Effective thermal conductivity of two-phase systems with cylindrical inclusions

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A theoretical model is presented to predict effective thermal conductivity of real two-phase materials from the values of thermal conductivity of the constituent phases and their volume fractions. Two-phase materials have been assumed to contain cylindrical particles arranged in a regular three-dimensional cubic geometry. The arrangement has been divided into unit cells, each of which contains a cylinder. The resistor model has been applied to determine the effective thermal conductivity (ETC) of the unit cell. A porosity correction term \( F \) is introduced in order to incorporate varying individual geometries and non-linear flow of heat flux lines generated by the difference in thermal conductivities of constituent phases. Theoretical calculations of the ETC have been carried out on a large number of samples and comparisons have been made with other models and experimental values cited in the literature. The values predicted by the proposed model are in close agreement with experimental values and more accurate than those obtained from existing models.

[Keywords: Correction term, Cylindrical inclusions, Effective thermal conductivity, Real two-phase systems, Unit cells]

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1 Introduction

The study of heat transfer through porous and composite materials is becoming increasingly important in many physical and industrial processes. Important fields where this study is of extensive use are oil exploration, distillation, water conservation, energy preservation and development of composite materials. Many diverse areas where the composite media have continued use are the production of integrated circuits, infrared absorbers and highly porous amorphous solids. Important classes of materials used are soils, ceramics, fiber-reinforced materials, silica aerogels, foamed polymers, metal foams and coated fiber composites. Such substances are composed of at least two components. In many of their applications knowledge of thermal conductivity is essential. Its dependence on porosity, grain size and shape of the particles etc. is a matter of concern to the engineers, architects and physicists. Theoretical modelling and accounting its dependence on such complex parameters is a challenging task to engineers and physicists. In the literature one finds several efforts in which the situation has been simplified by assuming that the particles are of specific shape and arranged in a particular geometries within the continuous phase.

The value of thermal conductivity in the solid-fluid composite is required in the numerical modelling of forced convection through porous media. Hunt et al. used an empirical stagnant conduction model developed by Tien & Vafai to define the effective thermal conductivity in the volume averaged homogeneous energy equation. Antohe has also emphasized the use of an empirical phase symmetry conduction that was developed by Hsu to create a numerical model for the simulation of cooling micro heat exchangers. The origins of the phase-symmetry conduction model by Hsu are based upon the original work done by Zehner et al. on packed beds of spheres. In a configuration with low solid volume fraction and order of magnitude difference between thermal conductivities of two phases, an accurate description of the geometry of the solid medium is the key in estimating the effective thermal conductivity of the medium. Zehner et al. did this technique successfully for a packed bed of spheres. Utilizing a geometrical estimate, a recent advancement in the estimation of the ETC specifically for metallic foams saturated with a fluid was developed by Calmidi and Mahajan and Boomsma and Poulikakos. For high porosity metal foams
Calmidi and Mahajan\textsuperscript{14} presented a one dimensional heat conduction model considering the porous medium to be formed of a two dimensional array of hexagonal cells. Whereas Boomsma and Poulikakos\textsuperscript{15} proposed a three dimensional model using metal foam structure in the form of tetrakaidecahedral cells with cubic nodes at the intersection of two fibers. Both the models involved a geometric parameter that was evaluated using the experimental data. Recently, Bhattacharya \textit{et al.}\textsuperscript{16} has extended the analysis of Calmidi and Mahajan\textsuperscript{14} with a circular intersection, which results in a six fold rotational symmetry. 

In the present paper we have tried to fill the space arrangement of cells of equal size with the minimal surface energy and a theoretical model has been proposed to predict ETC of the two-phase systems with cylindrical inclusions. In order to incorporate varying individual geometries and non-linear flow of heat flux lines generated by the difference in thermal conductivities of constituent phases, a correction term in place of the physical porosity has been introduced.

Expression for porosity correction term $F$ has been obtained empirically in terms of the ratio of thermal conductivities of the constituents and the physical porosity of the material\textsuperscript{17-22}.

\section*{2 Theory}

We assume the following while analyzing the problem:

1. The contact resistant between the solid and fluid phase is negligible; 
2. The mixture is homogeneous throughout and no transfer of heat occurs by way of convection or radiation; and 
3. The heat is flowing along the X-axis and the flux lines remain parallel during the heat flow.

