COMPUTATIONAL – EXPERIMENTAL DETERMINATION OF THE THERMOPHYSICAL PROPERTIES OF MATERIALS

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The problem is considered of the restoration of the coefficients of the quasilinear, one-dimensional equation of thermal conductivity over a given temperature field for "pure" and "composite" materials. The strong dependence of the solution on the errors in the specification of the initial temperature field is illustrated by a particular example. Algorithms are given for the numerical solution of the problem.

1. Formulation of the Problem. We shall consider the boundary problem for the thermal conductivity equation

$$
\begin{gathered}
P[u] \equiv c\frac{\partial u}{\partial \tau} - \frac{\partial}{\partial \xi}\left(\lambda \frac{\partial u}{\partial \xi}\right) = 0, \\
(\xi, \tau) \in G \equiv (\xi_0, \xi_1) \times (\tau_0, \tau_1), \\
u(\xi, \tau_0) = u^0(\xi), \; u(\xi_0, \tau) = u_0(\tau), \; u(\xi_1, \tau) = u_1(\tau).
\end{gathered} \tag{1}
$$

The solution $u(\xi, \tau)$ reaches the upper and lower bounds at the boundary G:

$$
\begin{gathered}
u_i = \inf_{(\xi,\tau)\in\overline{G}} u(\xi, \tau) = \inf_{(\xi,\tau)\in\overline{G}} \{u^0(\xi), \; u_0(\tau), \; u_1(\tau)\}, \\
u_s = \sup_{(\xi,\tau)\in\overline{G}} u(\xi, \tau) = \sup_{(\xi,\tau)\in\overline{G}} \{u^0(\xi), \; u_0(\tau), \; u_1(\tau)\}.
\end{gathered}
$$

Denoting by I_1 the interval (u_i, u_s), we shall assume that the coefficients c and λ belong to the classes $C(\overline{I_1})$ and $C^1(\overline{I_1})$ respectively. We shall suppose also that the functions occurring in the boundary conditions (1), satisfy the conditions of compatibility of first order [1]:

$$
\begin{gathered}
\exists\, v(\xi, \tau) \in C^{2,1}(\overline{G}): \; v(\xi, \tau_0) = u^0(\xi), \\
v(\xi_0, \tau) = u_0(\tau), \; v(\xi_1(\tau) = u_1(\tau), \; P[v]|_{\tau=0+} = 0.
\end{gathered} \tag{2}
$$

Within these assumptions there exists also a unique solution of the boundary problem (1) for every pair (c, λ) and, consequently, the functional mapping K of the set M of pairs (c, λ) can be introduced into the class $C^{2,1}(\overline{G})$:

$$
K[(c, \lambda)] = u, \tag{3}
$$

$$
u \in C^{2,1}(\overline{G}), \; (c, \lambda) \in M \equiv \{(c, \lambda) \mid c, \; \lambda > 0, \; (c, \lambda) \in C(\overline{I_1}) \times C^1(\overline{I_1})\}.
$$

In view of what has been stated, we shall consider the following reverse problem. For a given function $v \in C^{2,1}(\overline{G})$, satisfying the boundary conditions (1), it is necessary to find a pair $(c, \lambda) \in M$, making equation (1) identical, i.e., to solve relative to (c, λ) the functional equation $K[(c, \lambda)] = v$. In the general case, i.e., for the arbitrary function $v \in C^{2,1}(\overline{G})$, the solution of $(c, \lambda) \in M$ in the stated sense does not exist, but when it exists then, generally speaking, it is not unique. We note at once the obvious nonuniqueness of the solution (c, λ):

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$$K[(c,\ \lambda)] = K[\alpha c,\ \alpha\lambda],\ \forall\alpha > 0.$$

Nonuniqueness of this type cannot be removed by any choice whatever of $v \in C^{2,1}(\overline{G})$. Therefore, the two solutions (c, λ) and $(\tilde{c}, \tilde{\lambda})$ of equation (3) which are connected by the relation

$$\tilde{c} = \alpha c, \quad \tilde{\lambda} = \alpha\lambda, \ \alpha = \text{const} > 0, \tag{4}$$

we shall assume to be coincident. For those cases when the solution exists of the formulated reverse problem, the class of temperature fields $v \in C^{2,1}(\overline{G})$, for which the solution is unique with an accuracy up to the transformation of Eq. (4), can be described completely. In [2], the solution (c, λ) of Eq. (3) is nonunique when, and only when, the field $u(\xi, \tau)$ has the form $u = u(z)$, where the function $z(\xi, \tau)$ is determined by one of the relations:

$$z = \alpha_0\xi + \beta_0\tau + \gamma_0 \ \text{ or } \ z = \frac{\xi + \beta_0}{\sqrt{\alpha_0(\alpha_1 - \tau)}} + \gamma_0. \tag{5}$$

Here α_0, β_0, γ_0, α_1 are arbitrary constants.

