DETERMINATION OF THE PARAMETERS IN THE GENERALIZED HEAT-CONDUCTION EQUATION FROM TRANSIENT EXPERIMENTAL DATA

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The synthesis of an iterative algorithm for determining the parameters in the generalized heat-conduction equation from the results of temperature measurements is discussed.

Inverse heat-transfer problems have undergone vigorous theoretical development and broadening areas of practical application in recent years [1]. An important class of such problems comprises coefficient inverse heat-conduction problems, in which it is required to reconstruct the thermophysical coefficients from temperature measurements at interior points of the investigated body for a particular mathematical model of the heat-transfer process and given boundary conditions. Of particular significance is the analysis of transient coefficient inverse problems [2]. Inverse problems, as a rule, belong to the class of ill-posed problems of mathematical physics [3]. Iterative methods have been found to be highly effective for their solution [4, 5].

In this article we consider the problem of determining the constant values of the set of thermophysical coefficients c, λ, k, and Q from the conditions

$$c\frac{\partial T}{\partial \tau}=\lambda\frac{\partial^2 T}{\partial x^2}+k\frac{\partial T}{\partial x}+Q,\quad 0<x<b,\quad 0<\tau\leqslant\tau_m; \tag{1}$$

$$-\lambda\frac{\partial T(0,\ \tau)}{\partial x}=q_1(\tau); \tag{2}$$

$$-\lambda\frac{\partial T(b,\ \tau)}{\partial x}=q_2(\tau); \tag{3}$$

$$T(x,\ 0)=\varphi(x),\quad 0\leqslant x\leqslant b; \tag{4}$$

$$T(x_i,\ \tau)=f_i(\tau),\quad 0<x_i<b,\quad i=2,\ 3,\ \ldots,\ N-1, \tag{5}$$

where $q_1(\tau)$, $q_2(\tau)$, $f_i(\tau)$ are known functions.

We assume that the investigated coefficient inverse problem has a unique solution. This assumption is based on the results of [6], in which it is proved that the solution of the analogously stated problem for the nonlinear homogeneous heat-conduction equation is unique. The principal objective of this study is to carry out a practical analysis of the problems of the uniqueness of solution and the possibility of synthesizing iterative algorithms of the gradient type [5] for determining the set of thermophysical parameters from the solution of the inverse problem.

The assumption of constancy of the thermophysical characteristics imposes definite limitations on the domain of practical application of the analyzed statement of the problem, because in real situations the thermophysical properties depend on the temperature. The proposed algorithm can be used when the temperature range realized in the investigated sample does not exceed a specific value in a time interval in question. According to the results of, for example, [7], this range is 500-700°K.

We treat the inverse problem as an optimal control problem, where the control function is the vector of parameters $R = \{c, \lambda, k, Q\}$. As the criterion for the selection of the unknowns we consider the mean-square residual

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$$I(x,\ \tau,\ R) = \sum_{i=2}^{N-1} \int_0^{\tau_m} [T_i(x,\ \tau,\ R) - f_i(\tau)]^2\, d\tau. \tag{6}$$

We form the solution of the extremal problem (1)-(6) with the use of gradient minimization procedures. We derive an expression for the components of the gradient of the functional in terms of the unknown parameters.

We represent the system of Eqs. (1)-(5) as the problem of the heating of an unbounded multilayered plate with layers having identical thermophysical properties. We assume that "ideal" contact is established between the individual layers and that the contact thermal resistances are equal to zero. We then obtain

$$c\frac{\partial T_i}{\partial\tau} = \lambda\frac{\partial^2 T_i}{\partial x^2} + k\frac{\partial T_i}{\partial x} + Q,\quad x_i < x < x_{i+1},\quad 0 < \tau \leqslant \tau_m,$$
$$i = 1,\ 2,\ \ldots,\ N-1,\quad x_1 = 0,\ x_N = b; \tag{7}$$

$$-\lambda\frac{\partial T_1(0,\ \tau)}{\partial x} = q_1(\tau); \tag{8}$$

$$T_{i-1}(x_i,\ \tau) = T_i(x_i,\ \tau), \tag{9}$$
$$\frac{\partial T_{i-1}(x_i,\ \tau)}{\partial x} = \frac{\partial T_i(x_i,\ \tau)}{\partial x},\quad i = 2,\ 3,\ \ldots,\ N-1; \tag{10}$$

$$-\lambda\frac{\partial T_{N-1}(b,\ \tau)}{\partial x} = q_2(\tau); \tag{11}$$

$$T_i(x,\ 0) = \varphi_i(x),\quad i = 1,\ 2,\ \ldots,\ N-1; \tag{12}$$

$$T_i(x_i,\ \tau) = f_i(\tau),\quad x_1 < x_i < x_N,\quad i = 2,\ 3,\ \ldots,\ N-1. \tag{13}$$

The inverse problem entails calculating the vector R = {c, λ, k, Q} from the condition of minimization of the functional (6) subject to conditions (7)-(13).

