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A Proposed Model for Calculating Effective Thermal Conductivity of Nanofluids, Effect of Nanolayer and Non-Uniform Size of Nanoparticles

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ABSTRACT.

Nanofluids, containing nanometric metallic or oxide particles, exhibit extraordinarily high thermal conductivity that can be used for enhancing heat transfer performance of conventional systems. This work presents a proposed method for calculating the effective thermal conductivity of nanofluids. The thermal conductivity of nanofluids primarily depends on the properties of base fluids and nanoparticles, the volume fraction of nanoparticles, the interfacial layer, non-uniform sizes of nanoparticles, fractal dimension of particles, Brownian motion and temperature. In the resent study, the impact of non-uniform sizes of nanoparticles and interfacial layer is investigated simultaneously. Hence, this model has the capability of offering both analytical and numerical Predictions. Results of the present model show reasonably good and better agreements with available experimental data.

KEYWORDS: Nanofluid, Nanoparticle, Effective thermal conductivity, non-uniform size, Interfacial layer, Fractal dimension.

1. INTRODUCTION

Nanofluids, a term first proposed by Choi, are produced by dispersing nanoparticles in conventional fluids such as water, ethylene glycol, oil and etc. [1].

Classical models such as Maxwell [2], Hamilton–Crosser [3] and Bruggeman (Hui et al. [4]) were developed for predicting the effective thermal conductivity of a continuum medium with well-dispersed solid particles, but they were found to be unable to predict the anomalously high thermal conductivity of nanofluids. Hence, many studies try to suggest accepted models for the effective thermal conductivity of nanofluids.

Keblinski [5] proposed that the size effect, the clustering of nanoparticles, the surface adsorption and the Brownian motion are four main explanations for an anomalous increase of thermal conductivity. Yu and Choi [6, 7], Xue [8], Xie [9] modified classical models to include the effect of interfacial layer. By considering the existence of interfacial layer at the solid particle/liquid interface, Leong [10] and Murshed [11] developed new theoretical models. Murshed's model [11] takes into account most of possible parameters such as particle size, nanolayer, particle movements, interactions and surface chemistry of nanoparticles. They show that the major reasons for the enhanced thermal conductivity of nanofluids result from static parameters.

Most recent studies are done by consideration of uniform distribution of nanoparticles size. While, in fact, nanoparticles dispersed in nanofluids have different sizes and some of them may form clusters. Effect of clustering of nanoparticles on the effective thermal conductivity of nanofluids is investigated by Hong [12]. Based on the fractal theory, Wang [13] modified the Maxwell model and found that the size distribution of nanoparticles and clusters follow the fractal law. Based on the fractal distribution, Xu [14] proposed a model for the effective thermal conductivity of nanofluids. Recently, Feng [15] suggested a new model that takes into account the effect of convection caused by the Brownian motion and the fractal distribution of nanoparticle sizes. More recently, Tun-Ping Teng [16] investigated the effect of particle size, temperature, and volume fraction and proposed an empirical equation for the effective thermal conductivity of nanofluids.

Despite the great effect of interfacial layer and non-uniform size distribution of nanoparticles, no model is simultaneously considered these effects. In this paper, a new and improved model for the effective thermal conductivity of nanofluids is established considering the effective parameters such as non-uniform nanoparticle size distribution and existence of interfacial layer. However, modeling the effective thermal conductivity of nanofluids is separated to two parts: first considering the static and dynamic parameters a new model for calculating the effective thermal conductivity of nanofluids is proposed. Then based on the fractal nature of nanoparticle size distributions, the probability model for nanoparticle size distribution is derived. The predictions of the present model are then compared with the available experimental data.

2. Modeling effective thermal conductivity of nanofluids

In particle-fluid mixtures, the liquid molecules close to a particle surface are known to form layered structures. The thickness of nanolayer is at magnitude of nanometer. Here, both the interfacial shell and the

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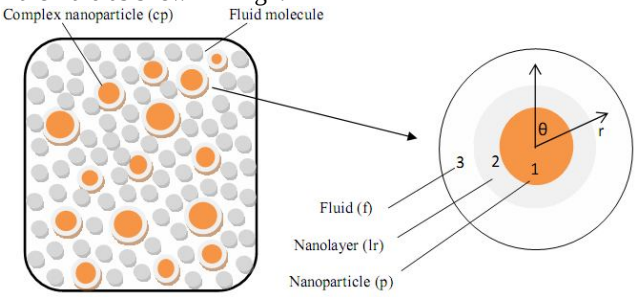
nanoparticle is considered as a "complex nanoparticle", so the nanofluid system is regarded as complex nanoparticles dispersed in the fluid as shown in Fig1.



