AN EXPERIMENTAL-COMPUTATIONAL SYSTEM FOR THE DETERMINATION OF THERMAL PROPERTIES OF MATERIALS. II. CONCEPTION AND REALIZATION OF COMPUTER CODE FOR EXPERIMENTAL DATA PROCESSING

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Abstract - In this part the conception and realization of a computer code for experimental data processing to estimate the thermal and radiative properties of thermal-insulating materials are given. The main purpose of this study was: to confirm operability and effectiveness of the methods developed and the corresponded software for determining the thermal properties of modern structural and thermal-insulating materials, as temperature-dependent. The most promising direction in further development of methods for non-destructive composite materials using the procedure of inverse problems is the simultaneous determination of a combination of their thermal and radiation properties. The general method of iterative regularization is concerned with application to the estimation of material properties (as example: thermal conductivity $\lambda(T)$, heat capacity $C(T)$ and emissivity $\varepsilon(T)$). Such problems are of great practical importance in the study of material properties used as non-destructive surface coating in objects of space engineering, power engineering, etc.

1. INTRODUCTION

In determining the thermal characteristics of modern structural and thermal-insulating materials, as temperature-dependent, the most effective methods are based on solving coefficient inverse heat conduction problems [1-2]. The initial data for such problems are based on the results of measurements and include boundary conditions (of the first or second kind) and temperature-time measurements at several internal points of the specimen. The types of boundary condition and the number of points of temperature measurement should meet the conditions of uniqueness of the inverse problem solution under analysis [3]. The conditions of uniqueness usually define the minimum number of measurements needed in one experiment. As an example: at the simultaneous determining of the dependencies of thermal conductivity and volumetric heat capacity on temperature, at least at one boundary, it is necessary to measure the non-zero heat flux density entering a specimen and make transient temperature measurements at not less than two internal points. Boundary conditions of the first kind, or a condition of heat insulation on both boundaries, can be assigned, but in this case a specimen should be multi-layered and contain one layer of the material with known thermal characteristics and the number of temperature measurement points in the material layer under study should be not less than two.

The procedure of inverse problems is a simultaneous determination of a combination of thermal and radiation characteristics of the material (thermal conductivity $\lambda(T)$, heat capacity $C(T)$ and emissivity $\varepsilon(T)$) [3-7]. The experimental equipment [8] and the method described below could be applied for the determination of three characteristics of the material; the availability of two specimens of the material allows us to provide uniqueness of the solution.

In designing new thermal-insulating materials, quite a number of comparative heat tests are carried out, the purpose of which is clear from the analysis of the thermal properties of materials in different heating conditions corresponding to service conditions. The experimental specimens for such tests are manufactured in the form of a flat plate of the material analyzed. Owing to the structural version and homogeneous surface heating in specimens, a one-dimensional heat transfer process is realized. In the tests, as a rule, a one-sided heating of specimens is run. To control the assigned heating condition, the temperature of the external heated surface is measured and to estimate the thermal properties of the material in the study, the temperature at two internal points of the specimens and on the internal surface are measured (the temperature of the external surface is also used). In addition, the heat flux density is assumed to be known for the warm-up of a specimen. Realization of this condition is possible through experimental means. The internal surface temperature is used as a boundary condition. In practice it is difficult to realize a uniform initial temperature distribution in specimens, hence the initial temperature distribution is approximated through recorded data at zero time.

2. INVERSE PROBLEM ALGORITHM USED IN COMPUTER CODE

The direct problems for the considered case is given by:
\[
C(T) \frac{\partial T}{\partial \tau} = \frac{\partial}{\partial x} \left( \lambda(T) \frac{\partial T}{\partial x} \right), \quad x \in (X_0, X_1), \quad \tau \in (\tau_{\text{min}}, \tau_{\text{max}}) \quad (1)
\]

\[
T(x, \tau_{\text{min}}) = T_0(x), \quad x \in [X_0, X_1] \quad (2)
\]

\[
- \beta \lambda(T) \frac{\partial T(x, \tau)}{\partial \tau} + \alpha_1 T(x, \tau) = q_1(\tau), \quad \tau \in (\tau_{\text{min}}, \tau_{\text{max}}) \quad (3)
\]

\[
- \beta \lambda(T) \frac{\partial T(x, \tau)}{\partial \tau} + \alpha_2 T(x, \tau) = q_2(\tau) + c(T) \sigma T^4(x, \tau), \quad \tau \in (\tau_{\text{min}}, \tau_{\text{max}}) \quad (4)
\]

