Numerical modelling in problems of thermal control for three-layer structures with defects

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Abstract. This article describes solutions to the direct and inverse problems of the three-dimensional non-stationary heat conduction problem in a three-layer structure, using the finite element method for the direct problem and the gradient descent method for the inverse problem. A comparison of the FEM-solution and the analytical solution for a solid with a simple geometry is presented. Here are presented solutions of the direct and inverse three-dimensional non-stationary heat conductivity problem for a free three-stage turbine. The accuracy of the found and exact solutions is compared.

1. Introduction

Non-destructive thermal testing is one of the most promising methods for detecting defects in three-layer structures. To solve the problem of determining the geometric parameters of such defects, it is necessary to determine unknown parameters from the thermal field obtained during thermal control. Such problems are an important part of the theory of inverse problems and its applications [1]. The solution of inverse problems allows using a mathematical model to replace the real experiment and estimate values that are not available to observations, using the measured parameters of the studied processes.

2. Conceptual statement of the problem of thermal control

Figure 1. Conceptual statement of the problem of thermal control. 1–the heat source; 2,3 - the left and right surface of the object; 4 - the defect to be restored; 5 - the device that controls the temperature of the object; 6 - the object under study; 7 - the Г contour.

Figure 1 shows the method of thermal control, which is carried out by heating the object 6 with specialized external heat sources to obtain heat flow during control by the device 5. Areas with a defect correspond to increased or reduced heating. This method of thermal control can be used, provided that the structure under study is not subjected to strong heating during its operation, or measurement and monitoring of the temperature distribution in the object during its operation is impossible by technical means.
The problem of determining temperature fields is reduced to a non-stationary problem of thermal conductivity in a three-layer structure. The geometric characteristics of the defect are assumed to be unknown. The determination of such defect parameters consists in solving the geometrically inverse problem.

3. Mathematical model of a direct problem

Consider the direct problem of three-dimensional non-stationary heat conductivity. Let \( \Omega \) be a multi-connected domain, \( \partial \Omega = \Sigma \) is the boundary and \( \lambda = \lambda_0 e_i \otimes e_j \) - thermal conductivity tensor. For the considered direct non-stationary heat conduction problem, taking into account the absence of mass heat sources, the complete system of equations can be written as follows.

Let \( \theta \in C^2(\Omega) \cap C(\bar{\Omega}) \) then:

\[
\begin{align*}
\rho(M) c_v(M) \frac{\partial \theta(M,t)}{\partial t} &= \vec{V} \cdot \left( \lambda(M) \cdot \nabla \theta(M,t) \right), M \in \Omega, t \in (t_0, t_{\text{max}}) \\
\theta(M,t)_{|_{t=0}} &= \theta_0(M), M \in \Omega \cup \Sigma; \\
\theta(M,t)_{|_{M \in \Sigma, t \geq t_0}} &= \theta_{\text{const}}(M,t), M \in \Sigma, t \geq t_0; \\
-\vec{n} \cdot \lambda(M) \cdot \nabla \theta(M,t)_{|_{M \in \Sigma_d, t \geq t_0}} &= q_\Sigma(M,t), M \in \Sigma_d, t \geq t_0; \\
-\vec{n} \cdot \lambda(M) \cdot \nabla \theta(M,t)_{|_{M \in \Sigma_d, t \geq t_0}} &= \alpha(M,t) \left[ \theta(M,t) - \theta_c(M,t) \right]_{|_{M \in \Sigma_0, t \geq t_0}}, \\
-\vec{n} \cdot \lambda(M) \cdot \nabla \theta(M,t)_{|_{M \in \Sigma_d, t \geq t_0}} &= \sigma_0 \left[ \varepsilon_{M0} \theta^4(M,t) - \varepsilon_{M1} \theta^4(M,t) \right]_{|_{M \in \Sigma_0, t \geq t_0}}, \\
\theta(M) &= \theta_{\text{cp}}(M), \\
-\vec{n} \cdot \lambda(M) \cdot \nabla \theta(M) &= -\vec{n} \cdot \lambda_{\text{cp}}(M) \cdot \nabla \theta_{\text{cp}}(M), M \in \Sigma_\text{cp}
\end{align*}
\]

\( \Sigma_\rho, \Sigma_\gamma \) – specified surfaces of the body on which the boundary conditions of constant temperature and convective heat exchange are set; 
\( \Sigma_d = \partial \Omega \cup \Sigma_d \) – the inner surface of the defect occupying region \( \Omega_d \).

