Numerical analytic method for solving the inverse coefficient problem of heat conduction in anisotropic half-space

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Abstract. The paper proposes a numerical-analytical method for solving the inverse problem of identification of the components of the thermal conductivity tensor in anisotropic materials on the basis of the earlier analytical solution of the heat conduction problem in anisotropic half-space when heated with a thermal flow. The method is based upon expansion of the residual functional into Taylor series and determination of incremental vectors of the target coefficients which are then used for application of iterative gradient descent algorithms. The solution demonstrates fine iteration convergence even if the initial approximation of the coefficients vector differs from the target one by several times, and even when there is some inaccuracy in the experimental data. The proposed method can be used for a wide range of problems in continuum mechanics.

1. Introduction

Mathematical model of direct problems of continuum mechanics in general and heat conduction in particular describes cause (initial and boundary conditions, coefficients, algebraic, differential or integral equations) and effect (in heat conduction problems — thermal flows, temperature fields, gas-dynamic characteristics etc.) relationship [1].

In the inverse problems, vice versa — the effect is used to identify causes which are not described with mathematical models, which often makes the inverse problems incorrect, because one of the following conditions (or all of them) is not satisfied: the solution exists, it is unique, there is a continuous dependence of the solution on the initial data (stability) [2,3].

When analyzing the thermal condition of structural elements of power and transport machinery in process of designing or in operation, we should be aware of the thermo-physical properties (TPP) of the materials they are made of [1]. This is particularly important for composite materials which TPP are often unknown. These properties, first of all, include the principal components and orientation angles of the principal axes of the thermal conductivity tensors of anisotropic materials, as well as volumetric heat capacity.

Under these conditions, the above-mentioned properties can be obtained from the solution of inverse heat conduction coefficient problems, if the temperature of the material is measured at several points as a function of time.

The difficulty is that the experimental temperature values depend on unknown thermo-physical properties which should be defined with the prescribed accuracy in the inverse problem.
in which the initial TPP values included into the iteration process may significantly (by several times) differ from the true values. Moreover, they should be within a certain tolerable error.

There are fairly large number of works devoted to inverse problems [2–5] concerning one-dimensional inverse heat conduction problems for the recovery of permanent and non-linear heat conduction coefficients in isotropic media. The works [6–8] suggest a numerical solution of the inverse coefficient and boundary problems based on parametric identification.

This paper proposes a method for solving the problem on recovery of the principal components and orientation angles of the principal axes of the thermal conductivity tensors based on the analytical solutions of the second initial-boundary value problem of anisotropic heat conduction obtained in [9].

2. Problem statement

We consider the following inverse heat conduction coefficient problem for determination of the components $\lambda_{11}$, $\lambda_{22}$, $\lambda_{12}$ of the thermal conductivity tensor in anisotropic half-space:

$$
\begin{align*}
\lambda_{11} \frac{\partial^2 T}{\partial x^2} + 2\lambda_{12} \frac{\partial^2 T}{\partial x \partial y} + \lambda_{22} \frac{\partial^2 T}{\partial y^2} &= c\rho \frac{\partial T}{\partial t}, \quad x \in (-\infty, +\infty), \quad y \in (0, +\infty), \quad t > 0, \\
- \left( \lambda_{21} \frac{\partial T}{\partial x} + \lambda_{22} \frac{\partial T}{\partial y} \right) &= q\eta (l - |x|), \quad x \in (-\infty, +\infty), \quad y = 0, \quad t > 0,
\end{align*}
$$

$$
T(\pm \infty, y, t) = 0, \quad \frac{\partial T(\pm \infty, y, t)}{\partial x} = 0, \quad x \to \pm \infty, \quad y \in (0, +\infty), \quad t > 0,
$$

$$
T(x, \infty, t) = 0, \quad \frac{\partial T(x, \infty, t)}{\partial y} = 0, \quad x \in (-\infty, +\infty), \quad y \to \infty, \quad t > 0
$$

$$
T(x, y, 0) = 0, \quad x \in (-\infty, +\infty), \quad y \in (0, +\infty), \quad t = 0.
$$

The equations for the determination of the $\lambda_{ij}$, $i,j = 1,2$ of the thermal conductivity tensor are as follows:

$$
\begin{align*}
\lambda_{11} &= \lambda_\xi \cos^2 \varphi + \lambda_\eta \sin^2 \varphi, \\
\lambda_{22} &= \lambda_\xi \sin^2 \varphi + \lambda_\eta \cos^2 \varphi, \\
\lambda_{12} &= (\lambda_\xi - \lambda_\eta) \sin \varphi \cos \varphi,
\end{align*}
$$

where $\lambda_\xi$, $\lambda_\eta$ are principal components of thermal conductivity tensor, $\varphi$ is orientation angle of the principal axes $O\xi$ and $O\eta$.