(a) (b)

Fig1. : (a) A schematic scheme of nanoparticles suspended in base fluid (b) A Single spherical particle with interfacial layer.

In addition, particles in nanofluids may have different sizes and this matter can influence the effective thermal conductivity of nanofluids. So, in this paper, nanoparticles are regarded to have different diameters. Based on these assumptions, a new model for calculating the effective thermal conductivity of nanofluids is presented.

2.1. Modeling static part of effective thermal conductivity

To Modeling the static part of effective thermal conductivity, the heat conduction equation should be solved. Leong [10] solved the two-dimensional steady-state heat conduction equation in spherical coordinates and obtained temperature gradients for each region (spherical nanoparticle (p), nanolayer (lr) and base fluid (f)) along the z-axis as follows:

$$\frac{dT_p}{dz} = \frac{3k_{lr}}{k_p + 2k_{lr}} T_\infty \tag{1}$$

$$\frac{dT_{lr}}{dz} = \left(1 + \frac{1}{\gamma_1^{\,3}} \frac{k_{lr} - k_p}{k_p + 2k_{lr}}\right) T_\infty \tag{2}$$

$$\frac{dT_f}{dz} = T_\infty \tag{3}$$

where $\gamma = 1 + \frac{t}{r_p}$, $\gamma_1 = 1 + \frac{t}{2r_p}$. By utilize the definition of spatial average the effective static thermal conductivity express as follows:

$$k_{st} = -\frac{q_z}{\nabla T_z} = -\frac{\int_V q_z dv}{\int_V \nabla T_z dv} = \frac{\sum_{p,lr,f} (k_{z,i} \frac{dT_{z,i}}{dz} v_i)}{\sum_{p,lr,f} (\frac{dT_{z,i}}{dz} v_i)} \tag{4}$$

Substituting Eq. (1-3) into Eq. (5), considering the total number of nanoparticles which dispersed in fluid is N_t and using $v_{lr,i} = v_{p,i}(\gamma^3 - 1)$, k_{st} is obtain as;

$$k_{st} = \frac{k_{lr} \sum_{i=1}^{N_t} \frac{V_{p,i}}{\gamma_{1,i}^3} \left[(k_p + 2k_{lr}) \gamma_{1,i}^3 \gamma_i^3 + (k_p - k_{lr})(2\gamma_{1,i}^3 - \gamma_i^3 + 1) \right] + v_f k_f (k_p + 2k_{lr})}{\sum_{i=1}^{N_t} \frac{V_{p,i}}{\gamma_{1,i}^3} \left[(k_p + 2k_{lr}) \gamma_{1,i}^3 \gamma_i^3 - (k_p - k_{lr})(\gamma_{1,i}^3 + \gamma_i^3 - 1) \right] + v_f (k_p + 2k_{lr})} \tag{5}$$

Volume fraction of fluid can be expressed as, $\phi_f = 1 - \gamma^3 \phi_p$ and from the definition of volume fraction we know that $\phi_{p,lr,f} = \frac{V_{p,lr,f}}{V_{total}}$, where $V_p = \sum_{i=1}^{N_t} v_{p,i}$. So we have

$$v_f = (1 - \gamma^3 \phi_p) \frac{V_p}{\phi_p} \tag{6}$$

There are no available correlations for calculating the thermal conductivity of nanolayer. The interfacial layer would be expected to have an intermediate thermal conductivity between the bulk liquid and the nanoparticle. By use of empirical factor ($\omega > 1$), thermal conductivity of nanolayer is defined as $k_{lr} = \omega k_f$. It is demonstrated that the thickness of the interfacial shell between the particles and fluid is several nm [13]. In this study, an interfacial layer thickness of 1 nm is used to predict the thermal conductivity of nanofluids.