Suppose the grains of the solid phase be cylindrical having radius $a$ and length $2c$ ($a < c$), respectively. Furthermore, assume that these grains be located at the corners of a simple cube of side $2b$. Their distribution in two dimensions is shown in Fig. 1(i). The geometry of a unit cell is shown in Fig. 1(ii).

Fig. 1 — The resistor model for two-phase systems with cylindrical particles [(i) particles distribution in two dimensions, (ii) geometry of a unit cell, (iii) one section of unit cell and (iv) rectangular bar]
Let the origin of cartesian coordinates has been placed at the centre of the cylinder. We divide the unit cell into eight parts. One such part is shown in Fig. 1(iii). This is further sub-divided into rectangular bars. One such bar is shown in Fig. 1(iv). Let the length of the bar be \( b \), its area of cross section will be \( dxdz \). The shaded portion of the element in the Fig. 1(iii) represents the solid phase and the non-shaded portion represents the fluid phase. Let us suppose that the heat flux is incident normally on the cubic cell.

The volume fraction of the solid phase of the bar will be 
\[
\text{Volume fraction of solid phase} = \frac{(c dxdz)}{(b dxdz)} = \frac{c}{b} \quad \ldots (1)
\]

Similarly the volume fraction of the fluid phase will be 
\[
\text{Volume fraction of fluid phase} = \frac{(b - c) dxdz}{(b dxdz)} = \frac{1 - c}{b} \quad \ldots (2)
\]

The terms \( \frac{c}{b} \) and \( \frac{1 - c}{b} \) are equivalent to one-dimensional porosity as used by Cheng and Vachon. Considering that these elements form parallel resistors with respect to the direction of heat flow, one can take a combination of such resistors to predict the ETC utilizing the thermal conductivities of the constituent phases as
\[
\lambda' = \lambda_1 \left( \frac{c}{b} \right) + \lambda_2 \left( 1 - \frac{c}{b} \right) \quad \ldots (3)
\]

where \( \lambda_1 \) and \( \lambda_2 \) are the thermal conductivities of solid and fluid phase respectively. In reference to the Fig. 1(iii), the thermal conductivity of the section will be
\[
\lambda'' = \frac{(abd)}{b^2 dx} \lambda'_{av} + \frac{(b - a)bdx}{b^2 dx} \lambda_2
\]
or
\[
\lambda' = \frac{(a/b)\lambda'_{av} + (1-a/b)\lambda_2}{b^2 dx} \quad \ldots (4)
\]

where \( \lambda'_{av} = (1/a) \int_0^a \lambda' \, dz \) 
\[
\ldots (5)
\]

Combining Eqs (4) and (5) yields the following result
\[
\lambda'' = \frac{(a/b)\lambda'_{av} + (1-a/b)\lambda_2}{b^2 dx} \quad \ldots (6)
\]

With reference to Fig. 1(iii), we have:

Volume fraction of portions numbered
\[
I = (abdx)/(b^2 \, dx) = (a/b) \quad \ldots (7)
\]

Volume fraction of portions numbered
\[
II = ((b^2-ba)dx)/(b^2 \, dx) = (1-a/b) \quad \ldots (8)
\]

These elements form equivalent series resistors perpendicular to the direction of heat flow, therefore the effective thermal conductivity \( \lambda_e \) of the unit cell will be
\[
\frac{1}{\lambda} = \frac{(a/b)\lambda'_{av}}{\lambda''_{av}} + \frac{(1-a/b)\lambda_2}{\lambda_2} \quad \ldots (9)
\]

For a cylindrical particle taking \( Y \)-axis as the axes we have \( x^2 + z^2 = a^2 \)

Therefore
\[
x = \sqrt{(a^2 - z^2)} \quad \ldots (10)
\]

Since \( \lambda'' \) varies as \( x \) changes from 0 to \( \sqrt{(a^2 - z^2)} \), then, on averaging
\[
\lambda''_{av} = (1/a) \int_0^{\sqrt{(a^2 - z^2)}} \lambda'' \, dx \quad \ldots (11)
\]

Combining Eqs (6) and (11) yields the following result:
\[
\lambda'' = \frac{(a/b)\lambda'_{av} + (1-a/b)\lambda_2}{b^2 dx} \quad \ldots (12)
\]

Combining Eqs (3) and (12) yields the following result:
\[
\lambda''_{av} = (1/a) \int_0^{\sqrt{(a^2 - z^2)}} [(1/b)
\[
\int_0^a \lambda' \, dz + (1-a/b)\lambda_2] \, dx + (1-a/b)\lambda_2 \, dx
\]