4. Solution of a direct problem

A variational formulation of the direct problem.

\[
\int_\Omega \left( \rho c_v \frac{\partial \theta}{\partial t} \right) d\Omega + \int_\Omega \left( \vec{V} \lambda \nabla \theta \right) + \int_{\Sigma_\rho} \alpha \nu \theta d\Sigma = \int_{\Sigma_\gamma} v q_{\Sigma} d\Sigma + \int_{\Sigma_\rho} \alpha \nu \theta_c d\Sigma - \int_{\Sigma_\gamma} \sigma(\varepsilon_{M0} \theta^4 - \varepsilon_{M1} \theta^4) d\Sigma
\]

Global system of linear algebraic equations of the problem.

\[
T_k^T (v_h) R_h = T_k^T (v_h) C_h T_k (\theta_h) + T_k^T (v_h) K_h T_k (\theta_h) - T_k^T (v_h) P_h
\]

where \( C_h = \int_{v_h} \rho c_v \phi^T \phi dV_h \) – element heat capacity matrix;

\[
K_h = \int_{v_h} B^T \lambda B dV_h + \int_{\Sigma_h} \alpha \phi^T \phi d\Sigma_h
\]

- matrix of thermal conductivity of the element («stiffness»);

\[
P_h = \int_{\Sigma_h} \phi^T q_{\Sigma} d\Sigma_h + \int_{\Sigma_h} \alpha \phi^T \theta d\Sigma_h
\]

- vector of the reduced nodal thermal loads of the element, on the border section with the specified conditions of the 2nd and 3rd kind.
To solve the problem of thermal conductivity, a 10-node tetrahedron is used. Next, to calculate the integrals included in formula (2), we use the transition to the unit affine-equivalent finite element. For simplex CES, this allows you to use the following formula:

$$\int_{\Omega} f(\tau) = |detB| \int_{0}^{1} dL_1 \int_{0}^{1-L_1} dL_2 \ldots \int_{0}^{1-L_1-L_2-\ldots-L_{n-1}} f(L_1,\ldots,L_n) dL_n$$  \hspace{1cm} (4)

5. Result of the FEM-Solution

Figure 2. Geometry of a solid body with an indication of the boundary conditions that are set in this problem.

Figure 3. EM - mesh node by reducing the size of the elements in places of possible defects.

We solve a SLAE using the conjugate gradient method and using LU-preconditioning [7]. The initial data are as follows: material-molybdenum, $\rho = 10210 \text{kg/m}^3$, $\lambda = 135 \text{W/(m} \cdot \text{K)}$ - coefficient of thermal conductivity, $\theta_0 = 298K$ and $\theta_0 = 298K$ - the temperature at the initial time and the temperature of the medium are assumed to be the same. $\theta_{const} = 340K$ - Temperature in the boundary condition of the 1st kind.

$q_{\Sigma} = 30W / m^2$, $\alpha = 10W / (m^2 \cdot K)$, $c_v = 244J / (kg \cdot K)W / (m^2 \cdot K)$, $c_f = 244J / (kg \cdot K)$
- conditions defined based on the source material — molybdenum, and the working environment - the air.

Figure 4. Temperature distribution in a three-layer structure obtained by solving the problem of thermal conductivity.
6. Mathematical model of the inverse problem

Let’s assume that for a certain point in time $t_1$ it is necessary to know the geometric characteristics $E_{g_1}$ application $\Omega_1$ at the temperature of $\tilde{\theta}$ the surface of the body part $\Sigma_1$. Also, let the surface $\Sigma_1: g(x) = 0$, which describes the defect, is smooth, and belongs to the class $\Sigma_1 \in C^1(\Omega)$. 

Note that the direct three-dimensional non-stationary heat conduction problem implicitly defines a certain well-known operation (we denote it as $J_{inv}$), using which the specified $E_{g_1}$ is set to match $\theta_{t_1}$.

Then the problem of thermal nondestructive testing will take the form:

$$J_{inv}(g) = \tilde{\theta}, \tilde{\theta} \in \tilde{\Theta}, g \in G \quad (5)$$

This problem is an incorrectly set Hadamard problem.

Then we define the quasi-solution of the problem as:

$$g_* = \arg\inf_{\rho_{\tilde{\theta}}} J_{inv}(g), g \in \hat{G} \quad (6)$$

7. Inverse problem solution

We define an elliptic defect by the following formula:

$$\frac{(x-x_0)^2}{\delta^2} + \frac{(y-y_0)^2}{d^2} + \frac{(z-z_0)^2}{d^2} = 1$$

We assume that the parameters $x_0, z_0$ - are known and equal $x_0 \equiv C_1$, $z_0 \equiv C_2$. Then we will restore the defect by 3 parameters: $d$ - the radius of the ellipsoid along the axis Y and Z (the radius of the defect opening), $\delta$ - radius of the ellipsoid on the X-axis (defect scale), $y_0$ - position of the center of the ellipsoid on the Y axis (depth of the defect).

