HEAT CONDUCTION IN ISOTROPIC HETEROGENEOUS MEDIA

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ABSTRACT

In this study, the effective thermal conductivity of aluminum or tin filled high-density polyethylene composites is investigated numerically as a function of filler concentration. The obtained values are compared with experimental results and the existing theoretical and empirical models. The thermal conductivity is measured by a modified hot-wire technique. For numerical study, the effective thermal conductivity of particle-filled composites were calculated numerically using the microstructural images of them. By identifying each pixel with a finite difference equation and accompanying appropriate image processing, the effective thermal conductivity of composite material is determined numerically. As a result of this study, numerical results, experimental values and all the models are close to each other at low particle content. For particle content greater than 10%, the effective thermal conductivity is exponentially formed. All the models fail to predict thermal conductivity in this region. But, numerical results give satisfactory values in the whole range of aluminum particle content.

Key Words: Composite material, Thermal conductivity, Image processing, Finite difference method

1. INTRODUCTION

The effective thermal conductivity of high-density polyethylene containing particulate fillers is obtained numerically at several filler concentrations. A numerical approach was used to determine the effective thermal conductivity of particle composites in this study. The effective thermal conductivity of the material was determined using the Laplace equation, as were the temperature and flux fields within the control volume. A finite difference method was used in this study. Calculation is carried out on two-dimensional geometric spaces. The
results obtained from this calculation were compared to results found in prior literature.

Knowing physical properties of the composite materials have gained significant importance in the design of new systems. For many materials applications, information is needed on their thermal properties. Determining the thermal conductivity of composite materials is crucial in a number of industrial processes. The temperature fields in composite materials cannot be determined unless the thermal conductivities of the media are known. Despite the importance of this material property and the considerable number of studies that have been carried out, the determination of effective thermal conductivity of a composite material is partially understood. The effective thermal conductivity of a composite material is a complex function of their geometry, the thermal conductivity of the different phases, distribution within the medium, and contact between the particles. Numerous theoretical and experimental approaches have been developed to determine the precise value of this parameter.

Maxwell was studied the effective thermal conductivity of heterogeneous materials. By solving Laplace's equation, he determined the effective conductivity of a random suspension of spheres within a continuous medium. The model developed by Maxwell assumes that the particles are sufficiently far apart that the potential around each sphere will not be influenced by the presence of other particles (Maxwell, 1954). Russell developed one of the early model systems using the electrical analogy. Assuming that the discrete phase are isolated cubes of the same size dispersed in the matrix material and that the isothermal lines are planes (Russell, 1935). Based on Tsao’s probabilistic model (Tsao, 1961), Cheng and Vachon assumed a parabolic distribution of the discontinuous phase (Cheng and Vachon, 1969). Lewis and Nielsen derived a semi-theoretical model by a modification of the Halpin-Tsai equation (Ashton et all., 1969) to include the effect of the shape of the particles and the orientation or type of packing for a two-phase system (Lewis and Nielsen, 1970). Baschirov and Selenew developed the equation for the case when the particles are spherical and the two phases are isotropic (Baschirov and Manukian, 1974). In real composite material, the isothermal surfaces present a very complex shape and cannot be analytically determined. The models used to calculate thermal conductivities are thus highly simplified models of the real media. Veyret, Cioulachtjian, Tadrist and Pantaloni characterized conductive heat transfer through composite, granular, or fibrous materials by using the finite element method (Veyret et all., 1993). Terada, Miura and Kikuchi generated the finite element model by identifying each pixel with a finite element and accompanying appropriate image processing (Terada et all., 1997). Deissler and Boegli carried out the numerical studies. They proposed a solution to Laplace’s equation for a cubic array of spheres presenting a single point of contact (Deissler and Boegli, 1958). Deissler’s works were extended by Wakao and Kato for a cubic or orthorhombic array of uniform spheres in contact (Wakao and Kato, 1968). Shonnard and Whitaker have investigated the influence of contacts on two-dimensional models. They have developed a global equation with an integral method for heat transfer in the medium (Shonnard and Whitaker, 1989).

2. THERMAL CONDUCTIVITY MODELS

In this section are listed several models and a brief description of their basis. Many theoretical and empirical models have been proposed to predict the effective thermal conductivity of two phase mixtures. Comprehensive review articles have discussed the applicability of many of these models that appear to be more promising (Progelhof, et all., 1976; Ott, 1981).