We assume that the components of the vector R have acquired small increments Δc, Δλ, Δk, ΔQ. Then the temperature $T_i(x,\ \tau)$ acquires an increment $\vartheta_i(x,\ \tau)$. Using relations (7)-(13), we can show that the function $\vartheta_i(x,\ \tau)$ satisfies the following boundary-value problem in the linear approximation:

$$c\frac{\partial\vartheta_i}{\partial\tau} = \lambda\frac{\partial^2\vartheta_i}{\partial x^2} + k\frac{\partial\vartheta_i}{\partial x} + \Delta\lambda\frac{\partial^2 T_i}{\partial x^2} - \Delta c\frac{\partial T_i}{\partial\tau} + \Delta Q,\quad x_i < x < x_{i+1},$$
$$0 < \tau \leqslant \tau_m,\quad i = 1,\ 2,\ \ldots,\ N-1; \tag{14}$$

$$-\lambda\frac{\partial\vartheta_1(0,\ \tau)}{\partial x} = \Delta\lambda\frac{\partial T_1(0,\ \tau)}{\partial x}; \tag{15}$$

$$\vartheta_{i-1}(x_i,\ \tau) = \vartheta_i(x_i,\ \tau), \tag{16}$$
$$\frac{\partial\vartheta_{i-1}(x_i,\ \tau)}{\partial x} = \frac{\partial\vartheta_i(x_i,\ \tau)}{\partial x},\quad i = 2,\ 3,\ \ldots,\ N-1; \tag{17}$$

$$-\lambda\frac{\partial\vartheta_{N-1}(b,\ \tau)}{\partial x} = \Delta\lambda\frac{\partial T_{N-1}(b,\ \tau)}{\partial x}; \tag{18}$$

$$\vartheta_i(x,\ 0) = 0,\quad i = 1,\ 2,\ \ldots,\ N-1. \tag{19}$$

The linear part of the increment of the objective functional has the form

$$\Delta I = 2\sum_{i=2}^{N-1}\int_0^{\tau_m} [T_i(x_i,\ \tau) - f_i(\tau)]\,\vartheta_i(x_i,\ \tau)\, d\tau. \tag{20}$$

We now introduce the boundary problem adjoint to the system (7)-(13):

$$-c\frac{\partial\psi_i}{\partial\tau}=\lambda\frac{\partial^2\psi_i}{\partial x^2}-k\frac{\partial\psi_i}{\partial x},\quad 0<\tau\leqslant\tau_m,\ x_i<x<x_{i+1},$$
$$i=1,\ 2,\ \ldots,\ N-1; \tag{21}$$

$$\lambda\frac{\partial\psi_1(0,\ \tau)}{\partial x}=k\psi_1(0,\ \tau); \tag{22}$$

$$\psi_{i-1}(x_i,\ \tau)=\psi_i(x_i,\ \tau); \tag{23}$$

$$\lambda\left[\frac{\partial\psi_{i-1}(x_i,\ \tau)}{\partial x}-\frac{\partial\psi_i(x_i,\ \tau)}{\partial x}\right]=2\left[T_i(x_i,\ \tau)-f_i(\tau)\right],$$
$$i=2,\ 3,\ \ldots,\ N-1; \tag{24}$$

$$\lambda\frac{\partial\psi_{N-1}(b,\ \tau)}{\partial x}=k\psi_{N-1}(b,\ \tau); \tag{25}$$

$$\psi_i(x,\ \tau_m)=0,\quad i=1,\ 2,\ \ldots,\ N-1. \tag{26}$$

Then, making use of relations (24), (22), and (17), we write the increment of the objective functional (20) in the form

