + \frac{3(\alpha-1)}{(\alpha+2)-(\alpha-1)v}[v + f(\alpha)v^2 + O(v^3)]$	High-order terms represent pair interaction of dispersed spheres
Xue [4]	$\frac{k_{eff}}{k_m} = \frac{1-f+2f\frac{k_c}{k_c-k_m}\ln\frac{k_c+k_m}{2k_m}}{1-f+2f\frac{k_c}{k_c-k_m}\ln\frac{k_c+k_m}{2k_m}}$	CNTs-based composites based on Maxwell theory

II. EXPERIMENTAL DATA

In this study, experimental data presented by Lee et al [3] for Al_2O_3/EG system and H.Q. Xie [4] for Al_2O_3/Water system has been used. To measure the thermal conductivity of nanofluids transient hot-wire method has been employed. The fundamental principle of the transient hot-wire technique is based on the calculation of the transient temperature field around a thin wire, this thin wire generates heat and can be treated as a line source. A constant current is supplied to the wire to generate needed temperature rise. The wire is put in nanofluid, whose thermal conductivity is to be measured. The wire treats as both the heat source and the temperature sensor. The heat dissipated in the wire increases the temperature of the wire and also that of the sample. The temperature rise in the wire depends on the thermal conductivity of the sample through which the wire is inserted [3,4].

In the calculations, the thermal conductivity of Al_2O_3 nanoparticle is taken as 76.5 W/mK, and that of water and EG as 0.604 and 0.258 W/mK, respectively [3,4].

III. THEORETICAL DISCUSSION

A. Al_2O_3/Water

1) Nanoparticle morphology

Corundum is the most common form of crystalline alumina. AL^{3+} in center, is octahedral and oxygen ions form a hexagonal close-packed. Form crystallography aspect, corundum adopts a trigonal Bravais lattice with a space group of R-3c. Figure 1 illustrates Al_2O_3 molecular structure [16].

Figure 2 shows Al_2O_3 nanoparticle TEM image provided by J.H. Lee et al [17]. As it can be seen, assuming Al_2O_3 as a ball, as some models are based on [18,19, 20], is not accurate assumption.

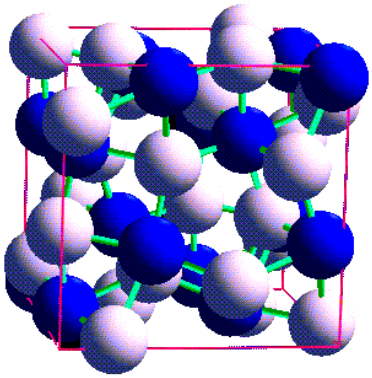

Fig 1. Molecule geometric structure of Al_2O_3 [16]

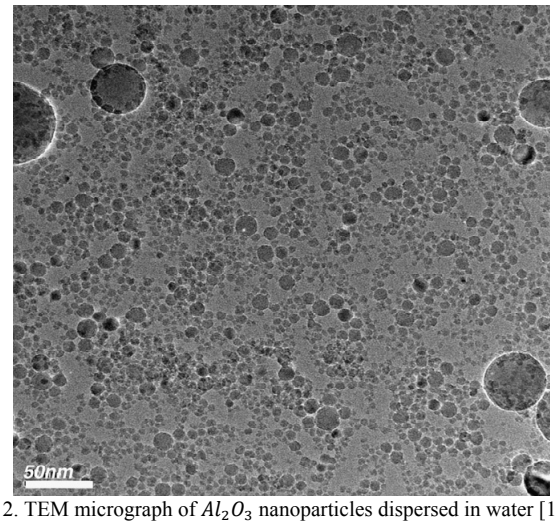

Fig 2. TEM micrograph of Al_2O_3 nanoparticles dispersed in water [16].