In the model (1)-(4), the relations \(C(T), \lambda(T)\) and \(c(T)\) are unknown. For the additional information necessary to solve an inverse problem, the results of temperature measurements inside a specimen are assigned, namely

\[
T_{\text{exp}}(x, \tau) = f_m(\tau), \quad m = 1, M \quad (5)
\]

In the inverse problem (1)-(5) it is necessary first of all to indicate a domain of defining the unknown functions as a temperature range \([T_{\text{min}}, T_{\text{max}}]\), general for all experiments, at which the inverse problem analysis has a unique solution. For \(T_{\text{min}}\) the minimum value of the initial temperature is used. Of much greater importance is a correct sampling of value \(T_{\text{max}}\). Proceeding from the necessity to provide uniqueness of solution, it appears possible to sample for \(T_{\text{max}}\) the maximum temperature value gained on the control thermocouple positioned on the heated surface. Suppose then that the unknown characteristics are given in their parametric form. With this purpose three uniform difference grids with the number of nodes \(N_i, i=1,2,3\) are introduced in the interval \([T_{\text{min}}, T_{\text{max}}]\):

\[
\omega = \{T_k = T_{\text{min}} + k \Delta T, k = -2, -1, 0, \ldots, N + 3, \Delta T = (T_{\text{max}} - T_{\text{min}})/N\} \quad (6)
\]

The function

\[
B^{(j-1)}(T) = B^{(j-1)}(T_k, T_{k+1}, \ldots, T_{k+j}, \tau) = \sum_{s=k}^{k+j} \left( T_s - T_k \right)^{s-k} / \omega_s(T_k) \quad (7)
\]

where \(\omega_s(T_k) = (T - T_k, \ldots, T - T_{k+j})\) and \(\left( T_s - T_k \right)^{s-k} = \max \left( 0, \left( T_s - T_k \right)^{s-k} \right)\) is called the B-spline of the \((j-1)\) degree relative to the nodes \(T_k, T_{k+1}, \ldots, T_{k+j}\). When solving practical problems, B-splines are used with so-called "natural" boundary conditions:

\[
u^*(T_{\text{min}}) = u^*(T_{\text{max}}) = 0 \quad (8)
\]

where \(u\) is the desired function.

Then, in the case of cubic B-splines \((j = 3)\), the unknown function is presented as follows:

\[
u_i(T) = \sum_{k=1}^{N_i} u_k \phi_{i,k}(T) \quad (9)
\]

where

\[
\phi_1(T) = 2B_0(T + \Delta T) - B_0(T) \quad (10a)
\]

\[
\phi_2(T) = -B_0(T + \Delta T) + B_0(T - \Delta T) \quad (10b)
\]

\[
\phi_3(T) = B_{k-1}(T), \quad k = 3, \ldots, N_i - 2 \quad (10c)
\]

\[
\phi_{N_i-1}(T) = B_0(T - (N_i - 2)\Delta T) - B_0(T - N_i\Delta T) \quad (10d)
\]

\[
\phi_{N_i}(T) = B_0(T - (N_i - 1)\Delta T) + 2B_0(T - N_i\Delta T) \quad (10e)
\]

The function \(B_0(T)\) has the property

\[
B_0(T) = \begin{cases} > 0, & \text{if } -2\Delta T < T < 2\Delta T \\ = 0, & \text{if } |T| \geq 2\Delta T \end{cases} \quad (10j)
\]

This property makes the computational algorithm simpler.

