Physical-Statistical Model of Thermal Conductivity of Nanofluids

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A physical-statistical model for predicting the effective thermal conductivity of nanofluids is proposed. The volumetric unit of nanofluids in the model consists of solid, liquid, and gas particles and is treated as a system made up of regular geometric figures, spheres, filling the volumetric unit by layers. The model assumes that connections between layers of the spheres and between neighbouring spheres in the layer are represented by serial and parallel connections of thermal resistors, respectively. This model is expressed in terms of thermal resistance of nanoparticles and fluids and the multinomial distribution of particles in the nanofluids. The results for predicted and measured effective thermal conductivity of several nanofluids (Al₂O₃/ethylene glycol-based and Al₂O₃/water-based; CuO/ethylene glycol-based and CuO/water-based; and TiO₂/ethylene glycol-based) are presented. The physical-statistical model shows a reasonably good agreement with the experimental results and gives more accurate predictions for the effective thermal conductivity of nanofluids compared to existing classical models.

1. Introduction

Fluids with nanoparticles suspended in them are known as nanofluids. The thermal properties of nanofluids, that is, thermal conductivity and specific heat, are very important parameters for estimating the heat transfer coefficient [1–4], because nanofluids are proposed for various uses in important fields such as electronics, space technology, medicine, and HVAC (heating, ventilation, and air conditioning). Hence, there is a need for fundamental understanding of the heat transfer behaviour of nanofluids in order to exploit their potential benefits and applications [5, 6]. Earlier studies show that the enhancement of thermal conductivity of the base fluid is essential in order to improve the thermal efficiency of different systems [2, 7].

In this paper, we present a physical-statistical model and its performance in predicting the thermal conductivity of various fluids with nanoparticles suspended in them. We hope that this model should find wider practical application in the study of nanofluids.

2. Physical-Statistical Model of Thermal Conductivity

The study employs the physical-statistical model of soil thermal conductivity proposed by Usowicz et al. [8, 9]. The model is expressed in terms of thermal resistance (Ohm’s law and Fourier’s law), two laws of Kirchhoff, and the multinomial distribution [10]. The volumetric unit of soil in the model consists of solid, liquid, and gas particles and is treated as a system made up of regular geometric figures, spheres, filling the volumetric unit by layers (Figure 1).

The model assumes that connections between layers of the spheres and between neighbouring spheres in the layer are represented by serial and parallel connections of thermal resistors, respectively. A comparison of resultant resistance, considering all possible configurations of sphere with
Figure 1: Schematic diagram of the physical-statistical model construction: (a) unit volume of soil, (b) the system of spheres that form overlapping layers, and (c) parallel connection of resistors in the layers and series between layers.

Figure 2: Number of the required parallel connections "\( u \)" as a function of nanoparticle volume concentration \( \frac{\theta_V}{\phi} \). \( \theta_V \): volume content of nanoparticles; \( \phi \): volume content of nanofluids. #: photo from [11].

a mean thermal resistance of a given unit soil volume, allows estimating the thermal conductivity of soil \( k \) (in \( \text{W m}^{-1} \text{K}^{-1} \)) according to the equation below [8, 9]:

\[
k = \frac{4\pi}{u \sum_{j=1}^{L} \left( P(x_{1j}, \ldots, x_{kj}) / \left(x_{1j}k_1(T)r_1 + \cdots + x_{kj}k_k(T)r_k \right) \right)}.
\]

where \( u \) is the number of parallel connections of soil particles treated as thermal resistors, \( L \) is the number of all possible combinations of particle configuration, \( x_1, x_2, \ldots, x_k \) are numbers of particles of individual particles of a soil with thermal conductivities \( k_1, k_2, \ldots, k_k \) and particle radii \( r_1, r_2, \ldots, r_k \), where \( \sum_{i=1}^{k} x_{ij} = u, j = 1, 2, \ldots, L, \) and \( P(x_{ij}) \) is the probability of occurrence of a given soil particle configuration calculated from the multinomial distribution [10]:

\[
P(x_{1j}, \ldots, x_{kj}) = \frac{u!}{x_{1j}! \cdots x_{kj}!} f_1^{x_{1j}} \cdots f_k^{x_{kj}}.
\]

The condition \( \sum_{j=1}^{L} P(X = x_j) = 1 \) must be fulfilled. The probability of selection of a given particle \( f_i, i = s, l, g, \) in a single sample is determined based on soil properties. In the case of nanofluids, the values of \( f_s, f_l, \) and \( f_g \) are taken individually for composing fractions of minerals as—\( f_s = \theta_s, \) \( \theta_V \)—volume content of nanoparticles, for liquids as—\( f_l = \theta_l, \theta_f \)—volume content of fluids, and for air or gases as—\( f_g = \phi - \theta_V - \theta_f \) inside the volume content of nanofluids—\( \phi \) (\( \text{m}^3 \text{m}^{-3} \)). When the content of nanoparticles and the base fluid equals the content of nanofluids, the gas content is then equal to zero.