In order to complete the inverse coefficient heat conduction problem we should set the experimental temperature values as a function of time on an interior of a set $(x, y)_i, i = 1, I$. 

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{Computational scheme}
\end{figure}
Since the body is two-dimensional, we should take at least two points with experimental values on each coordinate axis, and since the body is anisotropic the minimal number of points with experimental temperature values on the coordinate axes is three (in accordance with spatial distribution for finite-difference schemes). Thus we take the minimum allowable number of spatial points, which is nine, with experimental temperature values as a function of time

\[ T((x, y)_i, t^j) = \tilde{T}_{i,j}, \quad i = 3 \times 3 = 9, \quad j = \overline{1, J}. \]  

(7)

Analytical solution for the direct problem of heat conduction (1)–(5) is described by the following equation [9]:

\[ T(x, y, t) = \frac{q}{2\sqrt{\pi}\gamma\lambda_{22}} \int_0^t \frac{1}{\sqrt{t-\tau}} \exp \left[ -\frac{\gamma y^2}{4(t-\tau)} \right] \left[ \text{erf} \left( \frac{1+(x-\alpha y)}{2\sqrt{\beta(t-\tau)/\gamma}} \right) + \text{erf} \left( \frac{l-(x-\alpha y)}{2\sqrt{\beta(t-\tau)/\gamma}} \right) \right] d\tau, \]  

(8)

where \( \alpha = \lambda_{12}/\lambda_{22}, \beta = (\lambda_{11}\lambda_{22} - \lambda_{12}^2)/\lambda_{22}^2 = \lambda_\xi \lambda_\eta/\lambda_{22}^2, \gamma = c\rho/\lambda_{22}. \)

In order to determine the thermo-physical properties of the anisotropic half-space — the components of the thermal conductivity tensor \( \lambda_{11}, \lambda_{12} = \lambda_{21}, \lambda_{22} \) — we apply the same analytical solution (8). Since the thermo-physical properties (TPP) \( \lambda_\xi, \lambda_\eta, \varphi \) are included into the complexes \( \alpha = \lambda_{12}/\lambda_{22}, \beta = (\lambda_{11}\lambda_{22} - \lambda_{12}^2)/\lambda_{22}^2, \gamma = c\rho/\lambda_{22}, \) after defining of the coefficient \( \lambda_{22} \) and the properties \( \alpha, \beta, \gamma, \) we can define all the TPP as follows:

\[ \lambda_{12} = \alpha \lambda_{22}, \quad \lambda_{11} = \left[ \beta + \frac{(\lambda_{12}/\lambda_{22})^2}{\lambda_{22}} \right] \lambda_{22}, \quad A \rho = \gamma \lambda_{22} \]  

(9)

and, moreover, the principal components \( \lambda_\xi, \lambda_\eta \) and the orientation angle \( \varphi \) of the main axes \( O\xi, O\eta, \) of the thermal conductivity tensor from the relations (6) under the Jacobi rotation method [10], according to which we can determine the eigenvalues of \( \lambda_\xi, \lambda_\eta, \) rotation angle \( \varphi \) and eigen vectors for the symmetric matrix \( \Lambda = \left( \begin{array}{cc} \lambda_{11} & \lambda_{12} \\ \lambda_{21} & \lambda_{22} \end{array} \right) \) by means of rotation of prime vectors, where the matrix columns are coordinate columns of some of the vectors, through the angle \( \varphi \) until the prime vectors match with the eigen basis of the matrix \( \Lambda: \)

\[ \varphi = \frac{1}{2} \arctan \frac{2\lambda_{12}}{\lambda_{11} - \lambda_{22}}, \]  

(10)

\[ \lambda_\xi = \lambda_{11} \cos^2 \varphi + \lambda_{22} \sin^2 \varphi + \lambda_{12} \sin(2\varphi), \]  

(11)

\[ \lambda_\eta = \lambda_{11} \sin^2 \varphi + \lambda_{22} \cos^2 \varphi - \lambda_{12} \sin(2\varphi). \]  

(12)

Thus, as soon as the parameters \( \lambda_{22}, \alpha, \beta \) are defined, we can define the thermo-physical properties \( \lambda_{12}, \lambda_{11}, \varphi, \lambda_\xi, \lambda_\eta \) from the relations (9)–(12).