Let us introduce in the interval \([T_{\text{min}}, T_{\text{max}}]\) three uniform difference grids with the number of nodes \(N_i, i=1,2,3\), namely

\[
\omega_i = \{T_k = T_{\text{min}} + (k - 1)\Delta T, k = 1, N_i\}, \quad i=1,3 \quad (11)
\]
We now approximate the unknown functions on grids (6) using cubic B-splines as follows:

\[ C(T) = \sum_{k=1}^{N_1} C_k \phi_k^1(T), \quad \lambda(T) = \sum_{k=1}^{N_2} \lambda_k \phi_k^2(T), \quad \varepsilon(T) = \sum_{k=1}^{N_3} \varepsilon_k \phi_k^3(T) \]  

where \( C_k, k=1,N_1, \lambda_k, k=1,N_2, \varepsilon_k, k=1,N_3 \) are parameters. As a result of the approximation, the inverse problem is reduced to a search for the vector of unknown parameters \( \bar{p} = \{ p_k \}, k=1,N_p \), which has dimension \( N_p = N_1+N_2+N_3 \). Write down a mean-square error of the design and experimental temperature values at points of thermal sensors positioning, namely

\[ J(C(T), \lambda(T), \varepsilon(T)) = J(\bar{p}) = \sum_{m=1}^{M} \int_{\tau_{\min}}^{\tau_{\max}} (T(x_m, \tau) - f_m(\tau))^2 d\tau \]  

where \( T(x_m, \tau) \) is determined from the solution of the boundary-value problem (1)-(5) using the approximations (12). It is assumed that the conditions of uniqueness of the inverse problem solving are satisfied.

Proceeding from the principle of iterative regularization, the unknown vector \( \bar{p} \) can be determined through the minimization of the functional (13) by gradient methods of the first-order prior to the fulfilment of the condition:

\[ J(\bar{p}) \leq \delta_f \]  

An analytical form for the minimized functional gradient is given by

\[ J_p^{(s)} = \int_{\tau_{\min}}^{\tau_{\max}} \int_{x_{\min}}^{x_{\max}} \psi(x, \tau) \cdot \frac{\partial^2 T}{\partial \tau^2} \cdot \phi_k^2(T) \cdot \frac{\partial^2 T}{\partial \tau^2} \cdot \phi_k^2(T) \cdot \frac{\partial^2 T}{\partial \tau^2} \cdot \phi_k^2(T) \cdot \frac{\partial^2 T}{\partial \tau^2} \cdot \phi_k^2(T) \cdot \frac{\partial^2 T}{\partial \tau^2} \cdot \phi_k^2(T) \cdot \frac{\partial^2 T}{\partial \tau^2} \cdot \phi_k^2(T) \cdot \frac{\partial^2 T}{\partial \tau^2} \cdot \phi_k^2(T) \cdot \frac{\partial^2 T}{\partial \tau^2} \cdot \phi_k^2(T) \cdot \frac{\partial^2 T}{\partial \tau^2} \cdot \phi_k^2(T) \cdot \frac{\partial^2 T}{\partial \tau^2} \cdot \phi_k^2(T) \cdot \frac{\partial^2 T}{\partial \tau^2} \cdot \phi_k^2(T) \cdot \frac{\partial^2 T}{\partial \tau^2} \]  

where \( \psi(x, \tau) \) is the solution of a boundary-value problem adjoint to a linearized form of the initial problem (1)-(4):
To calculate the descent step a linear estimation is used:

\[ y^* = \left( \sum_{m=1}^{M} \int_{r_{\min}}^{r_{\max}} (x_m, r) \mathcal{G}(x_m, r) dT \right) \left( \sum_{m=1}^{M} \int_{r_{\min}}^{r_{\max}} \mathcal{G}^2(x_m, r) \right) \]

using the boundary-value problem for the Frechet differential of \( T(x, \tau) \) at the point \( \{C(T), \lambda(T), \phi(T)\} \) (noted as \( \mathcal{G}(x, \tau) \)), and assumed to be given by

\[ dC(T) = \sum_{k=1}^{N_1} g_{k1}^1(\mathcal{G}) \]
\[ d\lambda(T) = \sum_{k=1}^{N_2} g_{k2}^2(\mathcal{G}) \]
\[ d\phi(T) = \sum_{k=1}^{N_3} g_{k3}^3(\mathcal{G}) \]

