THE INVERSE DETERMINATION OF THE VOLUME FRACTION
OF FIBERS IN A UNIDIRECTIONALLY REINFORCED COMPOSITE
FOR A GIVEN EFFECTIVE THERMAL CONDUCTIVITY

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THE INVERSE DETERMINATION OF THE VOLUME FRACTION OF FIBERS IN A UNIDIRECTIONALLY REINFORCED COMPOSITE FOR A GIVEN EFFECTIVE THERMAL CONDUCTIVITY

MAGDALENA MIERZWICZAK AND JAN ADAM KOŁODZIEJ

We consider the problem of determining the volume fraction of fibers in a unidirectionally reinforced composite in order to provide the appropriate effective thermal conductivity. The problem is formulated in such a way as to be treated as an inverse heat transfer problem. The thermal conductivities of the constituents (fibers and matrix) and fiber arrangement are known. The calculations are carried out for a perfect thermal contact between the fibers and matrix.

1. Introduction

In the literature the following problems are considered to be classical inverse heat conduction problems:

- determination of heat sources [Yan et al. 2008],
- determination of the heat transfer coefficient [Hon and Wei 2004],
- the Cauchy problem [Marin 2005], and
- determination of the temperature dependent thermal conductivity [Chantasiriwan 2002].

These problems usually apply to homogeneous media. In the case of composite materials (nonhomogeneous media) other practically important issues might have to be considered. One of them is the inverse problem of determination of the volume fraction of constituents in order to obtain the appropriate effective thermal conductivity. Let’s consider a unidirectional fibrous composite with regular arrangement of fibers (Figure 1, left). If the thermal conductivity coefficients of constituents and their volume fractions are known then the composite can be treated as a homogeneous region for which effective thermal conductivity can be determined as a function of known parameters. Currently there are many papers in which the effective thermal conductivity coefficient is determined for a regular arrangement of fibers for given thermal conductivity of constituents and volume fraction of fibers (the direct problem). The method of determination is usually based on the solution of the heat transfer equation at a microstructure level in repeated elements of an array [Han and Cosner 1981]. But to our knowledge no paper has considered the inverse problem of determination of the volume fraction of fibers for a given effective thermal conductivity. Here we propose an analytic-numerical algorithm for determination of the volume fraction of fibers in order to obtain a given value of the transverse effective thermal conductivity \( \lambda_z \) (the inverse problem).

Keywords: effective thermal conductivity, inverse heat transfer problem, boundary collocation method, Newton’s method.
2. Direct problem: determination of the effective thermal conductivity coefficient of the composite material

Consider a unidirectional composite with fibers arranged in a matrix in a regular, square array with imperfect thermal contact between the fiber and matrix (Figure 1, left), where $a$ is radius of the fibers, $2b$ is the distance between neighboring fibers, $E = a/b$, and $\varphi = \pi E^2/4$ is the volume fraction of the fibers. The ratio of the thermal conductivity of fibers $\lambda_f$ to matrix $\lambda_m$ is denoted as $F = \lambda_f/\lambda_m$, $R = r/b$ is the dimensionless radius, $X = x/b$ and $Y = y/b$ are the dimensionless Cartesian coordinates, $T = (\hat{T} - \hat{T}_R)/(\hat{T}_R - \hat{T}_L)$ is the dimensionless temperature field, and $\hat{T}_R$ and $\hat{T}_L$ are the temperatures on the left and right boundaries of the repeated element, respectively. In order to solve the boundary value problem in the repeated element of the composite (Figure 1) the boundary collocation method is used [Kołodziej and Zieliński 2009]. The general solution of the Laplace equation in a polar coordinate system has the form

$$T = A_0 + A_1 \theta + A_2 \theta \ln R + A_3 \ln R + \sum_{k=1}^{\infty} \left( B_k R^k + C_k R^{-k} \right) \cos(k\theta) + \left( D_k R^k + E_k R^{-k} \right) \sin(k\theta),$$

(2-1)

where $A_0, A_1, \ldots, E_k$ are integral constants.