According to TEM image presented in figure 2 and also other images provided by Premkumar and Geckeler [21], Al_2O_3 nanoparticles are not complete spherical particles. Therefore, using n_i=3 for Al_2O_3 cannot be acceptable. In fact, their shape is a little far from sphere.

Xue expressed that in the nano-size particles, 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 [9]. So, the nanofluid system should be regarded as complex nanoparticles dispersed in the fluid Therefore the fact that particles are spherical or not should be regarded.

B. Model Development

To have a better understanding of nanofluid behavior, considering nanoparticle structure is essential. It is believed that a liquid film covers the nanoparticle so that this phenomenon changes the surface shape of the particle and consequently, the shape factor will change. Another factor in this modeling is that either liquid phase is continuous or nanoparticles.

In this work, since volume fraction of nanoparticles is low, it is assumed that base liquid is continuous phase and nanoparticles have been dispersed randomly in it.

The effective thermal conductivity for the nanofluid (K_e) is considered to be a function of thermal conductivities of the base fluid (k_2), solid particle (k_1), shape factor (n_i), and volume fraction of the particle (v):

$$K_e = f(k_1, k_2, n_i, v) \quad (1)$$

Brailsford and Major [22] presented general equation for multi-component materials (Eq. (2));

$$K_e = \frac{\sum_{i=1}^{m} k_i v_i \frac{n_i \tilde{k}}{(n_i - 1)\tilde{k} + k_i}}{\sum_{i=1}^{m} v_i \frac{d_i \tilde{k}}{(n_i - 1)\tilde{k} + k_i}} \quad (2)$$

d_i is shape factor and $\tilde{k}$ indicates that which phase is considered as continuous phase.

By selecting suitable data for n and $\tilde{k}$, a novel correlation for Al_2O_3/water system was investigated. If the empirical shape factor which illustrates non-spherical matter of nanoparticles is assumed to be around 4.1 (by try and error method this value gives the best correlation for the thermal conductivity) then, resulted equation will predict thermal conductivity of system more accurate. This value theoretically confirms non-spherical matter of nanoparticles, however it is in contrast by some other researches [16,21]. Since water was as a continuous phase in this research so, $\tilde{k} = k_1$ were defined for water. Equation (3) was specialized for the applicable current systems as following:

$$K = \frac{\frac{4.1k1k2v}{3.1k2 + k1} + k2(1 - v)}{v\left(\frac{4.1k2}{3.1k2 + k1} - 1\right) + 1} \quad (3)$$

In this equation, v, k_1 and k_2 are volume fraction of nano particles, thermal conductivity of nano particles and water, respectively.

C. Al_2O_3/Ethylene Glycol

At first, above model has been used for predicting thermal behavior of Al_2O_3 / Water system but the results were not acceptable enough. The same method employed for resulting the model of thermal conductivity for Al_2O_3 / Water system, has been used to find suitable shape factor for new system. d=3.5 was found to be the best shape factor consideration. Therefore, the equation Al_2O_3 /Ethylene Glycol system changes as follow:

$$K_e = \frac{\frac{3.5k1k2v}{2.5k2 + k1} + k2(1 - v)}{v\left(\frac{3.5k2}{2.5k2 + k1} - 1\right) + 1} \quad (4)$$

IV. Results And Discussions

Both models show linear dependence of thermal conductivity on Al_2O_3 volume fraction. Figure 3 shows the prediction of five models including presented model for Al_2O_3 / Water system. As illustrated, the model especially in lower concentrations has good enough agreement with empirical data.

As expected, the enormous enhancement in the thermal conductivity of nanofluids in low concentration for mention system has been observed.