The problem of finding the global minimum of the following functional:

$$L(g_k) = \rho_{\tilde{\theta}} J_{inv}(g_k, \tilde{\theta}) \rightarrow \min, \ g_k \in \hat{G}, \tilde{\theta} \in \tilde{\Theta} \quad (7)$$

The distance between the functions in the space $G$:

$$\rho_{\tilde{\theta}}(J_{inv}(D_i(d_i, \delta_i, y_0)), \tilde{\theta} = \|J_{inv}(D_i(d_i, \delta_i, y_0)) - \tilde{\theta}\|_2 \quad (8)$$

Let $w_i = (d_i, \delta_i, y_0)^T$ - the vector be a column of optimization parameters. Then the gradient descent step will take the form:

$$w_{i+1} = w_i - \eta \frac{\nabla L_{inv}(w_i)}{\nabla L_{inv}(w_i)} \quad (9)$$

Where $\eta$ is the speed of gradient descent.

The algorithm for solving the inverse problem will look like this:

We solve the direct non-stationary heat conductivity problem for a solid with known defect parameters by the finite element method. Further considers this to be experimental data $\tilde{\theta}$ with unknown defect parameters, which we will approximate numerically:

- enter the initial approximation of the defect parameters $w_0$;
counting the error at the initial iteration;
• we calculate the gradient of the functional at the point $\nabla L_{inv}(w_0)$;
• calculate the parameter $\eta_0$ - the speed of gradient descent;
• updating the values of the defect parameters $w_{i+1} = w_i - \eta \nabla L_{inv}(w_i)$;
• calculate $J_{inv}(D_l(d_i, \delta_i, y_0))$ – solution of the direct non-stationary heat conduction problem for a test defect by the finite element method;
• we consider an error $\rho_0(J_{inv}(D_l(d_i, \delta_i, y_0)), \tilde{\theta}) = \|J_{inv}(D_l(d_i, \delta_i, y_0)) - \tilde{\theta}\|^2$;

If $\rho_0(J_{inv}(D_l(d_i, \delta_i, y_0)), \tilde{\theta}) < \varepsilon$, then we stop, otherwise we return to the 3rd point.

8. Results of solving the inverse problem
Consider the results of solving the inverse problem, which were obtained using the solution algorithm. Let's set some value of the parameters $w_{true}$ and find a solution to the direct problem for these parameters.

![Figure 5](image.png)
**Figure 5.** A given temperature distribution in a three-layer structure with an elliptical defect inside. Distortion of the temperature field due to the presence of a defect is highlighted in a red circle.

Now we will choose an arbitrary initial approximation and optimize the defect parameters according to the developed algorithm. Figure 6 shows the temperature distribution over the body at the initial approximation of the defect with the parameters $w_0$. And figure 7 shows the final optimization result, which can be visually compared with the exact value.

![Figure 6](image.png)
**Figure 6.** Temperature distribution in a three-layer structure with an elliptical defect inside for some initial approximation of the defect parameters $w_0$.

![Figure 7](image.png)
**Figure 7.** Restored temperature distribution in a three-layer structure with an elliptical defect inside.
Now let's look at the changes in the parameters of the $w_i$, defect, the graphs of which are shown in figures 8-10. Red is the exact parameter value, and blue is the values of parameter approximations at each iteration of gradient descent.

![Figure 8](image1.png) \hspace{1cm} ![Figure 9](image2.png)

**Figure 8.** Changing the parameter $y_{0i}$ - the depth of the defect at each iteration. \hspace{1cm} **Figure 9.** Changing the parameter $d_i$ - the radius of the defect opening at each iteration.

![Figure 10](image3.png)

**Figure 10.** Changing the metric at each optimization iteration

9. Conclusions
The article describes the solution of the direct and inverse three-dimensional non-stationary heat conduction problem in a three-layer structure using the finite element method for the direct problem and the gradient descent method for the inverse one. The accuracy of the FEM-solution for a body with a simple geometry was tested.

On average, searching for the global minimum required about 30-40 iterations of descent to obtain an accuracy of approximately $10^{-3}$[3]. Of course, to obtain a global minimum, a good initial approximation was also required, otherwise the method converged to a local minimum, which was most often observed in bodies with complex geometries. You can also see that the resulting algorithm works well for simple bodies, and for complex and composite structures, the accuracy is approximately $10^{-1}$.

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