Given the repetitive element of the square array $\Omega = \Omega_m + \Omega_f$ in the region of the fiber $\Omega_f$ and the matrix $\Omega_m$, a solution is predicted with the form of (2-1). Some of the constants must be determined
strictly by the conditions at the bottom and on the left side of the repeated element:

\[
\frac{\partial T_f}{\partial \theta} = \frac{\partial T_m}{\partial \theta} = 0 \quad \text{for} \quad \theta = 0, \quad T_f = T_m = 1 \quad \text{for} \quad \theta = \frac{\pi}{2},
\]

(2-2)

and the contact conditions of the fiber-matrix:

\[
F \frac{\partial T_f}{\partial R} = \frac{\partial T_m}{\partial R} \quad \text{for} \quad R = E, \quad T_f = T_m \quad \text{for} \quad R = E.
\]

(2-3)

After determining the constants from the boundary conditions (2-2) and from the contact conditions (2-3) of fiber-matrix, marking the remaining constants as \( w_k \), and cutting off an infinite number of test functions to \( N \) expressions, we obtain a solution for the temperature field of the fiber and matrix:

\[
T_f = 1 + \sum_{k=1}^{N} w_k R^{(2k-1)} \cos((2k-1)\theta),
\]

(2-4)

\[
T_m = 1 + \sum_{k=1}^{N} \frac{w_k}{2} \left[ (1 + F) R^{(2k-1)} + (1 - F) \frac{E^2(2k-1)}{R^{(2k-1)}} \right] \cos((2k-1)\theta).
\]

(2-5)

The constants \( w_k \) are determined by fulfillment of the condition on the collocation points on the upper \( \Gamma_2 \) and on the right \( \Gamma_1 \) edges of the concerned region (Figure 2):

\[
T_m = 0 \quad \text{for} \quad X = 1,
\]

(2-6)

\[
\frac{\partial T_m}{\partial Y} = 0 \quad \text{for} \quad Y = 1.
\]

(2-7)

Figure 2. The collocation points at the upper and right boundaries of the matrix in a repeated element in which the boundary conditions are collocated.
The condition (2-7) can be written for polar coordinates:

$$\frac{\partial T_m}{\partial Y} = \frac{\partial T_m}{\partial R} \sin(\theta) + \frac{1}{R} \frac{\partial T_m}{\partial \theta} \cos(\theta).$$

Choosing $N_1$ points on the right boundary $\Gamma_1$ and $N_2$ points on the upper boundary $\Gamma_2$ and collocating the conditions (2-6) and (2-8) we obtain the system of $N_1 + N_2$ linear equations with $N$ unknown coefficients $w_k$, $k = 1, \ldots, N$:

$$Aw = b.$$ (2-9)

The constants $w_k$ obtained by the Gaussian elimination method provide estimates of the value of the global heat flux through the unit region of the considered element:

$$q = \frac{1}{b} \left[ -\lambda_f \int_0^a \frac{\partial T_f}{\partial x} \bigg|_{x=0} \, dy + \lambda_m \int_a^b \frac{\partial T_m}{\partial x} \bigg|_{x=0} \, dy \right].$$ (2-10)

The transverse effective thermal conductivity is defined by the formula

$$\lambda_z = \frac{qb}{\Delta \hat{T}},$$ (2-11)

where $b$ is the distance between the isothermal boundaries and $\Delta \hat{T} = \hat{T}_L - \hat{T}_R$ is the difference of the temperatures at the isothermal edges. After taking into consideration in formula (2-11) the definition of the nondimensional temperature and coordinates, the value of the effective thermal conductivity in relation to the thermal conductivity of the matrix can be calculated from the relationship:

$$\frac{\lambda_z}{\lambda_m} = -F \int_0^E \frac{1}{R} \frac{\partial T_f}{\partial \theta} \bigg|_{\theta=\pi} \, dR + \int_0^1 \frac{1}{R} \frac{\partial T_m}{\partial \theta} \bigg|_{\theta=\pi} \, dR,$$ (2-12)

or

$$\frac{\lambda_z}{\lambda_m} = \sum_{k=1}^N \frac{w_k}{2} (-1)^k \left[ (F + 1) + (F - 1) E^{2(2k-1)} \right].$$ (2-13)