$$\Delta I=2\sum_{i=2}^{N-1}\int_0^{\tau_m}\left[T_i(x_i,\ \tau)-f_i(\tau)\right]\vartheta_i(x_i,\ \tau)\,d\tau=\sum_{i=1}^{N-1}\int_{x_i}^{x_{i+1}}\int_0^{\tau_m}\left[\lambda\vartheta_i(x,\ \tau)+\lambda\frac{\partial\psi_i(x,\ \tau)}{\partial x}\frac{\partial\vartheta_i(x,\ \tau)}{\partial x}\right]dxd\tau+$$
$$+k\psi_1(0,\ \tau)-k\psi_{N-1}(b,\ \tau)=\sum_{i=1}^{N-1}\int_{x_i}^{x_{i+1}}\int_0^{\tau_m}\left[-c\frac{\partial\psi_i(x,\ \tau)}{\partial\tau}+\right.$$
$$\left.+k\frac{\partial\psi_i(x,\ \tau)}{\partial x}\vartheta_i(x,\ \tau)+\lambda\frac{\partial\psi_i(x,\ \tau)}{\partial x}\frac{\partial\vartheta_i(x,\ \tau)}{\partial x}\right]dxd\tau+k\psi_1(0,\ \tau)-k\psi_{N-1}(b,\ \tau),$$

or, on the basis of Eqs. (14), (21) and relations (26), (18), and (23):

$$\Delta I=\sum_{i=1}^{N-1}\int_{x_i}^{x_{i+1}}\int_0^{\tau_m}\left[\Delta\lambda\frac{\partial^2T_i}{\partial x^2}+\Delta k\frac{\partial T_i}{\partial x}-\Delta c\frac{\partial T_i}{\partial\tau}+\Delta Q\right]\psi_i\,dxd\tau+$$
$$+\int_0^{\tau_m}\psi_1(0,\ \tau)\frac{\partial T_1(0,\ \tau)}{\partial x}\Delta\lambda d\tau-\int_0^{\tau_m}\psi_{N-1}(b,\ \tau)\frac{\partial T_{N-1}(b,\ \tau)}{\partial x}\Delta\lambda d\tau. \tag{27}$$

Inasmuch as in the linear approximation $\Delta I = I'_c\Delta c + I'_\lambda\Delta\lambda + I'_k\Delta k + I'_Q\Delta Q$, where $I'_c = \partial I/\partial c$, $I'_\lambda = \partial I/\partial\lambda$, $I'_k = \partial I/\partial k$, $I'_Q = \partial I/\partial Q$, we have

$$\frac{\partial I}{\partial c}=-\sum_{i=1}^{N-1}\int_{x_i}^{x_{i+1}}\int_0^{\tau_m}\frac{\partial T_i}{\partial\tau}\psi_i\,dxd\tau, \tag{28}$$

$$\frac{\partial I}{\partial\lambda}=\sum_{i=1}^{N-1}\int_{x_i}^{x_{i+1}}\int_0^{\tau_m}\psi_i\frac{\partial^2T_i}{\partial x^2}dxd\tau+\int_0^{\tau_m}\psi_1(0,\ \tau)\frac{\partial T_1(0,\ \tau)}{\partial x}d\tau-\int_0^{\tau_m}\psi_{N-1}(b,\ \tau)\frac{\partial T_{N-1}(b,\ \tau)}{\partial x}d\tau; \tag{29}$$

$$\frac{\partial I}{\partial k}=\sum_{i=1}^{N-1}\int_{x_i}^{x_{i+1}}\int_0^{\tau_m}\frac{\partial T_i}{\partial x}\psi_i\,dxd\tau; \tag{30}$$

$$\frac{\partial I}{\partial Q}=\sum_{i=1}^{N-1}\int_{x_i}^{x_{i+1}}\int_0^{\tau_m}\psi_i\,dxd\tau. \tag{31}$$

Knowing the values of the gradients of the functional, we can construct a successive-approximation procedure on the basis of one of the gradient methods, for example, the method of conjugate gradients [8].

The results of preliminary calculations have shown that with the conventional choice of descent step common to all unknown parameters the convergence of the given algorithm to the true values of the unknown parameters depends strongly on the predetermined values of the initial approximation. Moreover, the rate of convergence is strongly affected by the relations between the separate unknowns, a fact that characterizes any real material. As a result, in the approach described here every specific practical problem can evolve into a laborious process of numerical parametric modeling.