2.2. Modeling dynamic part of effective thermal conductivity

For two particles in the same size, the net axial heat flux due to the movement of particles can be written as

$$q_{net-dy,l}'' \approx -\frac{1}{2}\rho_{cp} c_{p-cp} d_s U_B \nabla T \tag{7}$$

where ρ_{cp} and c_{p-cp} are density and specific heat of complex nanoparticles, respectively, d_s is the distance between two particles and U_B is the Brownian particle motion. Thus, the total net axial heat flux due to movement of all particles in a nanofluid can be obtained by use of the weighted average method,

$$q_{net-dy,total}'' \approx \sum_{l=1}^{m}\left(-\frac{1}{2}\rho_{cp} c_{p-cp} d_s U_B \nabla T\right)\frac{n_{p,l}}{N_t} \tag{8}$$

where m is the number of particle group which have the same size, $n_{p,l}$ is the number of particle in the l^{th} group and N_t is the total number of particle.

Based on the effective diffusion coefficient, the modified Brownian motion can be expressed as,

$$U_B = \sqrt{\frac{2K_B\left(1-1.5\phi_{cp}\right)}{m}} \tag{9}$$

where K_B is the Boltzmann's constant and equal to 1.38×10^{-23} and m is the mass of complex nanoparticles. Substituting Eq. (9) into Eq. (8) and knowing that $q_{net-dy,total} = k_{dy}\nabla T$,

$$k_{dy} = \sum_{l=1}^{m}\left(-\frac{1}{2}\rho_{cp} c_{p-cp} d_s \sqrt{\frac{2K_B\left(1-1.5\phi_{cp}\right)}{m}}\right)\frac{n_{p,l}}{N_t} \tag{10}$$

By using of $r_{cp} = \gamma r_p, \phi_{cp} = \phi_p \gamma^3$ and knowing that $d_s = 0.893 r_{cp}\phi_{cp}^{-1/3}$,

$$k_{dy} = \sum_{l=1}^{m}\left(-\frac{1}{2}\rho_{cp} c_{p-cp} d_s \sqrt{\frac{3K_B\left(1-1.5\gamma^3\phi_p\right)}{2\pi\rho_{cp}\gamma^3 r_p^{\,3}}}\right)\frac{n_{p,l}}{N_t} \tag{11}$$

Now we can combine both static and dynamic part and obtain a new expression for the thermal conductivity of nanofluids as below

$$k_{nf} = k_{st} + k_{dy} \tag{12}$$

Finally we can find the effective thermal conductivity of nanofluids by definition as $k_{eff} = k_{nf} / k_f$.

2.3. Fractal proposed model

As Wang [13] proposed, we consider that the size distribution of nanoparticles obeys the fractal theory. The fractal dimension (D_f) is given by [18],

$$D_f = 2 - \frac{\ln\ln\phi_p}{\ln\ln\left(\frac{d_{min}}{d_{max}}\right)} \tag{13}$$

Where d_{min} and d_{max} are the minimum and maximum diameters of nanoparticles. The diameter of i^{th} nanoparticle which chosen randomly can be expressed as

$$d_i = \frac{d_{min}}{1-R_i^{1/D_f}} = \left(\frac{d_{min}}{d_{max}}\right)\frac{d_{max}}{1-R_i^{\frac{1}{D_f}}} \tag{14}$$

where R point out the set of random numbers of $0\sim1$ produced by computer, $d_{min} \le d_i \le d_{max}$, and N_t is the number of nanoparticles. The iteration process is terminated until the specified stopping criterion is satisfied, as the following expression,

$$\bar{d} = \frac{1}{N_t}\sum_{i=1}^{N_t} d_i \ge d_{av} \tag{15}$$

where $\bar{d}$ is the average of produced diameters and d_{av} is obtained from Eq. (12). The algorithm repeats for several runs (N) and the averaged effective thermal conductivity is obtained as,

$$\overline{k_{eff}} = \frac{1}{N}\sum_{i=1}^{N} k_{eff}^{(n)} \tag{16}$$

3. RESULT AND DISSCUSSION

The proportion of static and dynamic parameters is presented in Table 1. Results show that static mechanisms have the main contribution on the effective thermal conductivity of nanofluids. On the other hand, Table 1 demonstrates that static contribution increases with increasing volume fraction while a dynamic contribution decreases.