### 3. The results of the numerical experiment

The results of the calculations of the effective thermal conductivity of the fibrous composite are shown in Figure 3. The value of the effective thermal conductivity in relation to the thermal conductivity of the matrix $\lambda_z/\lambda_m = (\lambda_z/\lambda_m)(\varphi)|_{F}$ is presented as a function of the volume fraction of fibers $\varphi$ for the desired value of thermal conductivity ratio $F$ of the fiber $\lambda_f$ to the matrix $\lambda_m$, with $F \in \{0.5, 2, 10, 20\}$. In order to compare the results, for a flat layer composite consisting of two components with different
The comparative results for a flat layer of composite are shown in Figure 3 by the dotted line. The value of the effective thermal conductivity $\lambda_z$ depends not only on the constants characterizing the composite, $F$ and $E$, but also on the coefficients $w_k$ involved in fulfilling the boundary conditions at the $N_1 + N_2$ collocation points. Table 1 shows the influence of the number of collocation points on the maximum error fulfilling the collocation boundary conditions calculated at the control points (between the collocation points). The analysis of the results shows that increase in the number of collocation points doesn’t lead to an increase in the accuracy of the calculations. Increasing the number of collocation points entails a rise in the dimension of the matrix system of equations. In all four examples presented in Table 1, the smallest maximum error satisfying the boundary conditions was obtained for 7 collocation points on the right edge and for 6 points on the upper edge of the region considered.

4. Inverse problem: determination of the volume fraction of fibers in a composite for a given effective thermal conductivity

At times, when designing composites with specific properties of the fibers and matrix we must estimate the fraction of the volume of fibers to obtain effective thermal conductivity values. Assuming that $E = a/b$ is unknown, we use the known value of the effective thermal conductivity in relation to the thermal conductivity of the matrix $\lambda_z/\lambda_m$. From the collocation of the boundary conditions in the $N_1 + N_2$ points on the right and upper edges of the considered region and from condition (2-11) we obtain a system of $N_1 + N_2 + 1$ nonlinear equations with the $N + 1$ unknowns $w_k$ and $E$: 
Table 1. The impact of the number of collocation points on the value of the effective thermal conductivity of the composite and the maximum error of fulfilling the boundary conditions at control points.

\[
f_j = 1 + \sum_{k=1}^{N} \frac{w_k}{2} \left[ (1 + F) R_j^{(2k-1)} + (1 - F) \frac{E^{2(2k-1)}}{R_j^{(2k-1)}} + \right] \cos((2k-1) \theta_j) = 0,
\]
\[
(R_j, \theta_j) \in \Gamma_1 \quad j = 1, \ldots, N_1,
\]

\[
f_j = \sum_{k=1}^{N} w_k (2k - 1) \left[ (1 + F) R_j^{(2k-1)} \sin((2k-1) \theta_j) + (1 - F) \frac{E^{2(2k-1)}}{R_j^{(2k-1)}} \cos(2k \theta_j) \right] = 0,
\]
\[
(R_j, \theta_j) \in \Gamma_2 \quad j = N_1 + 1, \ldots, N_1 + N_2,
\]

\[
f_{N_1+N_2+1} = \sum_{k=1}^{N} \frac{w_k}{2} (-1)^k \left[ (1 + F) + (F - 1) E^{2(2k-1)} \right] - \frac{\lambda_z}{\lambda_m} = 0.
\]
The nonlinear system of \( N_1 + N_2 + 1 \) equations \( f \) with \( N + 1 \) unknowns \( W = [w_1, \ldots, w_N, E]^T \) is solved by using Newton’s iterative method:

\[
\left[ \begin{array}{c} w_1 \\ \vdots \\ w_N \\ E \end{array} \right]^{(i+1)} = \left[ \begin{array}{c} w_1 \\ \vdots \\ w_N \\ E \end{array} \right]^{(i)} - \left[ \begin{array}{c} f_1^{(i)} \\ \vdots \\ f_{N+1+N_2}^{(i)} \end{array} \right] \left[ \begin{array}{ccc} J_{1,1}^{(i)} & \ldots & J_{1,N+1}^{(i)} \\ \vdots & \ddots & \vdots \\ J_{N+1+N_2,1}^{(i)} & \ldots & J_{N+1+N_2+1,N+1}^{(i)} \end{array} \right]^{-1}, 
\]

(4-2)

\[
W^{(i+1)} = W^{(i)} - f(W^{(i)}) J(W^{(i)})^{-1} \quad \Rightarrow \quad W^{(i+1)} = W^{(i)} - Y(W^{(i)}),
\]

\[
Y(W^{(i)}) = f(W^{(i)}) J(W^{(i)})^{-1} \quad \Rightarrow \quad J(W^{(i)})^{-1} Y(W^{(i)}) = f(W^{(i)}).
\]

The functions \( f_i \) are described by (4-1), while the Jacobi elements have the following form:

\[
J_{j,k} = \frac{\partial f_j}{\partial w_k} = \frac{1}{2} \left[ (1 + F) R_j^{2(k-1)} + (1 - F) \frac{E^{2(k-1)}}{R_j^{(2k-1)}} \right] \cos((2k-1)\theta_j), \quad j = 1, \ldots, N_1, \quad k = 1, \ldots, N,
\]

\[
J_{j,N+1} = \frac{\partial f_j}{\partial E} = \sum_{k=1}^{N} w_k (2k-1)(1 - F) \frac{E^{(4k-3)}}{R_j^{(2k-1)}} \cos((2k-1)\theta_j), \quad j = 1, \ldots, N_1,
\]

\[
J_{j,k} = \frac{\partial f_j}{\partial w_k} = \frac{(2k-1)}{2} \left[ (1 + F) R_j^{2(k-1)} \sin(2(k-1)\theta_j) + (1 - F) \frac{E^{2(k-1)}}{R_j^{(2k)}} \sin(2k\theta_j) \right], \quad j = N_1 + 1, \ldots, N_1 + N_2, \quad k = 1, \ldots, N,
\]

(4-3)

\[
J_{j,N+1} = \frac{\partial f_j}{\partial E} = \sum_{k=1}^{N} w_k (2k-1)^2 \left[ (1 - F) \frac{E^{(4k-3)}}{R_j^{(2k)}} \sin(2k\theta_j) \right], \quad j = N_1 + 1, \ldots, N_1 + N_2,
\]

\[
J_{j,k} = \frac{\partial f_j}{\partial w_k} = \frac{(-1)^k}{2} \left[ (1 + F) + (F - 1) E^{2(2k-1)} \right], \quad j = N_1 + N_2 + 1, \quad k = 1, \ldots, N,
\]

\[
J_{j,N+1} = \frac{\partial f_j}{\partial E} = \sum_{k=1}^{N} w_k (2k-1)(-1)^k (F - 1) E^{(4k-3)}, \quad j = N_1 + N_2 + 1.
\]

To start the Newton’s iteration we need to know \( W^{(0)} = [w_1^{(0)}, \ldots, w_N^{(0)}, E^{(0)}]^T \) as an initial condition. As an initial value of the constants \( w_k^{(0)}, k = 1, \ldots, n \), the solution of the linear problem for \( E = 0.1 \) has been adopted. The condition for the end of the iteration was adopted at \( \delta_{\text{Newt}} = \| W^{(i+1)} - W^{(i)} \|_{\text{max}} \leq 10^{-7} \), where \( \| \cdot \|_{\text{max}} \) means the maximum norm.