where

\[ C \frac{\partial \mathcal{G}}{\partial \tau} = \left( \frac{\partial C}{\partial \tau} \right) + \frac{\partial \lambda}{\partial \mathcal{T}} \frac{d \lambda}{d \mathcal{T}} \frac{d \mathcal{G}}{d \mathcal{T}} + \left( \frac{d^2 \lambda}{d \mathcal{T}^2} \right) \frac{\partial \mathcal{C}}{\partial \tau} \frac{d \mathcal{G}}{d \mathcal{T}} + \frac{\partial \phi}{\partial \mathcal{G}} \frac{d \phi}{d \mathcal{G}} \frac{d \mathcal{C}}{d \mathcal{G}} \frac{d \mathcal{G}}{d \tau} \]

\[ \mathcal{G} = \mathcal{G}(x, \tau), x \in (x_0, x_1), \tau \in (r_{\min}, r_{\max}) \]

\[ \mathcal{G}(x, r_{\min}) = 0, x \in [x_0, x_1] \]

\[ -\beta_1 \frac{d \mathcal{G}}{d \mathcal{T}}(X_0, r) + \frac{d \lambda}{d \mathcal{T}} d \mathcal{T} \mathcal{G}(X_0, r) + \alpha_1 \mathcal{G}(X_0, \tau) = 0, \tau \in (r_{\min}, r_{\max}) \]

\[ -\beta_2 \frac{d \mathcal{G}}{d \mathcal{T}}(X_1, r) - \frac{d \lambda}{d \mathcal{T}} d \mathcal{T} \mathcal{G}(X_1, r) + \alpha_2 \mathcal{G}(X_0, r) = \]

\[ -4 \mathcal{G}(T) \sigma T^3(X_1, r) + \sum_{k=1}^{N_3} g_{k3}^3(\mathcal{G}) = 0, \tau \in (r_{\min}, r_{\max}) \]

3. COMPUTER CODE

The authors started a prototype of the computer code, intended for the development of algorithms for the estimating of material thermal properties, in 1990. Developed software is the set of problem-oriented blocks for numerical solving various inverse problems in the processing of transient thermal experiments, data processing and of optimal experiment design with respect to different optimality criterion. The software consists of individual modules and has multi-level structure. Software is made of the segments “Task”, “Data”, “Core”, “Model coefficient”, “Logistics” (Figure 1):
The presented structure is stipulated by the need to adjust the software to new problems to be solved and the role by each segment in the iterative procedure. The “Task” segment is intended for the following operations: to allocate required resources, to configure the software version to be used, namely to define the titles of subprograms, shaping the mathematical model and dimensions of the used arrays (mesh nodes, approximation parameters). The “Task” segment is made of a set of commands and basis programs, which define the model to be used, allocates resources and controls the operations by the “Model coefficient” segment. The “Data” segment modules are the sets of the input data to be used by other segments. The structure of input data is a very important question for users, and data input module generates a data description table, their basis characteristics as well as tables of connection with heat transfer mathematical model (Figure 2). Entire information is piled together in a single data array. Individual modules are united into so-called segments. The “Core” segment does not depend on the considered problem, that is achieved through the special procedure of input data processing and the system of interconnections among individual program modules. In this segment are realized the algorithms: optimization, one-dimensional and multi-dimensional search, statistic identification, etc. A particular problem is defined at the computation of the model coefficients. Programs, used for coefficient computing, make up the segment “Model coefficients”. Modules, realizing conventional mathematical methods to be used by all programs, are united into the segment “Logistics”. Software structure is an open-end one and can be enhanced or modified if needed. Software is realized into FORTRAN and C++ programming language. The segment “Logistics” includes the following functions:
- Linear/spline interpolation;
- Approximation/basis functions (B-splines with free and natural boundary conditions, polynomials);
- Calculation of matrix eigenvalues and eigenvectors;
- Various simulators of random values;
- Solving systems of linear algebraic equations and non-linear algebraic equations.

Programs of the “Model Coefficients” segment defined by the type of heat conduction equation:
- Programs to compute coefficients of heat transfer direct problem;
- Programs to compute coefficients of the adjoint problem,
- Programs to compute coefficients of the problem of temperature variations.

The “Core” programs are universal for the class of problem, considered here. The change of heat transfer mathematical model demands the modifications of the problems making up the second “Model Coefficients” segment (all these programs make up less then 2% of total software).