Table 1: proportion of static and dynamic parameters to k_{eff} predicted by proposed model

Material	ϕ_p	k_{eff}	$k_{st}(\%)$	$k_{dy}(\%)$
$Al_2O_3(13nm)/water$	0.01	1.051	99.97	0.0297
$CuO(35nm)/EG$	0.02	1.0914	99.94	0.0057

In Fig. 3, Result of proposed model for the effective thermal conductivity of nanofluid Al_2O_3/EG with $d_{av} = 15nm$ and volume fraction v in 150 runs, is demonstrated. Whereas the nanoparticles size is produced randomly, amount of effective thermal conductivity oscillates about experiment value. No matter how the diameter is chosen (randomly), the average thermal conductivity can be calculated as 1.0332.

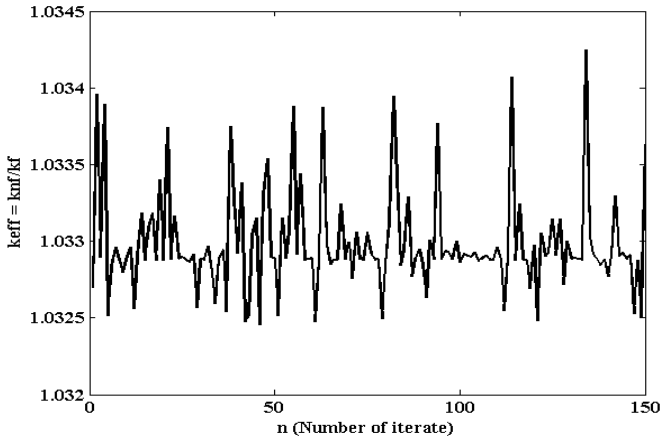


Figure 3: The effective thermal conductivity in 150 runs at $\phi_p = 0.01$ for $Al_2O_3(15nm)/EG$

Figs. 4-8 demonstrate that the present model shows reasonably good agreement with the experimental results. Fig. 4 indicates that the predicted thermal conductivities of nanofluids for $Al_2O_3(13nm)/Water$ are well in accord with the experimental measurements which are completely under-predicted by Maxwell's model. It can be seen that the present model has better predictions than other models such as Feng's model [15] and Murshed's model [11]. Since Murshed's model is developed by considering uniform size distribution. Figs. 4-6 depict that the predicted thermal conductivities of nanofluids after the fractal size distribution is considered are well in accord with the experimental measurements. Hence, if more accurate prediction is desirable, the nonuniform size effect should be considered. On the other hand, Feng's model does not consider the effect of interfacial layer which plays the significant role in suspensions containing nanoparticle.

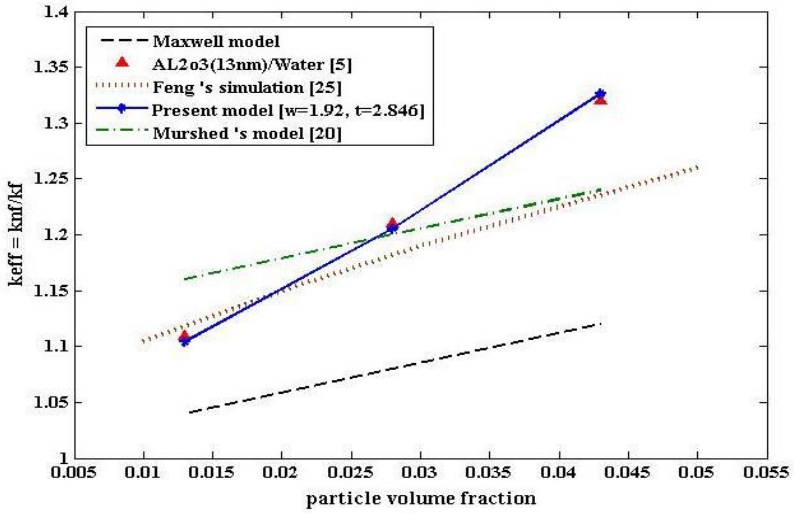


Figure 4: Comparison of present model's predictions with experimental data of Masuda [20] and predictions of other models for $Al_2O_3(13nm)/Water$ nanofluid