For the purposes of solving the inverse coefficient thermal conductivity problem, the following notations are introduced:

\[ \lambda_1 \equiv \lambda_{11}, \quad \lambda_2 \equiv \lambda_{22}, \quad \lambda_3 \equiv \lambda_{12}, \]  

(13)

and the \( \partial T_{i,j}(\lambda^{(m)})/\partial \lambda_k, i = \overline{1, I}, j = \overline{1, J}, k = \overline{1, K}, \) elements of sensitivity matrix are calculated at a known iteration, where \( I = 9, J = 2, K = 3, \) by differentiating the equation (8) with respect to the variables \( \lambda_k, k = \overline{1, 3}. \)

3. Solution method

For the purpose of identification of the properties (13), a quadratic functional in introduced

\[ S(\lambda_1, \lambda_2, \lambda_3) = \frac{1}{2} \sum_{i=1}^{I} \sum_{j=1}^{J} [T_{i,j}(\lambda_1, \lambda_2, \lambda_3) - \tilde{T}_{i,j}]^2, \]  

(14)
where $T_{i,j}(\lambda_1, \lambda_2, \lambda_3) \equiv T((x, y)_i, t^j, \lambda_1, \lambda_2, \lambda_3)$, as a sum of space-time variables of squared deviations of the experimental values $\bar{T}_{i,j}$ at the points $(x, y)_i, t^j$ from the estimated values $T_{i,j}(\lambda_1, \lambda_2, \lambda_3)$ obtained from the analytic formula (8) in the listed points using arbitrary input data $\lambda_1, \lambda_2, \lambda_3$. The experimental values $\bar{T}_{i,j}$ at the same space-time points (these experimental values are considered to be accurate) are the calculations according to the same formula (8) based on the values $\lambda_1, \lambda_2, \lambda_3, \lambda_4$ which are considered accurate.

Denote the vector of unknowns as $\lambda = (\lambda_1, \lambda_2, \lambda_3)^T$. Then according to the gradient descent method [10] we can write the following algorithm for minimization of the functional (14):

$$
\lambda^{(n+1)} = \lambda^{(n)} - \alpha_n \text{grad} S(\lambda^{(n)}),
$$

where $\alpha_n$ are parametric pitches which are sufficiently small and are subject to the condition

$$
S(\lambda^{(n+1)}) < S(\lambda^{(n)}).
$$

If we follow the condition (17), the initial value $\alpha_0$ can be selected arbitrarily, for example $\alpha_0 = 2$. Then, if the condition (17) is not fulfilled in the result of the next iteration, the $\alpha_n$ at this iteration is multiplied by ten, and the calculation is repeated at this iteration, otherwise (when (17) is fulfilled) $\alpha_n$ it is divided by 10 for the next iteration.

The iterative process stops in proximity to zero that is, when the following condition is met

$$
|\text{grad} S(\lambda^{(n)})| \leq \varepsilon,
$$

where $\varepsilon$ is the prescribed accuracy.

In order to calculate the gradient of the functional (14) followed by substitution into (16) and definition of vector $\Delta \lambda^{(n)} = \lambda^{(n+1)} - \lambda^{(n)}$, we expand the following function $T_{i,j}(\lambda^{(n)}) \equiv T_{i,j}(\lambda_1, \lambda_2, \lambda_3, \lambda_4)$ in a Taylor series in the neighborhood of $\lambda^{(n)}$, while preserving the components linear to $\Delta \lambda^{(n)}$ and we obtain

$$
S(\lambda^{(n+1)}) = \frac{1}{2} \sum_{i=1}^{I} \sum_{j=1}^{J} \left\{ T_{i,j}(\lambda^{(n)}) + \sum_{k=1}^{K} \left( \frac{\partial T_{i,j}(\lambda^{(n)})}{\partial \lambda_k} \right) \Delta \lambda_k^{(n)} \right\} - \bar{T}_{i,j} \right\}^2.
$$