2.1. Parallel, Series and Geometric Mean Models

For a two-component composite, the simplest alternatives would be with the materials arranged in either parallel or series with respect to heat flow, which gives the upper or lower bounds of effective thermal conductivity. For the parallel conduction model:

$$k_c = (1 - \phi)k_f + \phi k_m$$

and for series conduction model:

$$\frac{1}{k_c} = \frac{1 - \phi}{k_f} + \frac{\phi}{k_m}$$

In the case of geometric mean model, the effective thermal conductivity of the composite is given by:

$$k_c = k_f \left(1 - \phi\right)$$
2.2. Cheng and Vachon Theoretical Model

Starting with Tsao's basic probabilistic model, Cheng and Vachon assumed the discontinuous phase had a parabolic distribution. Based upon this assumption, Tsao's constants were evaluated and a closed form expression for effective thermal conductivity of a two phase mixture as a function of discontinuous phase volume fraction were obtained (Cheng and Vachon, 1969):

\[ k_f > k_m \]

\[ \frac{1}{k_e} = \frac{1}{\sqrt{C(k_m - k_f)[k_m + B(k_f - k_m)]}} \ln \left( \frac{\sqrt{k_m + B(k_f - k_m)} + \frac{B}{2} \sqrt{C(k_m - k_f)}}{\sqrt{k_m + B(k_f - k_m)} - \frac{B}{2} \sqrt{C(k_m - k_f)}} \right) + \frac{1 - B}{k_m} \]  \hspace{1cm} (4)

where for both equations:

\[ B = \sqrt{3\phi}/2 \quad C = -4\sqrt{2/(3\phi)} \]

2.3. Lewis and Nielsen Semi-Theoretical Model

Lewis and Nielsen modified the Halpin-Tsai equation to include the effect of the shape of the particles and the orientation or type of packing for a two-phase system (Lewis and Nielsen, 1970).

\[ k_e = k_m \left[ 1 + A\psi \right] \left[ 1 - B\phi \right] \]  \hspace{1cm} (5)

where

\[ A = k_c - 1 \quad B = \left( \frac{k_f - 1}{k_m} \right) \frac{k_f + A}{k_m} \quad \psi = 1 + \left( \frac{1 - \phi_m}{\phi_m} \right) \phi \]

The values of \( A \) and \( \phi_m \) for many geometric shapes and orientation are given in the following tables:

Table 1. Value of \( A \) for Various Systems

<table>
<thead>
<tr>
<th>Type of dispersed phase</th>
<th>Direction of Heat Flow</th>
<th>( A )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cubes</td>
<td>Any</td>
<td>2.0</td>
</tr>
<tr>
<td>Spheres</td>
<td>Any</td>
<td>1.50</td>
</tr>
<tr>
<td>Aggregates of spheres</td>
<td>Any</td>
<td>2.5</td>
</tr>
<tr>
<td>Randomly oriented rods</td>
<td>Any</td>
<td>1.58</td>
</tr>
<tr>
<td>Aspect ratio = 2</td>
<td></td>
<td>2.08</td>
</tr>
<tr>
<td>Randomly oriented rods</td>
<td>Any</td>
<td>2.8</td>
</tr>
<tr>
<td>Aspect ratio = 6</td>
<td></td>
<td>4.93</td>
</tr>
<tr>
<td>Randomly oriented rods</td>
<td>Any</td>
<td>8.38</td>
</tr>
<tr>
<td>Aspect ratio = 10</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Uniaxially oriented fibers</td>
<td>Parallel to fibers</td>
<td>2L/D</td>
</tr>
<tr>
<td>Uniaxially oriented fibers</td>
<td>Perpendicular to fibers</td>
<td>0.5</td>
</tr>
</tbody>
</table>

Table 2. Value of \( \phi_m \) for Various Systems

<table>
<thead>
<tr>
<th>Shape of Particle</th>
<th>Type of Packing</th>
<th>( \phi_m )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spheres</td>
<td>Hexagonal close</td>
<td>0.7405</td>
</tr>
<tr>
<td>Spheres</td>
<td>Face centered cubic</td>
<td>0.7405</td>
</tr>
<tr>
<td>Spheres</td>
<td>Body centered cubic</td>
<td>0.60</td>
</tr>
<tr>
<td>Spheres</td>
<td>Simple cubic</td>
<td>0.524</td>
</tr>
<tr>
<td>Spheres</td>
<td>Random close</td>
<td>0.637</td>
</tr>
<tr>
<td>Spheres</td>
<td>Random close</td>
<td>0.601</td>
</tr>
<tr>
<td>Rods or fibers</td>
<td>Uniaxial hexagonal close</td>
<td>0.907</td>
</tr>
<tr>
<td>Rods or fibers</td>
<td>Uniaxial simple cubic</td>
<td>0.785</td>
</tr>
<tr>
<td>Rods or fibers</td>
<td>Uniaxial random</td>
<td>0.82</td>
</tr>
<tr>
<td>Rods or fibers</td>
<td>Three dimensional random</td>
<td>0.52</td>
</tr>
</tbody>
</table>