Therefore
\[
\lambda''_{av} = \{(\lambda_1 - \lambda_2)/(ab^2)\} \int_0^{\sqrt{(a^2 - z^2)}} c dxdz + \lambda_2
\]
\[
\lambda_e = \frac{(\lambda_1 - \lambda_2)(\pi a^2 c)/(4b^2) + \lambda_2}{\pi a^2 c}/(4b^2)} + \lambda_2 \quad \text{(13)}
\]

or

\[
\lambda''_e = \frac{(\lambda_1 - \lambda_2)\pi ac}/(4b^2) + \lambda_2 \quad \text{(14)}
\]

Combining Eqs (9) and (14) yields the following result:

\[
\lambda_e = \lambda_2\left[\frac{(\lambda_1 - \lambda_2)(\pi ac)/(4b^2) + \lambda_2}{[1 - (a/b)(\lambda_1 - \lambda_2)(\pi ac)/(4b^2)]} + \lambda_2\right] \quad \text{(15)}
\]

The unit cell contains one cylinder that lies inside. Therefore, fractional volume of the solid phase will be

\[
\phi_1 = \frac{2\pi a^2 c}{8b^3} \quad \text{(16)}
\]

Putting the limiting condition into Eq. (16), if \( c = b \), then we get

\[
\phi_1 = (\pi/4)(a^2/b^2)
\]

Therefore

\[
(a/b) = \sqrt{\pi/4} \phi_1^{1/2} \quad \text{(17)}
\]

Combining Eqs (15) and (17) yields the following result:

\[
\lambda_e = \lambda_2\left[\frac{(\lambda_1 - \lambda_2)(\sqrt{\pi/4})\phi_1^{1/2} + \lambda_2}{[1 - (\sqrt{\pi/4})\phi_1^{1/2}(\lambda_1 - \lambda_2)(\sqrt{\pi/4})\phi_1^{1/2} + \lambda_2]} + \lambda_2\right] \quad \text{(18)}
\]

For cubic packing of cylindrical inclusions the maximum value of the packing fraction will be less than 0.785 (because \( a < b \)). Therefore, Eq. (18) is valid for \( 0 < \phi_1 < 0.785 \) which is a low and medium dispersion case. In the limiting case, it can be seen that, when \( \phi_1 \) tends to 0, \( \lambda_e \) approaches \( \lambda_2 \), and when \( \phi_1 \) tends to 0.785, \( \lambda_e \) leads to the arithmetic mean of the phases. Noting that the expression given in Eq. (18) is based on rigid geometry, which does not represent the true state of affairs of a real two-phase system. The ETC depends upon various characteristics of the system. The most prominent amongst them being the volume fraction and thermal conductivity of the constituent phases. Thus, for practical utilization, we have to modify the expression given in Eq. (18) by incorporating some correction term. Tareev\textsuperscript{24} has shown that, during the flow of electric flux from one dielectric to another dielectric medium, the deviation of flux lines in any medium depends upon the ratio of their dielectric constants. By the analogy we can have the concentration of thermal flux altered from its previous value as it passes through another medium and that the amount is a function of the thermal conductivity of the constituent phases. Such a deviation causes a zig-zag path of flux lines in the bulk and also alters the density of flux lines in the constituent phases. The concentration of flux lines is greater in the phase of higher conductivity than it is in the phase of lower conductivity. If the flow of flux lines were linear then this porosity function would have been numerically equal to the physical porosity of the sample. In cases where curvature in the flow lines occurs, the porosity function will not be equal to the physical porosity of the sample but it should be a function of the ratio of the thermal conductivity of the constituent phases as well as of the physical porosity of the sample. Considering random packing of phases, non-uniform shape of particles and the flow of heat flux lines not restricted to be parallel, we here replace physical volume fraction of solid phase by porosity correction term \( F \). \( F \) in general should be a function of the physical volume fraction of the solid phase and the ratio of the thermal conductivity of the constituent phases. Therefore, expression given in Eq. (18) may be written as:

\[
\lambda_e = \lambda_2\left[\frac{(\lambda_1 - \lambda_2)(\sqrt{\pi/4})F^{1/2} + \lambda_2}{[1 - (\sqrt{\pi/4})F^{1/2}(\lambda_1 - \lambda_2)(\sqrt{\pi/4})F^{1/2} + \lambda_2]} + \lambda_2\right] \quad \text{(19)}
\]

Rearranging Eq. (19) we get

\[
A F + B F^{1/2} + C = 0 \quad \text{(20)}
\]

where \( A = [\lambda_2(\lambda_1 - \lambda_2)] \), \( B = [\sqrt{\pi/4}(\lambda_1 - \lambda_2)(\lambda_2 - \lambda_e)] \) and \( C = \lambda_2(\lambda_2 - \lambda_e) \).