The components of the gradient of the functional (19) are as follows

$$
\frac{\partial S(\lambda^{(n+1)})}{\partial \lambda_k} = \sum_{i=1}^{I} \sum_{j=1}^{J} \left[ T_{i,j}(\lambda^{(n)}) - \bar{T}_{i,j} + \sum_{k=1}^{K} \left( \frac{\partial T_{i,j}(\lambda^{(n)})}{\partial \lambda_k} \right) \Delta \lambda_k^{(n)} \right]
$$

$$
\times \left\{ \frac{\partial T_{i,j}(\lambda^{(n)})}{\partial \lambda_k} + \frac{\partial}{\partial \lambda_k} \left[ \sum_{k=1}^{K} \left( \frac{\partial T_{i,j}(\lambda^{(n)})}{\partial \lambda_k} \Delta \lambda_k^{(n)} \right) \right] \right\}, \quad k = 1, 4.
$$

where $\varepsilon$ is the prescribed accuracy.
Let us represent (20) in the following vector-matrix form:

\[ S(\lambda^{(n)}) = Z^T(\lambda^{(n)}[T(\lambda^{(n)}) - \bar{T}] + Z^T(\lambda^{(nt)})Z(\lambda^{(n)})\Delta \lambda^{(n)}), \]  

(21)

\[ Z(\lambda^{(n)}) = \left( \begin{array}{cccc}
\frac{\partial T_{11}(\lambda^{(n)})}{\partial \lambda_1} & \frac{\partial T_{11}(\lambda^{(n)})}{\partial \lambda_2} & \cdots & \frac{\partial T_{11}(\lambda^{(n)})}{\partial \lambda_k} \\
\frac{\partial T_{12}(\lambda^{(n)})}{\partial \lambda_1} & \frac{\partial T_{12}(\lambda^{(n)})}{\partial \lambda_2} & \cdots & \frac{\partial T_{12}(\lambda^{(n)})}{\partial \lambda_k} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{\partial T_{I,J}(\lambda^{(n)})}{\partial \lambda_1} & \frac{\partial T_{I,J}(\lambda^{(n)})}{\partial \lambda_2} & \cdots & \frac{\partial T_{I,J}(\lambda^{(n)})}{\partial \lambda_k}
\end{array} \right), \]  

(22)

\[ (T(\lambda^{(n)}) - \bar{T})^T = ((T_{1,1}(\lambda^{(n)}) - \bar{T}_{1,1}), \ldots, (T_{I,1}(\lambda^{(n)}) - \bar{T}_{I,1}), \\
(T_{1,2}(\lambda^{(n)}) - \bar{T}_{1,2}), \ldots, (T_{I,2}(\lambda^{(n)}) - \bar{T}_{I,2}), \ldots, (T_{I,J}(\lambda^{(n)}) - \bar{T}_{I,J})), \]  

(23)

\[ \Delta \lambda^{(n)} = (\Delta \lambda_1^{(n)} \Delta \lambda_2^{(n)} \cdots \Delta \lambda_K^{(n)})^T, \]  

(24)

where \( K = 4 \). By inserting (21) into the (16), we get

\[ \Delta \lambda^{(n)} = -\alpha_n [E + \alpha_n Z^T(\lambda^{(n)})Z(\lambda^{(n)})]^{-1}Z^T(\lambda^{(n)})[T(\lambda^{(n)}) - \bar{T}] . \]  

(25)

The elements of the matrix (22) (it can be called the matrix of sensitivity coefficients) at the points \((x, y)_i, t^j\) are calculated as derivatives with respect to \( \lambda_1, \lambda_2, \lambda_3 \) from the analytic solution (8) at the specified space-time points and are temperature sensitivity coefficients for the parameters \( \lambda_1, \lambda_2, \lambda_3 \).

The unique solution of the system (25) is possible when the matrix \( E + \alpha_n Z^T(\lambda^{(n)})Z(\lambda^{(n)}) \) is non-degenerate, which means that there is an inverse of the matrix or its determinant is not equal to zero.

4. Numerical solution results

Calculations for the recovery of the components of the thermal conductivity tensor in anisotropic half-space were performed based on the described method. In order to obtain the experimental temperature values from the equation (8), the following input data were taken \( \lambda_\xi = 0.08 \text{W/(m-K)}, \lambda_\eta = 0.02 \text{W/(m-K)}, \varphi = \pi/6, \epsilon \rho = 1000 \text{J/(K-m^2)}, q = 20 \text{W/m^2}, l = 0.02 \text{m}. \)

The temperature values were calculated at the points with the following coordinates \((x, y)_i = \{(0, 0.01), (0.01, 0.01), (0.01, 0.02), (0.02, 0.02), (0.02, 0.02), (-0.01, 0.03), (0.01, 0.03), (-0.01, 0.03)\} \) at the time points \( t^j = 50 \) and \( 60 \text{s}. \)

The calculation results are shown in tables 1 and 2. In the first table the descent coefficient \( \alpha^k = 2 \) and the experimental data error equals to zero, in the second table the same data is used but the error equals to \( \delta = 0.05 \).