The number of the required parallel and serial connections of thermal resistors in the model depends strongly on the volume content of nanoparticles in the nanofluids. Increase in volume fraction of nanoparticles results in a greater number of bridges between the solid particles and a greater number of contact points and thus contact area between the solid particles, respectively. The model was identified as a model that adjusts the number of parallel connections of thermal resistors (e.g., from 3 to 13, Figure 2) along with the change of the ratio of volume content of nanoparticles in the volume content of nanofluids. The radius of the equivalent spheres was adopted equal to \( r_k = 0.08 \).

The stepwise transition of the value of "\( u \)" as a function of nanoparticles saturation with base fluid causes a respective step increase of calculated values of the thermal conductivity.
Table 1: Values and expressions for parameters used in calculating the 𝑘 of medium (°C in °C).

<table>
<thead>
<tr>
<th>Source</th>
<th>Thermal conductivity Parameters (W m⁻¹ K⁻¹)</th>
<th>Expression, value a</th>
</tr>
</thead>
<tbody>
<tr>
<td>[2]</td>
<td>𝐴12, 𝑘np,</td>
<td>40</td>
</tr>
<tr>
<td>[2]</td>
<td>𝐶𝑢O, 𝑘np,</td>
<td>32.9</td>
</tr>
<tr>
<td>[2]</td>
<td>𝑇𝑖O2, 𝑘np,</td>
<td>8.4</td>
</tr>
<tr>
<td>[2]</td>
<td>ethylene glycol, 𝑘f,</td>
<td>0.253</td>
</tr>
<tr>
<td>[13]</td>
<td>Water, 𝑘f,</td>
<td>0.552 + 2.3410⁻³ °C = 1.1 · 10⁻³ °C²</td>
</tr>
<tr>
<td>[13]</td>
<td>air, 𝑘g,</td>
<td>0.0237 + 0.000064 °C</td>
</tr>
<tr>
<td>[12]</td>
<td>Brownian motion, 𝑘bm,</td>
<td></td>
</tr>
</tbody>
</table>

Where: 𝑑 = 0.893𝑟φ−1/3 = 0.893𝑟φ−1/3, 𝜌cp and 𝑐𝑝 are the density and specific heat of complex nanoparticles, 𝜃 — the particle volume fraction, 𝑘np is the Boltzmann’s constant, 𝑦 = 1 + 𝑉/𝑖, 𝑖 is the radius of nanoparticle, 𝑠 is the interfacial layer of thickness and the fluid medium, °C — temperature, respectively.

of nanofluids. To avoid such transition, a procedure of intermediate determination of thermal conductivity in a range of nanoparticles saturations was proposed. According to the procedure the thermal conductivity is determined for two succeeding values: 𝑢 and 𝑢 + 1 and then the values corresponding to the volume content of nanoparticles θ(𝑢), θ(𝑢+1). The linear equation given below determines thermal conductivity for the needed value of the volume content of nanoparticles θcr:

\[ k_{uf} = k(u) + \frac{\theta_v - \theta(u)}{\theta(u) + 1} (k(u + 1) - k(u)). \]

3. Brownian Motion of Nanoparticles in Base Fluids

The thermal conductivity related to Brownian motion [12], 𝑘bm, and thermal conductivity of base fluids, 𝑘f, may be combined as one input variable to the physical-statistical model. The resulting thermal conductivity of such a fluid, 𝑘fapp, can be expressed as a sum of both conductivities (Table 1): 𝑘fapp = 𝑘f + 𝑘bm.

4. Input Data

The input data needed for calculating the thermal conductivity using the computer software [14] based on (1)–(3) comprise content of nanoparticles, temperature, and content of the base fluid. Moreover, the model requires reference data on the thermal conductivity of nanoparticles (𝑘np), base fluid (𝑘f), and air/gas (𝑘g) (Table 1). The data given in Table 1 was used to calculate the thermal conductivity of nanofluids using physical-statistical model.

Classical and other models presented in this paper are described in more detail in the following works: Gowda et al. [11], Leong et al. [15], Murshed et al. [16], and Tinga et al. [17].

5. Results

The effective thermal conductivity of nanofluids is compared with values predicted by physical-statistical, classical, and other models as well as experimental data obtained from the literature [11, 15, 16, 18–26]. The predicted and measured effective thermal conductivity of several nanofluids (𝐴12, 𝑓/ethylene glycol-based and 𝐴12, 𝑓/water-based; 𝐶𝑢O/ethylene glycol-based and 𝐶𝑢O/water-based; and 𝑇𝑖O2/ethylene glycol-based) are presented in Figures 3, 4, and 5. Generally, the experimental results and predicted data show a substantial increase in thermal conductivity with increasing particle volume fraction for all nanofluids with nonmetallic (oxide) nanoparticles. Murshed and Nieto de Castro [12] demonstrated that Brownian motion plays a significant role in enhancing the thermal conductivity of nanofluids especially at a low concentration of nanoparticles or their smaller sizes. This is due to the fact that smaller-sized particles perform larger motions in a fluid.