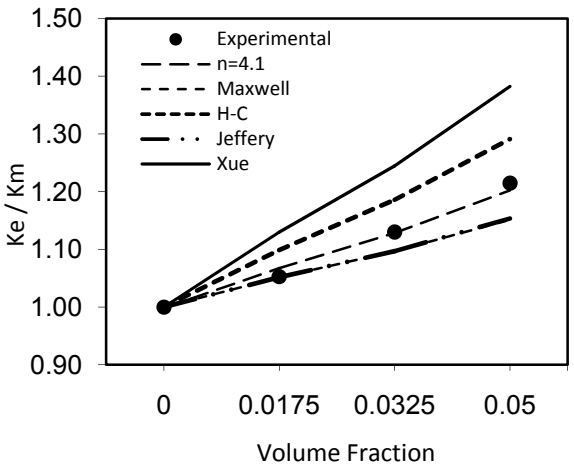

Fig.3 Prediction of four models including presented model for Al_2O_3 / Water system

Table 2 illustrates the deviation of each model from experimental data. As shown in the table, presented model with n=4.1 Al_2O_3/Water system has less deviation among all models.

TABLE 2 Each models deviation from experimental data.

Model	RD %
Presented Model (n=4.1)	0.6830
Maxwell	2.0860
Hamilton-Crosser	3.8917
Jeffrey	2.0290
Xue	7.8085

An interesting phenomenon observed was that the model could not predict thermal conductivity of Al_2O_3 nanoparticle dispersed in different base fluid. It seems that considering based fluid molecular in determination of shape factor value is necessary. So, idea of covering nanoparticles by molecules of based fluid and therefore considering them as a complex comes true. Therefore the amount of shape factor is depended on based fluid and from based fluid to other it varies. This can be explain by different molecular structure of EG and water. When nanoparticles are covered by either of these fluids, its shape factor changes but it seems that EG molecules do not cover Al_2O_3 nanoparticle as water molecules do. Figure 4 shows the prediction of five models including presented model for Al_2O_3 / EG system

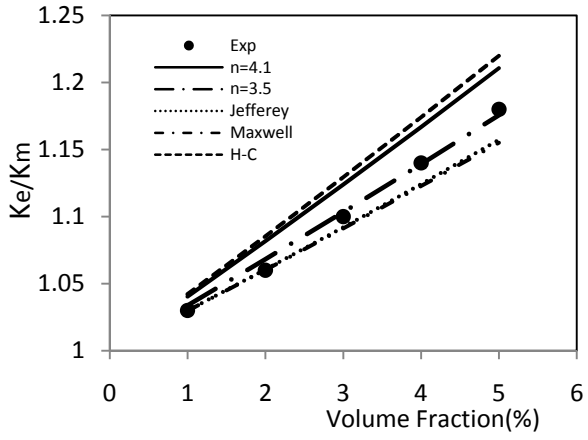

Fig.4 Prediction of five models including presented model for Al_2O_3 / EG system

As it can be seen from figure, presented model with n=3.5, has better agreement with experimental data than any other model of this system of suspension.

Table 3 illustrates the deviation of each model from experimental data. As it can be seen from the table, the model considering shape factor equals to 3.5 has less deviation in comparison of one with one with n=4.1.

TABLE 3 EACH MODELS DEVIATION FROM EXPERIMENTAL DATA.

Model	RD %
Presented Model (n=3.5)	1.007
Presented Model (n=4.1)	2.037
Maxwell	1.080
Hamilton-Crosser	3.451
Jeffrey	2.774

V. CONCLUSION

In this article, regarding Brailsford and Major general equation for multi-component materials, a new equation for predicting effective thermal conductivity for Al_2O_3 nanoparticles dispersed in ethylene glycol (EG) and water based on shape factor and volume fraction of nanoparticles, is developed. It has been proved that assuming Al_2O_3 particles as spherical molecules is not acceptable. Also, according to morphology of Al_2O_3, a new shape factor for these nanoparticles witch is more realistic, is given. Finally, theoretical results have been compared with experimental data and it is shown that shape factor value applied for Al_2O_3 / Water system cannot be used for Al_2O_3/ EG system. Therefore, EG molecules cover Al_2O_3 nanoparticles differently and base fluids molecular structure must be considered in nanoparticle shape factor.

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