This approach reduces software maintenance costs and simplifies its modification, even general ones.

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Figure 2. Data input: right boundary conditions (heat flux as a function of time: 1- the first experiment, 2 - the second experiment).

4. NUMERICAL ANALYSIS OF THE ALGORITHM AND COMPUTER CODE EFFECTIVENESS

Effective application of heat transfer research techniques based on inverse problem solutions demands accurate development of computing algorithms and the selection of the number of simultaneously processed specimens and that of the thermal sensors. At this stage of research the most effective method is a computational experiment. Assuming that all coefficients of the mathematical model are known, we can solve a direct heat transfer problem in the specimen. Then, using the temperature field, this obtained at the assumed points of thermal sensors setting, we form the additional information necessary for inverse problem solving and, afterwards, we solve an inverse problem of heat transfer [2]. Such an approach provides a means of analyzing the error effect on the results of inverse problem solving.

The domains of function definition in the case under consideration for all unknown characteristics are identical and equal to the interval: [293 K, 1150 K]. Figure 2 illustrates the external heat fluxes for two experiments processed simultaneously. Time of each experiment is 300 s. The internal boundaries of specimens were considered as thermally insulated. The exact values of the recovered functions are given in Figure 3. The number of experiments needed for the recovery of the above pointed heat transfer characteristics surface is two. Hence, for numerical studies we considered the complexity of unsteady thermal experiments taken two at a time (N=2). By mathematical modeling we considered specimens of 0.015 m thickness. Thermocouples were assumed to be installed at points with the coordinates:

1st specimen $X_1 = 0.0075m$, $X_2 = 0.0102m$, $X_3 = 0.015m$.

2nd specimen $X_1 = 0.01265m$, $X_2 = 0.01365m$, $X_3 = 0.015m$.

The inverse problem solving error in the given study is defined as

$$\delta C = \frac{\|C(T) - \overline{C}(T)\|_{L_2}}{\|\overline{C}(T)\|_{L_2}}$$

(34)
\[
\delta \lambda = \left\| \lambda(T) - \mathcal{X}(T) \right\|_{L_2} / \left\| \mathcal{X}(T) \right\|_{L_2}
\]
\[
\delta \varepsilon = \left\| \varepsilon(T) - \mathcal{E}(T) \right\|_{L_2} / \left\| \mathcal{E}(T) \right\|_{L_2}
\]

(35)

(36)

where \( C, \overline{C}, \lambda, \varepsilon, \mathcal{E} \) are recovered and accurate values of functions in the corresponding domains of definition.

Let us consider the effect of the number of approximation parameters on the accuracy of the solution obtained for different error levels in input temperature \( \delta \), and compare different approximations. Figure 3 presents the results of the unknown function approximation by various numbers of approximation functions. As is seen, when the number of parameters is three for \( C(T) \) and \( \varepsilon(T) \) and five for \( \lambda(T) \), the recovered characteristics are more close to a prescribed value. The residual functional values in the iterative procedure, obtained using the different numbers of approximation parameters, are presented in Figure 4. These results allow confirmation of the following formalized approach to the choosing of the unknown parameters number: the unknown function approximation should be carried out by the minimum number of terms with which the residual level \( \delta^r \) is reached.

Next, we analyze the influence of errors in \( q_2(\tau) \) and \( f_n(\tau) \) on the inverse problem solution. We modeled two types of errors: for \( f_n(\tau) \) by a normal distribution, for \( q_2(\tau) \) at a positive bias, where the level of relative maximum error rate is \( \delta = 5\% \). Random errors in the input data under modeling are formed by the formula:

\[
f_n(\tau) = \tilde{f}_n(\tau)(1 + \sigma \delta(\tau)), \quad m = 1, M
\]

(37)

where \( \tilde{f}_n(\tau) \) is the «exact» reading of the thermal sensor obtained from the direct problem solution, \( \sigma \) is the random value distributed by normal distribution with a variance equal to 1 and a mean value 0, \( \delta(\tau) \) is the maximum-possible accidental error. So it is shown in Figure 5 how deviation \( f_n(\tau) \) behaves. The above results testify a sufficiently high computing stability of the suggested algorithm towards random errors occurring in solving coefficient inverse problems. For modeling the effect we used the expression

\[
q_2(\tau) = \tilde{q}_2(\tau)(1 + \delta)
\]

(38)

Figure 6 shows the results of the unknown functions determination at the bias of the heat flux delivered from the heated side. The results presented show a very weak effect of heat flux measurement errors on the output of inverse problem solving.