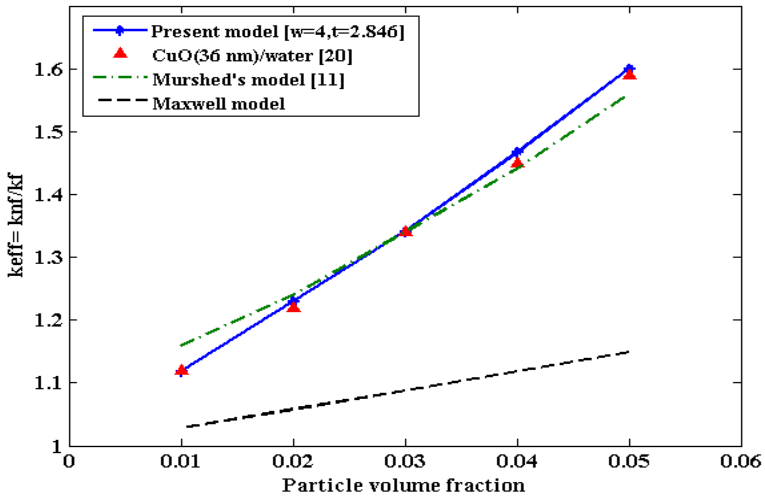


Figure 5: Comparison of present model's prediction with experimental data of Eastman [21] and predictions of other models for $CuO(36nm)/Water$ nanofluid

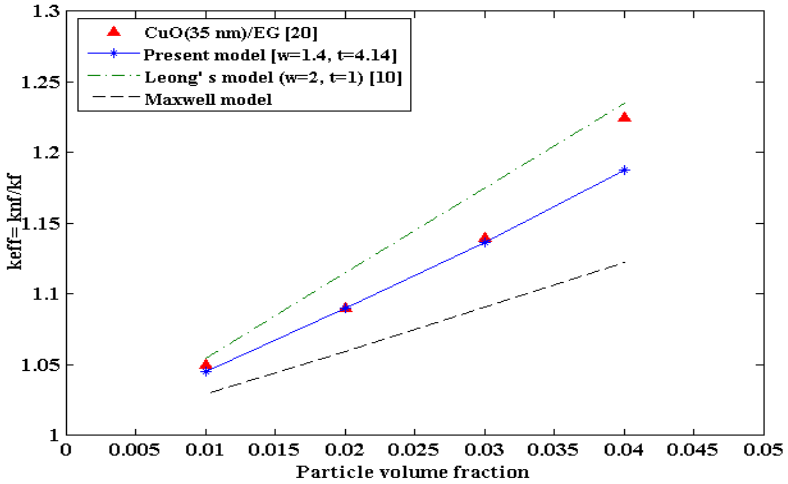


Figure 6: Comparison of present model's prediction with experimental data of Eastman [22] and predictions of other models for $CuO(35nm)/EG$ nanofluid

Figs. 5, 6 show better agreement between the predicted results of the present model and experimental data for $CuO(36nm)/Water$ and $CuO(35nm)/EG$ nanofluids, respectively. The figures also show that the effective thermal conductivity increases with increasing volume fraction. Like other types of nanofluids, Maxwell's model under-predicts the thermal conductivity of these nanofluids.

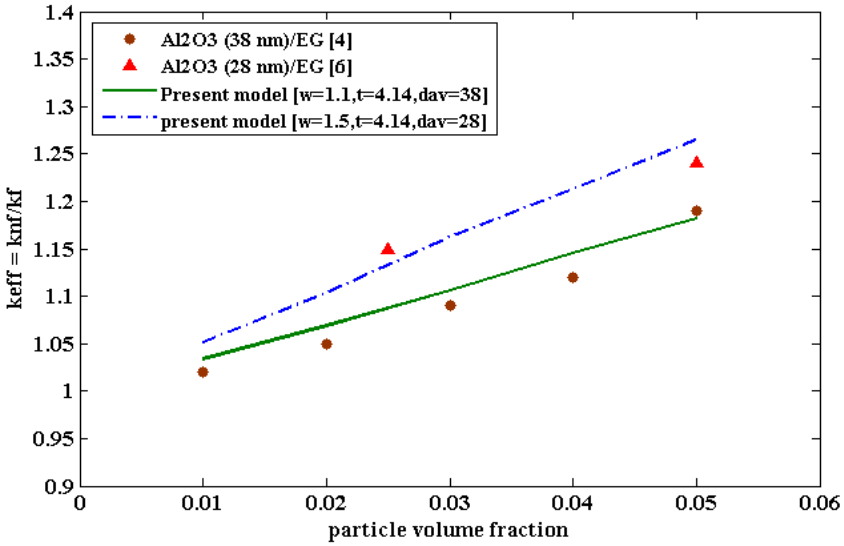


Figure 7: Comparison of predicted effective thermal conductivity with experimental data of Lee [22] and Wang [22] for $Al_2O_3(28,38nm)/EG$ nanofluids.