2.4. Maxwell Theoretical Model

Maxwell using potential theory obtained an exact solution for the conductivity of randomly distributed and non-interacting homogeneous spheres in a homogeneous medium (Maxwell, 1954):

\[ k_c = k_m \left[ k_f + 2k_m + 2\phi(k_f - k_m) \right] \left[ k_f + 2k_m + \phi(k_f - k_m) \right] \]  \hspace{1cm} (6)

2.5. Russell Theoretical Model

Assuming the pores are cubes of the same size and the isothermal lines are planes, Russell obtained the conductivity using a series parallel network:

\[ k_c = k_m \left[ \phi^{2/3} + \frac{k_m}{k_f} (1 - \phi^{2/3}) \right] \left[ \phi^{2/3} - \phi + \frac{k_m}{k_f} (1 + \phi - \phi^{2/3}) \right] \]  \hspace{1cm} (7)

3. IMAGE PROCESSING

An image is a spatial representation of an object (Haralick and Shapiro, 1994). Necessary information in engineering is usually given by an image or a set of several images that is obtained in a measurement...
or experimental procedure. The information is converted into a screen image on a digital computer. The digital image-based (DIB) finite element model (FEM) was originated by Hollister and Kikuchi, (1994) for studying a bone microstructure by the homogenization method.

Although there are many operations in image processing such as filtering, edge deduction, thresholding, and etc., we need only a few of them for the present study. Filtering and thresholding, which are the most important operations, in the first step are the operations directly related to the finite difference model. When an image is acquired by an imaging system, the vision system for which it is intended is unable to use it directly. The image may be corrupted by random variations in intensity or poor contrast that must be dealt with in the early stages of vision processing.

3.1. Size Filter

It is very common to use thresholding for finding a binary image. In most cases, there are some regions in an image that are due to noise. Usually, such regions are small. In many applications, it is known that objects of interest are of size greater than $T_0$ pixels. In such cases one may use a size filter to remove noise after component labeling. All components below $T_0$ in size are removed by changing the corresponding pixels to 0. This simple filtering mechanism is very effective in removing noise. Figure 1 shows an example of the application of a size filter to a noisy character image (Jain et al., 1995).

![Figure 1. A noisy binary image and the resulting image after the application of a size filter (right). $T_0 = 10$](image1.png)

3.2. Thresholding

The thresholding is defined as an image operation which produces a binary image from a gray scale image. Furthermore, the thresholding can produce a binary one on the output digital image whenever a pixel value on the input digital image is below a specified threshold level. A binary zero is produced otherwise. Although a composite material is not always composed of two phases, we shall consider two-phase composites for simplicity. Nonetheless, the definition can be easily extended by increasing the number of thresholding values.

The threshold values may be determined interactively by the operator. While the video display affords direct comparison of the thresholded image with the working image, the software enables us to modify or fix the thresholded images. Since we have assumed that the phases of the composite could be distinctive in the original image, the thresholding is done by referring to the histogram on the video screen. If the original image has enough resolution and little noise, then the histogram can provide most of the information needed to choose the threshold value required for generating approximated geometry. Furthermore, if the volume fraction of each phase in the two dimensional image is given, the software may provide a function to calculate the ratio between pixel values, by which the threshold value is determined.

![Figure 2. Thresholding the digital image](image2.png)
Once a threshold value has been chosen, it is easy to convert the selected image into a binary image. If the obtained image does not seem to be a satisfactory representation of the original, new threshold values may be chosen until we are satisfied with the binary image (Terada et al., 1997), (Figure 2).

4. EXPERIMENTAL STUDY

The matrix material is a high-density polyethylene in powder form, with a density of 0.968 g/cm$^3$ and a melt index of 5.8 g/10 min. Its thermal conductivity at 36 °C is 0.543 W/m.K. The metallic filler is aluminum in the form of fine powder, with particles approximately spherical in shape and particle size in the range of 40-80 microns for aluminum. The solid density of aluminum is 2.7 g/cm$^3$ and its thermal conductivity 204 W/m.K. Samples are prepared by the mold compression process. HDPE and aluminum powders are mixed at various volumetric concentrations (Figure 3). The mixed powder is then melted under pressure in a mold and solidified by air cooling. The process conditions are molding temperature of 185 °C, pressure of 4 MPa. The resulting samples for thermal conductivity measurements are rectangular in shape of 100 mm length, 50 mm width, and 17 mm thickness because of the measuring probe. Homogeneity of the samples is examined using a light microscope. Aluminum particles are found to be uniformly distributed in high-density polyethylene matrix with no voids in the structure.