Without laying claim to whatever the generality, we introduce the following terminology. We shall say that to every pair $(c, \lambda) \in M$ there corresponds a certain pure material and vice versa, pure materials are only those whose properties are described by a certain pair $(c, \lambda) \in M$. From the physical point of view, a pure material is one for which the properties c and λ are functions of a state (in the case of the thermal conductivity process — of a state of temperature) and are independent of the path by which this state is achieved. For pure materials, the solution of Eq. (3) for a given field $v(\xi, \tau) \in C^{2,1}(\overline{G})$ is equivalent to finding the zero minima of the functional

$$J_1^2 = \iint\limits_G \left\{c(v)\frac{\partial v}{\partial \tau} - \frac{\partial}{\partial \xi}\left[\lambda(v)\frac{\partial v}{\partial \xi}\right]\right\}^2 dG. \tag{6}$$

We shall understand by composite materials, those materials whose properties are not functions of a state. The main reasons for composite materials not having such thermophysical characteristics as specific heat and thermal conductivity, are irreversible changes of microstructure of the composite material or of some of its components in extreme conditions of external thermal influences. Two methods for describing the properties of composite materials are possible.

A. Assuming some or other model for the microstructure of the material and using the representations of statistical physics, the problem can be reduced to the solution of the kinetic equations. This approach, with a successful choice of model, should give the most complete and accurate description of the medium being investigated. However, it is well-known that there are enormous computational difficulties in solving the kinetic equations. There is also the drawback that the choice of model is not a simple matter and, for different types of composite materials, a special physical consideration is necessary. The adequacy itself of the model for actual composite materials can confirm only a comparison between the calculated temperature fields and those observed experimentally.

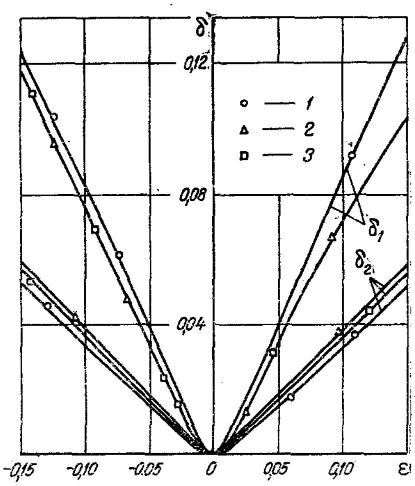

Fig. 1. Dependence of the fundamentals δ_1 and δ_2 on ε: 1) $N_\xi \times N_\tau = 6 \times 10$; 2) 21×21; 3) 51×21.

B. Phenomenological approach. Assuming that the temperature distribution in composite materials obeys the thermal conductivity equation, the coefficients of the equation in the temperature function are chosen in such a way that the solution of the equation differs minimally from the temperature field observed experimentally. Physically, this approach is justified in that the temperature is an energy, i.e., an integral, characteristic. It is clear from the most general considerations that a change of temperature must be described by an equation of the evolutionary type. The thermal conductivity equation, the coefficients of which are functionals of the temperature field, can serve as a special example of this equation. One of the variants of this phenomenological approach will be considered here.

Suppose that the temperature field $v(\xi, \tau) \in C(\overline{G})$ is given. The solution of the reverse problem in the case of a composite material, we shall call the pair $(c^*, \lambda^*) \in M$, providing the minimum to the functional

$$J_2^2 = \rho^2(v, u) \tag{7}$$

with the conditions

$$P[u] \equiv c\frac{\partial u}{\partial \tau} - \frac{\partial}{\partial \xi}\left(\lambda \frac{\partial u}{\partial \xi}\right) = 0, \ (\xi, \ \tau) \in G,$$

$$u(\xi, \ \tau_0) = v(\xi, \ \tau_0), \ u(\xi_0, \ \tau) = v(\xi_0, \ \tau),$$

$$u(\xi_1, \ \tau) = v(\xi_1, \ \tau).$$

That is, the condition determining the solution (c^*, λ^*) is written as

$$J_2^2(c^*, \ \lambda^*) = \rho^2(v, \ K(M)).$$

The metric ρ (v, u) in Eq. (7) is defined by one of the equivalent norms of the space C ($\overline{G}$).

2. Methods of Solution. In generalizing the problem, we shall not assume in future that the domain G is rectangular:

$$G \equiv \{(\xi, \ \tau) | \ \tau \in (\tau_0, \ \tau_1), \ \xi \in (\xi_0, \ \xi_1(\tau))\},$$

here $\xi_1(\tau)$ is a given continuously-differentiable function. Thus, the physical possibility of the removal (deposition) of mass from the surface of the sample is taken into account. We shall consider separately the cases of pure materials and composite materials.