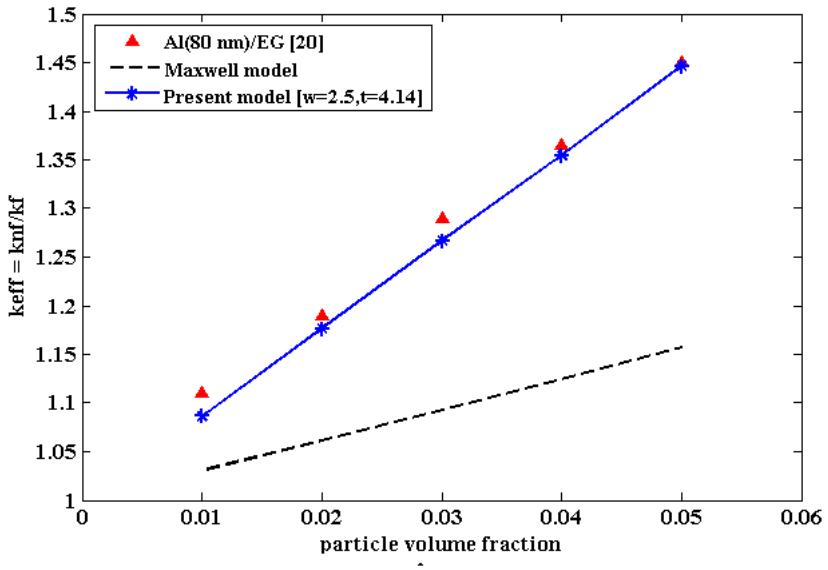


Figure 8: Comparison of present model's prediction with experimental data of Eastman [21] and predictions of other models for $Al(80nm)/EG$ nanofluid

Fig. 7 demonstrates the effect of particle sizes on the thermal conductivity for Al_2O_3/EG suspensions. It can be found that the effective thermal conductivity of nanofluid decreases with increasing nanoparticles sizes. Result of the present model for $Al(80nm)/EG$ nanofluid is demonstrated in Fig.8.

Table 2: Comparison of present model's prediction with experimental data [25]

Nanofluid	Volume fraction (%)	Predicted enhancement of thermal conductivity by present model	Observed enhancement of thermal conductivity	Error
Al_2O_3(28nm) / Water	3	12.50	12	2.02
Al_2O_3(33nm) / Water	5	28.20	29	2.74
Al_2O_3(60.4nm) / Water	5	22.97	23	0.01
Al_2O_3(80nm) / Water	5	24.25	24	1.00
Al_2O_3(29nm) / EG	4	17.88	18	0.65
Al_2O_3(38nm) / EG	5	18.60	18	3.00
Al_2O_3(60.4nm) / EG	5	29.16	30	2.71
CuO(12nm) / EG	1	5.70	6	5.00
CuO(29nm) / EG	5	22.35	23	2.82
CuO(35nm) / EG	4	22.51	22	2.33

The Comparison between the present model's prediction and experimental data is presented in Table 2. It indicates that the proposed model provides accurate results.

Finally, as a closing note, the effective thermal conductivity of nanoparticle suspensions is predicted successfully but the value of the thermal conductivity of interfacial factor ω was chosen to be between 1.1 and 4, because the exact thermal conductivity of the interfacial layer is not known and cannot be obtained neither experimentally nor theoretically. In short, further research would be needed for the prediction of effective thermal conductivity of adsorption nanolayer.

Conclusion

In this paper, a proposed method for calculating the effective thermal conductivity of nanofluids has been presented. The thermal conductivity of nanofluids primarily depends on the properties of base fluids and nanoparticles, the volume fraction of nanoparticles, the interfacial layer, non-uniform sizes of nanoparticles, and fractal dimension of particles, Brownian motion and temperature. Hence, this model has shown the capability of offering both analytical and numerical predictions. Results of the present model show reasonably good and better agreements with available experimental data.

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