3 Results and Discussion

Tables 1 and 2 cite experimental results of ETC and other data reported in literature. Without any
<table>
<thead>
<tr>
<th>S. No.</th>
<th>Type of the sample</th>
<th>$\phi_1$</th>
<th>$\lambda_1$</th>
<th>$\lambda_2$</th>
<th>$\lambda_e$ (expt.)</th>
<th>$\lambda_e$ (theo.) [Eq.(19)]</th>
<th>% Error</th>
</tr>
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<td>Cu/solder$^{25}$</td>
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<td>0.267</td>
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<td>22</td>
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<td>0.293</td>
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<td>0.385</td>
<td>0.433</td>
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*Contd...*
correction term Eq. (18) exhibits large deviations from the experimental results. This prompted the introduction of a correction in porosity. The correction term introduced for each sample has been computed using Eq. (20) and plotted with \( \phi_1^{1/2}\exp(\lambda_2/\lambda_1) \). Such plots of \( \phi_1^{1/2}\exp(\lambda_2/\lambda_1) \) versus \( \lambda_1/2 \) are shown in Figs 2 and 3. It is observed from Figs 2 and 3 that when \( \lambda_1 > \lambda_2 \), \( F^{3/2} \) increases roughly,

<table>
<thead>
<tr>
<th>S. No.</th>
<th>Type of the sample</th>
<th>( \phi_1 )</th>
<th>( \lambda_1 )</th>
<th>( \lambda_2 )</th>
<th>( \lambda_e ) (expt.)</th>
<th>( \lambda_e ) (theo.) [Eq.(19)]</th>
<th>% Error</th>
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<td>30</td>
<td>Bi. powder/Si rubber(^{23})</td>
<td>0.16</td>
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<td>39</td>
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<td>0.34</td>
<td>0.25</td>
<td>0.255</td>
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</table>

Average deviation 4.5%
linearly with increasing $\phi_1^{1/2}\exp(\lambda_2/\lambda_1)$ and when $\lambda_1 < \lambda_2$, $F^{1/2}$ decreases with increasing $\phi_1^{1/2}\exp(\lambda_2/\lambda_1)$. It clearly shows that there is a point of inflection near $\lambda_1 = \lambda_2$.

We have used the curve fitting technique and found that the expression

$$F^{1/2} = C_1 \phi_1^{1/2}\exp(\lambda_2/\lambda_1) + C_2 \quad \ldots(21)$$

best fits the curve obtained in Figs 2 and 3. Where $C_1$ and $C_2$ are constants. These constants are different for different type of materials. The values of these constants for solid-air, emulsion, suspension, granular and solid-solid two-phase systems are 0.8674 and -0.0409, for pineapple leaf fiber-phenolformaldehyde -0.3556 and 1.0411, for organic foam-air 1.3137 and -0.194, for organic foam-glycerin -0.0052 and 0.1836, for organic foam-engine oil -0.0226 and -0.4038 and for organic foam-mustard oil -0.0084 and -0.4038 respectively.

On putting Eq. (21) as the porosity correction term in Eq. (19) we have calculated values of the ETC for a large number of samples reported in the literature. Tables 1 and 2 show a comparison of experimental results of ETC and calculated values from Eq. (19). The error between experimental results reported in literature and the theoretical values lies in

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Fig. 2 — Variation of porosity correction term $F^{1/2}$ versus $\phi_1^{1/2}\exp(\lambda_2/\lambda_1)$. Squares are experimental data of solid-air, emulsion, suspension, granular and solid-solid two-phase systems and the full line is the theoretical simulation.

Fig. 3 — Variation of porosity correction term $F^{1/2}$ versus $\phi_1^{1/2}\exp(\lambda_2/\lambda_1)$. Squares are experimental data and the full line is the theoretical simulation.