5. The results of the numerical experiment

The results of the iterative calculation of the volume fraction of fibers for a composite are shown in Figure 4. The value of the volume fraction of fibers in a composite \( \phi \) is presented as a function \( \phi(\lambda_c/\lambda_m) \) of the effective thermal conductivity in relation to the thermal conductivity of the matrix.
\[ \varphi = \varphi \left( \frac{\lambda_z}{\lambda_m} \right)_F \]

\[ \varphi = \left( \left( \frac{\lambda_z}{\lambda_m} \right)^{-1} - 1 \right) \frac{F}{1 - F} \]

\[ \lambda_z/\lambda_m \text{ for the assumed value of the thermal conductivity ratio of the fiber to the matrix, } F = \lambda_f / \lambda_m \in \{0.5, 2, 10, 20\}. \]

In order to compare the results for a flat composite layer consisting of two components with different thermal conductivities, the volume fraction of the fibers for a known value of the effective thermal conductivity for an ideal contact with the components can be calculated from

\[ \varphi = \left( \left( \frac{\lambda_z}{\lambda_m} \right)^{-1} - 1 \right) \frac{F}{1 - F} \]

### Table 2

The impact of the number of collocation points on the value of the volumetric fraction of the fibers in the composite and the maximal error fulfillment of the boundary conditions at checkpoints.

<table>
<thead>
<tr>
<th>( N_1 )</th>
<th>( N_2 )</th>
<th>( \varphi )</th>
<th>( E )</th>
<th>( \delta_{\max} ) ( T_{m=0} )</th>
<th>( \delta_{\max} ) ( \partial T_m / \partial Y = 0 )</th>
<th>( \varphi )</th>
<th>( E )</th>
<th>( \delta_{\max} ) ( T_{m=0} )</th>
<th>( \delta_{\max} ) ( \partial T_m / \partial Y = 0 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>4</td>
<td>0.1904</td>
<td>0.4924</td>
<td>5.82 \times 10^{-5}</td>
<td>0.100879</td>
<td>0.5013</td>
<td>0.7989</td>
<td>1.74 \times 10^{-3}</td>
<td>2.688120</td>
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<tr>
<td>6</td>
<td>5</td>
<td>0.2036</td>
<td>0.5092</td>
<td>4.99 \times 10^{-5}</td>
<td>0.000256</td>
<td>0.6362</td>
<td>0.9</td>
<td>2.05 \times 10^{-2}</td>
<td>0.059686</td>
</tr>
<tr>
<td>7</td>
<td>6</td>
<td>0.2036</td>
<td>0.5092</td>
<td>6.72 \times 10^{-7}</td>
<td>8.91 \times 10^{-5}</td>
<td>0.6372</td>
<td>0.9007</td>
<td>5.68 \times 10^{-4}</td>
<td>0.016511</td>
</tr>
<tr>
<td>8</td>
<td>7</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
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</tr>
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<th>( \varphi )</th>
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<th>( E )</th>
<th>( \delta_{\max} ) ( T_{m=0} )</th>
<th>( \delta_{\max} ) ( \partial T_m / \partial Y = 0 )</th>
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<tr>
<td>5</td>
<td>4</td>
<td>0.1970</td>
<td>0.4774</td>
<td>1.49 \times 10^{-5}</td>
<td>0.026341</td>
<td>0.7876</td>
<td>1.0014</td>
<td>0.00025</td>
<td>0.32083</td>
</tr>
<tr>
<td>6</td>
<td>5</td>
<td>0.1915</td>
<td>0.4937</td>
<td>1.18 \times 10^{-5}</td>
<td>7.26 \times 10^{-5}</td>
<td>0.6327</td>
<td>0.8976</td>
<td>0.00025</td>
<td>0.0005</td>
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<tr>
<td>7</td>
<td>6</td>
<td>0.1915</td>
<td>0.4938</td>
<td>1.13 \times 10^{-7}</td>
<td>2.13 \times 10^{-5}</td>
<td>0.6328</td>
<td>0.8976</td>
<td>5.84 \times 10^{-5}</td>
<td>0.00204</td>
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<td>-</td>
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</tbody>
</table>
DETERMINATION OF THE VOLUME FRACTION OF FIBERS IN A COMPOSITE

\[ F = 10 \]