To circumvent these ahortcomings we have borrowed from [9] a procedure for selecting the descent step in vector form. In this case the new approximation of the unknown parameters is calculated according to the formula

$$R^{(S+1)} = R^{(S)} + \alpha^{(S)} G^{(S)}, \tag{32}$$

where

$$\alpha^{(S)} = \{\alpha_c^{(S)},\ \alpha_\lambda^{(S)},\ \alpha_k^{(S)},\ \alpha_Q^{(S)}\};\quad R = \{c,\ \lambda,\ k,\ Q\};\quad G^{(S)} = -I'^{(S)} + \beta^{(S)} G^{(S-1)};\ G^{(S)} = \{G_c^{(S)}, G_\lambda^{(S)}, G_k^{(S)}, G_Q^{(S)}\};\ I'^{(S)} = \{I_c'^{(S)}, I_\lambda'^{(S)}, I_k'^{(S)}, I_Q'^{(S)}\}$$

in which $\alpha^{(S)}$ is the depth of descent; and S is the number of iterations.

The increment problem is written

$$c\frac{\partial \vartheta_{i,j}}{\partial \tau} = \lambda \frac{\partial^2 \vartheta_{i,j}}{\partial x^2} + k\frac{\partial \vartheta_{i,j}}{\partial x} + \frac{\partial^2 T_{i,j}}{\partial x^2}\alpha_\lambda G_\lambda + \frac{\partial T_{i,j}}{\partial x}\alpha_k G_k - \frac{\partial T_{i,j}}{\partial \tau}\alpha_c G_c + \alpha_Q G_Q,\quad 0 < x < b,\quad 0 < \tau \leqslant \tau_m,\quad i = 1, 2, \ldots, N-1, \quad j = 1, 2, 3, 4; \tag{33}$$

$$-\lambda \frac{\partial \vartheta_{i,j}(0, \tau)}{\partial x} = \frac{\partial T_{1,j}(0, \tau)}{\partial x}\alpha_\lambda G_\lambda; \tag{34}$$

$$\vartheta_{i-1,j}(x_i, \tau) = \vartheta_{i,j}(x_i, \tau), \tag{35}$$

$$\frac{\partial \vartheta_{i-1,j}(x_i, \tau)}{\partial x} = \frac{\partial \vartheta_{i,j}(x_i, \tau)}{\partial x},\quad i = 2, 3, \ldots, N-1; \tag{36}$$

$$-\lambda \frac{\partial \vartheta_{N-1,j}(b, \tau)}{\partial x} = \frac{\partial T_{N-1,j}(b, \tau)}{\partial x}\alpha_\lambda G_\lambda; \tag{37}$$

$$\vartheta_{i,j}(x, 0) = 0,\quad i = 1, 2, \ldots, N-1. \tag{38}$$

By the linearity of (33)-(38) the solution of the problem can be written in the form

$$\vartheta(x, \tau, \alpha^{(S)}) = \vartheta_{i,1}(x, \tau, \alpha_c^{(S)}) + \vartheta_{i,2}(x, \tau, \alpha_\lambda^{(S)}) + \vartheta_{i,3}(x, \tau, \alpha_k^{(S)}) + \vartheta_{i,4}(x, \tau, \alpha_Q^{(S)}).$$

The values of the descent steps are selected from the condition of minimization of the objective functional (6). For the determination of $\alpha^{(S)}$ we obtain the system of linear algebraic equations

$$\alpha_c \sum_{i=2}^{N-1}\int_0^{\tau_m} \vartheta_{i,j}\vartheta_{i,1}d\tau + \alpha_\lambda \sum_{i=2}^{N-1}\int_0^{\tau_m} \vartheta_{i,j}\vartheta_{i,2}d\tau + \alpha_k \sum_{i=2}^{N-1}\int_0^{\tau_m} \vartheta_{i,j}\vartheta_{i,3}d\tau + \alpha_Q \sum_{i=2}^{N-1}\int_0^{\tau_m} \vartheta_{i,j}\vartheta_{i,4}d\tau = -\sum_{i=2}^{N-1}\int_0^{\tau_m} [T_i - f_i]\,\vartheta_{i,j}d\tau,\quad j = 1, 2, 3, 4. \tag{39}$$