5. NUMERICAL MODELING OF THE PROBLEM

Two-dimensional numerical analysis was carried out for the conductive heat transfer in the composite material. The temperature field in the composite material was defined by solving Laplace’s equation numerically using a finite difference formulation. The Laplace’s equation was solved by imposing the following boundary conditions:

(a) The vertical sides perpendicular to the direction of the heat flow are isothermal at the entrance to and the exit from the cell.
(b) The horizontal sides parallel to the direction of the heat flow are adiabatic. The heat flow moving into or out of the cell reaches its peak at the center of the isothermal faces. For an elementary two-dimensional cell with the dimensions of $L_x$ (along the x axis) and $L_y$ (along the y axis), the thermal conductivity is determined using the following relation:

$$ k_e \frac{L_y \Delta T_{cell}}{L_x} = \sum_i k_i y_i \frac{\partial T_i}{\partial x} \quad (7) $$

with \( \sum_i y_i = L_y \)

$$ k_i = \left\{ \begin{array}{l} k_m \text{ in the continuous phase} \\ k_f \text{ in the inclusions} \end{array} \right\} $$

Figure 3. Microscopic photograph of HDPE filled with 4 volume percent of Al

Figure 4. Two-dimensional model of the composite material

In the considered heat conduction problem the temperatures at the nodes along the boundaries $x = 0$ and $x = L_x$ are prescribed and known as $T_1$ and $T_2$, but the temperatures at the nodes in the interior region and on the adiabatic boundaries are unknown. Therefore, the problem involves many unknown temperatures. The equations needed for the determination of these temperatures are obtained by writing the appropriate finite-difference equation for each of these nodes.

Then, the finite-difference form of the energy equation without heat generation is written as;
\begin{equation}
\frac{(k_{i-l,j} + k_{i,j})}{2k_{i-l,j}k_{i,j}}(T_{i-l,j} - T_{i,j}) + \frac{(k_{i,j-1} + k_{i,j})}{k_{i,j-l,j}k_{i,j}}(T_{i,j-1} - T_{i,j}) + \frac{(k_{i,j+1} + k_{i,j})}{2k_{i,j+1}k_{i,j}}(T_{i,j+1} - T_{i,j}) = 0
\end{equation}

\begin{equation}
-\frac{(a_{i,j} + a_{2,i,j} + a_{3,i,j} + a_{4,i,j})}{a_{5,i,j}}T_{i,j} + a_{1,i,j}T_{i-1,j} + (a_{2,i,j} + a_{4,i,j})T_{i,j+1} + a_{3,i,j}T_{i+1,j} = 0
\end{equation}

The finite-difference equation for composite material on an adiabatic boundary

\begin{equation}
6. \text{ As seen from the Figure 6, some models give results approximate with the experimental data.}
\end{equation}

\begin{equation}
8. \text{ Similarly, the finite-difference form of the energy equation for } j = M \text{ is written as}
\end{equation}

\begin{equation}
-\frac{(a_{1,i,j} + a_{2,i,j} + a_{3,i,j} + a_{4,i,j})}{a_{5,i,j}}T_{i,j} + a_{1,i,j}T_{i-1,j} + (a_{2,i,j} + a_{4,i,j})T_{i,j+1} + a_{3,i,j}T_{i+1,j} = 0
\end{equation}

The finite-difference equation for composite material on an adiabatic boundary

\begin{equation}
10. \text{ Similarly, the finite-difference form of the energy equation for interior nodes is written as}
\end{equation}

\begin{equation}
-\frac{(a_{1,i,j} + a_{2,i,j} + a_{3,i,j} + a_{4,i,j})}{a_{5,i,j}}T_{i,j} + a_{1,i,j}T_{i-1,j} + (a_{2,i,j} + a_{4,i,j})T_{i,j+1} + a_{3,i,j}T_{i+1,j} = 0
\end{equation}

The finite-difference equation for composite material in the interior nodes

\begin{equation}
6. \text{ RESULTS AND DISCUSSION}
\end{equation}

In the Figure 5, the temperature distribution on the composite material composed of 4 % Aluminum filled high-density polyethylene is seen.

Results obtained from the experimental studies of Aluminum filled high-density polyethylene, several models and numerical studies are given in the Figure 6. As seen from the Figure 6, some models give results approximate with the experimental data.
If the results obtained from the numerical analysis are compared with the results obtained from the experimental study, it is seen that the numerical results are higher. It can be said that, since the quality of the pictures used in image processing carried out on the picture files in numerical study are not so good, the procedure was not so successful. Objects defined as noise in the picture will be accepted as Al particles added into the high-density polyethylene and in return, these additional objects will increase the thermal conductivity of the composite. Another reason for this value to be high can be the nonhomogeneous distribution of the Al particles into high-density polyethylene during the preparation of the specimens which effect the picture photographed of the piece taken from the specimen. Since the Al particles are not well mixed into that region, they may appear more dense. It is clear that this increases the thermal conductivity of the composite. All the models fail to predict thermal conductivity for particle content greater than 10 %.

7. REFERENCES