The researchers report that the minimal and maximum enhancement in thermal conductivity using 𝐴12, 𝑓 and 𝐶𝑢O (Figures 3 and 4), observed for 4 vol.% load in the case of ethylene glycol-based nanofluid, were about 12% and 30% and 18% and 23% and, in the case of water-based nanofluid, were about 20% and 32% and 14% and 47%, respectively. The effective thermal conductivities for 𝐴12, 𝑓/ethylene glycol-based and 𝐴12, 𝑓/water-based and 𝐶𝑢O/ethylene glycol-based and 𝐶𝑢O/water-based nanofluids predicted by the physical-statistical model are compared to experimental and theoretical results of other authors and are shown in Figures 3 and 4. It is found that the physical-statistical model with the number of parallel connections (number of particles), 𝑢 ≥ 2, for 𝐴12, 𝑓/ethylene glycol-based nanofluids (Figure 3(a)), shows good agreement with results obtained by Lee et al. [21, Eastman et al. [20], and Gowda et al. [11]. Also, good agreement is shown for the model with the number of parallel connections (number of particles), 𝑢 ≥ 3, for 𝐴12, 𝑓/ethylene glycol-based nanofluids (Figure 3(a)), with the data obtained by Wang et al. [26] and, for 𝐶𝑢O/ethylene glycol-based and 𝐶𝑢O/water-based nanofluids (Figures 4(a) and 4(b)), with the result obtained by Lee et al. [21], Liu et al. [23], Eastman et al. [19, 20], Wang et al. [26], and
Gowda et al. [11]. In the case of Al₂O₃/water-based nanofluids (Figure 3(b)) the physical-statistical model with the number of parallel connections (number of particles), \( u \geq 4 \), shows also good agreement with results obtained by Eastman et al. [19] and Leong et al. [15]. Results for Al₂O₃/ethylene glycol-based and Al₂O₃/water-based (Figures 3(a) and 3(b)) and CuO/water-based nanofluids (Figure 4(b)) obtained by Xie et al. [25], Masuda et al. [24], and Eastman et al. [19] differed significantly from the remaining data and were predicted by the physical-statistical model. Generally, most of the classical models presented in this work give less accurate predictions for the effective thermal conductivity of nanofluids than the physical-statistical model. Figures 3 and 4. Observed increase in the number of parallel connections, \( u \), with increasing nanoparticle volume in the physical-statistical model can be interpreted as a formation of thermal bridges between the nanoparticles, also between the nanoparticles and fluid, and, hence, it leads to an increase of the effective thermal conductivity of nanofluid.

As it is shown by Murshed et al. [16] and Lee et al. [22] for the particle volumetric loading of 5% (Figure 5) the maximum increase of thermal conductivity of TiO₂/ethylene glycol-based nanofluids is about 15–18%. Also, it can be seen that the physical-statistical model with the number of parallel connections (number of particles), \( u \geq 2 \), and Murshed et al.’s [16] model with spherical nanoparticle show reasonably good agreement with the experimental results. It is worth to notice, that in this case the predictions of Maxwell [27] and Prasher et al.’s [28] models for the effective thermal conductivity of nanofluids are slightly underestimated and significantly overestimated, respectively. As shown in the Figure 5, the physical-statistical model with a higher number of parallel connections (number of particles), \( u \geq 3 \), gives a slightly less accurate prediction than Murshed et al.’s [16] model, but more accurate than Prasher et al.’s [28] model.

6. Conclusion

A theoretical and modelling study on the effective thermal conductivity of nanofluids is conducted.

The effective thermal conductivity of nanofluids significantly increases with the nanoparticle volume fraction. The larger number of nanoparticles in the nanofluids corresponds to higher number of connections of thermal resistors. It can be interpreted as a formation of thermal bridges between
the nanoparticles, also between the nanoparticles and fluid. As a result, it leads to an increase of the effective thermal conductivity of nanofluid.

The physical-statistical model shows a reasonably good agreement with the experimental results and gives more accurate predictions for the effective thermal conductivity of nanofluids compared to existing classical models. This model also takes into account thermal conductivity related to Brownian motion.

The model requires further refinements, taking into account other variables which affect the effective thermal conductivity of nanofluids.

**Conflict of Interests**

The authors declare that there is no conflict of interests regarding the publication of this paper.

**References**