Fig. 4 — Comparison between experimental and theoretical values of ETC of the same samples (No. 1-14, Table 1)
Fig. 5 — Comparison between experimental and theoretical values of ETC of the same samples (No. 15-39, Table 1)

Fig. 6 — Comparison between experimental and theoretical values of ETC of the same samples (No. 1-12, Table 2)
the range 0-18% and the average deviation is 4.5% for solid-air, emulsion, suspension, granular, solid-solid and pineapple leaf fiber-phenolformaldehyde two-phase systems as shown in Table 1. For organic foams the average deviation is just 0.8%, which is shown in Table 2. The deviation is very low for pineapple leaf fiber-phenolformaldehyde and for organic foams from our model than other existing models. This is because, these composites are having fibers in cylindrical shape and in our model we have used the cylindrical shape of the solid phase, whereas modified Babanov1 considered the shape of the particle to be cubical, Singh12 considered the shape of the particle to be spherical and Bhattacharya et al.22 considered two-dimensional array of hexagonal cells with a circular intersection, which is not the true case for these materials. The deviation from the experimental results for modified Babanov’s model1, Singh’s model12 and Bhattacharya’s model22 has been calculated and shown is in Figs 4 and 5. For foam-like materials we have used Boomsma’s and calculated and shown is in Figs 4 and 5. For foam-like shape of the solid phase, whereas modified Babanov 1 shape and in our model we have used the cylindrical fiber-phenolformaldehyde and for organic foams from organic foams from pineapple leaf fiber-phenolformaldehyde two-

Table 2. The deviation is very low for pineapple leaf fiber-phenolformaldehyde and for organic foams from our model than other existing models. This is because, these composites are having fibers in cylindrical shape and in our model we have used the cylindrical shape of the solid phase, whereas modified Babanov1 considered the shape of the particle to be cubical, Singh12 considered the shape of the particle to be spherical and Bhattacharya et al.22 considered two-

Besides the success of the proposed model in predicting the ETC, it also has the merits in its favour.

(1) The model is capable of predicting ETCs close to the experimental values even for mixtures of higher conductivity ratios and high porosities, whereas one may find that other models give higher deviations in those situations; (2) This model enables one to avoid the introduction of sphericity or any other factor in the expression of ETC, making the model simple but powerful enough without compromising on the results.

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Appendix

1. The modified Babanov’s cubic particle model22 is

\[ \lambda_c = \frac{[\lambda_1 \{ \lambda_2 + F^{2/3} (\lambda_1 - \lambda_2) \}]}{[\lambda_2 + F^{2/3} (\lambda_1 - \lambda_2)(1 - F^{1/3})]} \]  

…(22)

where \( F = [1 - \exp\{-(0.92) \phi^2 \ln (\lambda_1/\lambda_2)\}] \)

2. The Singh’s spherical particle model22 is

\[ \lambda_c = \frac{[\lambda_1 \{ \lambda_2 + 0.8060F^{2/3} (\lambda_1 - \lambda_2) \}]}{[\lambda_2 + F^{2/3} \{0.8060(\lambda_1 - \lambda_2)(1 - 1.2407F^{1/3})\}]} \]  

…(23)

where \( F = [1 - \exp\{-(0.92) \phi^2 \ln (\lambda_1/\lambda_2)\}] \)

3. The Bhattacharya’s model16 is

\[ \lambda_c = F\{\phi_1 \lambda_1 + (1 - \phi_1) \lambda_2\} + \frac{(1 - F)}{\{\phi_1 / \lambda_1 + (1 - \phi_1) / \lambda_2\}} \]  

…(24)

where \( F = 0.35 \)

4. The Boomsma’s model15 is

\[ \lambda_c = \frac{\sqrt{2}}{2[R_A + R_B + R_C + R_D]} \]  

…(25)

where \( R_A = 4F/[\{2e^2 + \pi F(1-e)\} \lambda_1 + \{4 - 2e^2 - \pi F(1-e)\} \lambda_2] \)

\( R_B = (e - 2F)/[(e - 2F)e^2 \lambda_1 + \{2 - 4e - (e - 2F)e^2\} \lambda_2] \)

\( R_C = (\sqrt{2} - 2e)^2/[\{2\pi F(1 - 2e\sqrt{2})\lambda_1 + 2\sqrt{2} - 2\pi e^2 \lambda_2\} \lambda_2] \)

\( R_D = 2e[\{e^2 \lambda_1 + (4 - e^2) \lambda_2\}] F = \sqrt[3]{\{2 - (5/8)e^3 \}} \sqrt{2 - 2(1 - \phi)} / \{\pi (3 - 4e\sqrt{2} - e)\} \)

and \( e = 0.339 \)

Symbols involved in the formulae given in Eqs (22) – (25) have the same meaning as in the previous part in the paper.

References