To analyze the effect of the thermal sensor position on the accuracy of the inverse problem running solution we varied the coordinates of their position as follows:

\[
X_i = \overline{X}_i(1 + \delta_x)
\]

Also we assumed the temperature measurements on the external surface of the specimens. The minimum distance between thermal sensors was sampled from considerations of exclusion of their interference:

\[
\Delta X_m = X_m - X_{m-1},
\]

\[
\Delta X_m \geq 10d,
\]

where \( d \) is the thermal element hypothetic diameter (is taken equal to 0.0001 m). In the case under study, we assumed that \( \delta_x = 0.05 \). Computations for three thermal sensors in each experiment have been made at coordinate displacements of the left thermal sensor setting.

Figure 7 demonstrates the recovered functions of heat capacity, thermal conductivity and emissivity as a result of mathematical modeling for several possible displacements of the position of the thermal sensors. All computations have been carried out for initial data prescribed without error \( (\delta_x = 0.0) \).

The research performed shows that for the consideration under study, the accuracy of the solution being obtained becomes lower when the thermal sensors are shifted towards the heated surface, while the removal of additional thermal sensors from the heated surface is of lesser influence on the errors in their setting. However the above presented results cannot claim for completeness and fullness but only validate a need of a preliminary optimal experiment design in the case of defining a complex of insulation characteristics.

4. CONCLUSION

In this paper an algorithm and computer code are presented which were developed to process the data of unsteady-state thermal experiments. The algorithm is suggested for determining unknown thermal and radiative properties as a solution of the nonlinear inverse heat conduction problem in an extreme formulation. The computer code provides the using of the algorithm suggested for solving the applied problems [5].

The following main factors have an influence on the accuracy of the inverse heat conduction problem (in sequence of significance): the errors in coordinates of thermosensor positions; the errors in values of different
characteristics; the errors in estimating the residual level. It was shown that in the cases considered the accuracy of the solution of the inverse problem is compatible with the errors of the simulated "experimental measurements".

Figure 3. Results of reconstruction (measured temperature with error $\delta = 10\%$ relative to a current value): 1, 2, 3, 4, 5 – estimations of $C(T), \lambda(T), \epsilon(T)$ (number of parameters being 1, 2, 3, 5, 7); 6 – exact values.

Figure 5. Results of $C(T), \lambda(T), \epsilon(T)$ reconstruction: 1, 2 – measured temperature with error $\delta = 5\%, 10\%$ distributed by normal distribution, when error level is considered with respect to current value of disturbed function; 3 – exact values.

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Figure 4. The influence of the numbers of approximation parameters on the errors in the inverse problem solution (the residual functional value \([ K^2 \text{sec} ]\) as an iteration number): 1 – number of parameters is one for \(C(T)\), \(\lambda(T)\) and \(\varepsilon(T)\) (constants), 2 – number of parameters is two for \(C(T)\), \(\lambda(T)\) and \(\varepsilon(T)\) (linear functions), 3 – number of parameters is three for \(C(T)\) and \(\varepsilon(T)\) and five for \(\lambda(T)\), 4 – number of parameters is five for \(C(T)\), \(\lambda(T)\) and \(\varepsilon(T)\), 5 – number of parameters is seven for \(C(T)\), \(\lambda(T)\) and \(\varepsilon(T)\).

REFERENCES
Figure 6. Results of $C(T), \lambda(T), c(T)$ reconstruction: 1, 2 – bias $\delta = -10\%, +10\%$ at boundary condition (heat flux from the heated side); 3 – exact values.

Figure 7. Results of $C(T), \lambda(T), c(T)$ reconstruction with thermocouple displacements:
1 - $\delta_x = 0$; 2 - $\delta_x = -0.05$; 3 - $\delta_x = 0.05$;
4 – exact values.