Here the exact values of the sought parameters embedded into the “experimental” data were taken as follows:

\( \lambda_{11} = \lambda_\xi \cos^2 \varphi + \lambda_\eta \sin^2 \varphi = 0.065, \)

\( \lambda_{22} = \lambda_\xi \sin^2 \varphi + \lambda_\eta \cos^2 \varphi = 0.035, \)

\( \lambda_{12} = (\lambda_\xi - \lambda_\eta) \sin \varphi \cos \varphi \simeq 0.026. \)

The table shows that the relative error is \( \Delta \lambda_{11} = 1.69\%, \Delta \lambda_{22} = 0.95\%, \Delta \lambda_{12} = 2.18\%, \) which is significantly less than 5\%. 

Table 1.

| No. | $S(\lambda_{11}^{(n)}, \lambda_{22}^{(n)}, \lambda_{12}^{(n)})$ | $\lambda_{11}^{(n)}$ | $\lambda_{22}^{(n)}$ | $\lambda_{12}^{(n)}$ | $\alpha^k$ |
|-----|-------------------------------------------------|-----------------|-----------------|-----------------|--------|
| 0   | 1420.554127                                     | 0.01            | 0.01            | 0               | 0      |
| 1   | 263.7294772                                     | 0.02699266751   | 0.01465791762   | 0.0019293927    | 2      |
| 2   | 28.08914767                                     | 0.04859894177   | 0.02085204504   | 0.0085181015    | 2      |
| 3   | 1.381415239                                    | 0.06207530549   | 0.02844151399   | 0.01912625143   | 2      |
| 4   | 0.0247876840                                    | 0.06489041076   | 0.03390769286   | 0.02516176578   | 2      |
| 5   | 0.0000124024                                    | 0.06500385991   | 0.03497509207   | 0.02596756947   | 2      |
| 6   | 0.3739439 $\times 10^{-11}$                     | 0.06500000515   | 0.03499998548   | 0.02598075596   | 2      |

Table 2.

| No. | $S(\lambda_{11}^{(n)}, \lambda_{22}^{(n)}, \lambda_{12}^{(n)})$ | $\lambda_{11}^{(n)}$ | $\lambda_{22}^{(n)}$ | $\lambda_{12}^{(n)}$ | $\alpha^k$ |
|-----|-------------------------------------------------|-----------------|-----------------|-----------------|--------|
| 0   | 1437.476011                                     | 0.01            | 0.01            | 0               | 0      |
| 1   | 269.2519015                                     | 0.02706976128   | 0.01471455838   | 0.00193736711   | 2      |
| 2   | 29.92614833                                    | 0.04889747024   | 0.0210535897    | 0.00868620125   | 2      |
| 3   | 2.430334631                                    | 0.06273074694   | 0.02892504811   | 0.01975650552   | 2      |
| 4   | 1.003085658                                    | 0.06589872542   | 0.03450205605   | 0.02597721508   | 2      |
| 5   | 0.9808724323                                   | 0.0660996582    | 0.0353446815    | 0.02657168952   | 2      |
| 6   | 0.9808641222                                   | 0.06609572107   | 0.0353330821    | 0.02654742325   | 2      |

It is noteworthy that the initial TPP values were taken under the assumption that the space is isotropic and they differed by 3–7 times from the accurate values, and yet the iterative process has shown the accurate TPP values at 6 iterations.

Thus, the proposed method can be used for solving inverse coefficient problems of heat conduction in anisotropic half-space and band, including boundary inverse problems.

Conclusions

1. The paper proposes a method for solving the inverse problem of identification of the components of the thermal conductivity tensor in anisotropic materials on the basis of the earlier analytical solution of the direct problem of heat conduction in anisotropic half-space when heated with a thermal flow.

2. The results of the numerical experiments has shown good convergence of the method even when the initial TPP values differed from the accurate values, set by the experimental temperature values, by several times.

3. The proposed method can be recommended for use in a wide range of problems in continuum mechanics.

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