The iterative procedure is constructed as follows. We specify the initial values of the unknown parameters, solve the direct heat-conduction problem (7)-(13), and determine the temperature field. Then we solve the adjoint problem (21)-(26) and calculate the components of the gradient of the objective functional according to Eqs. (28)-(31). Next we solve problem (33)-(38) and from the solution of the system of equations (39) calculate the descent steps $\alpha^{(S)}$. The new approximation of the parameters is determined from expression (32), and the computational process is repeated. For the case in which the exact values of the input temperatures are known, the iteration process is halted when the unknown obtained in two successive iterations "hold." In the event that the input temperatures are given with errors, the process is stopped in accordance with the residual criterion, i.e., upon fulfillment of the condition

$$\sum_{i=2}^{N-1} \int_0^{\tau_m} [T_i(x_i, \tau) - f_i(\tau)]^2 \, d\tau \leqslant \delta^2,$$

where $\delta^2 = \sum_{i=2}^{N-1} \int_0^{\tau_m} \sigma_i^2 \, d\tau$ is the estimator of the generalized error of the initial data and $\sigma_i(\tau)$ is the standard deviation of the input temperatures at the points $x = x_i$ at time τ.

A regularized algorithm for the solution of the given inverse heat-conduction problem [4] is implemented under this approach.

The above-described algorithm formed the basis of a FORTRAN program for the BÉSM-6 computer. We used an implicit scheme for the approximation of the boundary-value problems [10] on a grid $\omega = \{x_i = hi,\ i = 0, 1, 2, \ldots, N;\ \tau_j = \Delta\tau j,\ j = 0, 1, 2, \ldots, m\}$.

We now give a few examples illustrating the efficiency of the proposed algorithm. The values of the reconstructed thermophysical parameters in the generalized heat-conduction equation (1) for perturbed input data are given in Table 1.

For the exact solution of the model example we consider the variant in which the following initial data are specified: $c = \lambda = k = Q = 1$, $q_1(\tau) = 2\tau$, $q_2(\tau) = 0$, $\tau_m = 1$, $b = 1$, $T_0 = 0$. The initial approximations of the unknown parameters are chosen within the limits of ±50% of their exact values. The input temperatures are specified at points with the coordinates $x_2 = 0.2$; $x_3 = 0.4$; $x_4 = 0.6$; $x_5 = 0.8$. The perturbations of the initial temperatures are modeled by a random number generator according to a uniform law within 5% error limits of the maximum temperature. It is essential to note that the results of determining the parameters c, λ, k, and Q agree with the sought-after values correct to four significant figures at the exact input data.

For a practical proof of the uniqueness of the solution in determining the thermophysical coefficients in the generalized heat-conduction equation we solve the following problem. As the exact solution we specify the temperature field obtained from the solution of the homogeneous heat-conduction equation, i.e., in Eq. (1) we put $k \equiv Q \equiv 0$.

In the initial approximation we specify four coefficients in the generalized equation and, as a result of the solution, obtain zero values for the convection term and source, along with the exact values of the reconstructed parameters. The results of solving the given problem are given in Table 1.

In using the algorithm for the data processing of real heat experiments for evaluating the coefficients in Eq. (1) the time to solve the problem did not exceed 2.5 min on a computing grid with parameters N = 51 and m = 61 for practically any values of the initial approximation.

TABLE 1. Values of Reconstructed Parameters (c, λ, k, Q = 0.5 in the first iteration)

No. of iterations	c	λ	k	Q
Perturbed input temperatures				
2	0,675	0,751	0,781	0,710
3	0,753	0,901	0,960	0,809
4	0,911	0,939	0,957	0,903
5	0,933	0,968	0,989	0,931
Homogeneous heat-conduction equation				
2	0,747	0,763	0,462	0,244
5	1,000	1,000	$9{,}703\cdot10^{-6}$	$1{,}085\cdot10^{-5}$
10	1,000	1,000	$8{,}309\cdot10^{-9}$	$1{,}147\cdot10^{-9}$

In conclusion we note that the proposed algorithm for solving the coefficient inverse heat-conduction problem is readily generalized to the case in which the thermophysical characteristics depend on the time, a space coordinate, or the temperature. In particular, the given method can be used directly for determining the piecewise-constant variations of the unknown characteristics as a function of the temperature [7] and the time.

NOTATION

c, volume specific heat; λ, thermal conductivity; k, a coefficient characterizing filtration; Q, distributed heat source (sink); T, temperature; x, coordinate; τ, time; T_0, initial temperature; q, heat flux; τ_m, right endpoint of time interval; $f(\tau)$, input temperatures; I, functional; δ, error of input data; q_1, q_2, values of heat flux at left and right boundaries, respectively; b, right endpoint of spatial interval; ϑ, temperature increment; ψ, adjoint variable; x_i, coordinate of layer boundary; α, descent step; i, space index; j, time index; N, number of layer boundaries.

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