<table>
<thead>
<tr>
<th>( \lambda_z/\lambda_m )</th>
<th>( \lambda_z/\lambda_m = 1.4 )</th>
<th>( \lambda_z/\lambda_m = 3.35 )</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Iter.</strong></td>
<td><strong>( \delta_{\text{Newton}} )</strong></td>
<td><strong>E</strong></td>
</tr>
<tr>
<td>1</td>
<td>0.456063</td>
<td>0.5439</td>
</tr>
<tr>
<td>2</td>
<td>0.032858</td>
<td>0.5111</td>
</tr>
<tr>
<td>3</td>
<td>1.89 \times 10^{-3}</td>
<td>0.5092</td>
</tr>
<tr>
<td>4</td>
<td>3.41 \times 10^{-6}</td>
<td>0.5092</td>
</tr>
<tr>
<td>5</td>
<td>1.13 \times 10^{-11}</td>
<td>0.5092</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>( \lambda_z/\lambda_m )</th>
<th>( \lambda_z/\lambda_m = 0.88 )</th>
<th>( \lambda_z/\lambda_m = 0.65 )</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Iter.</strong></td>
<td><strong>( \delta_{\text{Newton}} )</strong></td>
<td><strong>E</strong></td>
</tr>
<tr>
<td>1</td>
<td>0.357932</td>
<td>0.6421</td>
</tr>
<tr>
<td>2</td>
<td>1.31 \times 10^{-1}</td>
<td>0.5113</td>
</tr>
<tr>
<td>3</td>
<td>1.72 \times 10^{-2}</td>
<td>0.4941</td>
</tr>
<tr>
<td>4</td>
<td>2.99 \times 10^{-4}</td>
<td>0.4938</td>
</tr>
<tr>
<td>5</td>
<td>9.05 \times 10^{-8}</td>
<td>0.4938</td>
</tr>
</tbody>
</table>

**Table 3.** Convergence of Newton’s method for the test examples, with \( N_1 = 7 \) and \( N_2 = 8 \).

The results for a flat composite layer are presented by the dotted lines in *Figure 4*. As with the problem of identification of \( \lambda_z/\lambda_m \), so also for the iterative identification of the volume fraction of fibers \( \varphi \) in a composite; the number of collocation points \( N_1 + N_2 \) where the boundary condition is approximately fulfilled affects the accuracy of the calculations. *Table 2* shows the impact of the number of collocation points on the value of the volumetric fraction of fibers \( \varphi \) in the composite and the maximum error of fulfillment of boundary conditions at the checkpoints (between collocation points). As in the case of the direct problem, we obtain the best results for 7 collocation points at the right edge \( \Gamma_1 \) of a large finite element and 6 points at the upper edge \( \Gamma_2 \). In the case of the inverse problem for a large number of collocation points (greater than 7) the convergence of the algorithm is lost. *Table 3* presents the convergence of the used Newton’s iterative method for four test examples. The method proves to be convergent very quickly, and just after five iterations we get the correct result of the iteration with an error of less than \( 10^{-7} \).

6. Conclusions

The presented method of determining the volume fraction of fibers of a composite or the effective thermal conductivity except in the cases of maximal fiber density is easy to implement and efficient. It can be easily applied to other configurations of regular arrangement of fibers in the matrix, for example to a triangular or hexagonal mesh. This study compared the influence of the ratio of the thermal conductivity of fibers to the thermal conductivity of matrix \( F \) on the value of the volumetric fraction of the fibers and the value of the effective thermal conductivity of the composite. It was also shown that increasing the number of collocation points doesn’t reduce the error of the approximation of the boundary conditions; it leads to the ill-conditioning of the system of equations.
References


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