For pure materials, the solution (c, λ) is written in the form of cubic splines [3] $c_D(u)$ and $\lambda_D(u)$, defined by the lattice D

$$u_i \equiv u_0 < u_1 < u_2 < \ldots\ldots < u_N \equiv u_s.$$

The cubic spline [3] c_D on the intercept $[u_{k-1}, \ u_k]$ is given by the formula

$$c_D(u) = c_k^{(1)} f_1^k + c_k^{(2)} f_2^k + c_{k-1}^{(1)} g_1^k + c_{k-1}^{(2)} g_2^k, \ k = 1, \ 2, \ \ldots, N,$$

where

$$f_1^k = \frac{(u - u_{k-1})^2 \left[2(u_k - u) + h_k\right]}{h_k^3}, \ f_2^k = \frac{(u - u_{k-1})^2 (u - u_k)}{h_k^2};$$

$$g_1^k = \frac{(u_k - u)^2 \left[2(u - u_{k-1}) + h_k\right]}{h_k^3}, \quad g_2^k = \frac{(u_k - u)^2 (u - u_{k-1})}{h_k^2};$$

$$c_k^{(1)} = c(u_k), \ c_k^{(2)} = \frac{dc}{du}(u_k); \ h_k = u_k - u_{k-1}.$$

The spline $\lambda_D(u)$ is written similarly:

$$\lambda_D(u) = \lambda_k^{(1)} f_1^k + \lambda_k^2 f_2^k + \lambda_{k-1}^{(1)} g_1^k + \lambda_{k-1}^{(2)} g_2^k, \ k = 1, \ 2, \ \ldots, N,$$

with the same functionals f_i^k and g_i^k, and with the meaning of the coefficients $\lambda_k^{(i)}$.

The minimized functional (6) can be represented in the form of a sum:

$$J_1^2 = \sum_{k=1}^{N} \iint_{G_k} \left[c\frac{\partial v}{\partial \tau} - \frac{\partial}{\partial \xi}\left(\lambda \frac{\partial v}{\partial \xi}\right)\right]^2 dG_k \equiv \sum_{k=1}^{N} \iint_{G_k} F_k^2 dG_k \equiv \sum_{k=1}^{N} j_k^2,$$

where G_k is a Lebesque set of the function $v(\xi, \tau)$:

$$G_k \equiv \{(\xi, \ \tau) | \ (\xi, \ \tau) \in G; \ u_{k-1} \leqslant v(\xi, \ \tau) \leqslant u_k\}.$$

We introduce the following notations:

$$x_i = \begin{cases} c_\alpha^{(k)}, \ i = 4\alpha + k, \alpha = 0, \ 1, \ 2, \ \ldots, N, \\ \lambda_\alpha^{(k)}, \ i = 4\alpha + k + 2, \ k = 1, \ 2; \end{cases}$$

$$h^{\alpha, j} = \begin{cases} g_j^{\alpha} \dfrac{\partial v}{\partial \tau}, & j = 1, 2, \\ -\dfrac{\partial}{\partial \xi}\left(g_{j-2}^{\alpha} \dfrac{\partial v}{\partial \xi}\right), & j = 3, 4, \\ f_{j-4}^{\alpha} \dfrac{\partial v}{\partial \tau}, & j = 5, 6, \\ -\dfrac{\partial}{\partial \xi}\left(f_{j-6}^{\alpha} \dfrac{\partial v}{\partial \xi}\right), & j = 7, 8, \end{cases} \qquad H_p^{i, k} = \iint_{G_p} h^{p, i} h^{p, k}\, dG_p.$$

The integral of j_k^2 in these notations assumes the form:

$$j_k^2 = \iint_{G_k} \Big[\sum_{j=1}^{8} x_{j+4(k-1)} h^{k, j}\Big]^2 dG_k.$$

The condition for minimum of the function J_1^2 of the variables $\{x_k\}$ is represented by a linear system of algebraic equations (grad $J_1^2 = 0$):

$$\begin{gathered} \sum_{j=1}^{8} a_1^{k, j} x_j = 0, \ k = 1, 2, 3, 4, \\ \sum_{j=1}^{12} a_p^{k, j} x_{j+4(p-1)} = 0, \ p = 1, 2, \ldots, N-1, \ k = 5, 6, 7, 8, \\ \sum_{j=1}^{8} a_N^{k, j} x_{j+4(N-1)} = 0, \ k = 5, 6, 7, 8. \end{gathered} \tag{8}$$

the coefficients $a_i^{k, j}$ are determined by the equations:

$$a_1^{k, j} = H_1^{k, j},$$

$$a_p^{k, j} = \begin{cases} H_p^{k, j}, & 1 \leqslant j \leqslant 4, \\ H_p^{k, j} + H_{p+1}^{k-4, j-4}, & 5 \leqslant j \leqslant 8, \\ H_{p+1}^{k-4, j-4}, & 9 \leqslant j \leqslant 12. \end{cases}$$

$$a_N^{k, j} = H_N^{k, j}.$$

Thus, the procedure for finding the coefficients determining the splines $c_D(u)$ and $\lambda_D(u)$ has been reduced to the evaluation of 72N double integrals $H_p^{i,k}$ ($H_p^{i,k} = H_p^{k,i}$) and the solution of the linear equation (8). Both these operations are carried out easily numerically by standard methods. As the set of splines on $\bar{I}_1$ is everywhere dense in $C(\bar{I}_1)$ and in $C^1(\bar{I}_1)$, then when $N \to \infty$ the splines $c_D(u)$ and $\lambda_D(u)$ tend to the solution of the problem of minimization of the functional (6).

Let us now consider the case of a composite material. In the formulation of the problem, the solution (c^*, λ^*) minimizes the functional

$$J_2^2 = \iint_G (u - v)^2 dG \tag{9}$$

with the isoperimetric conditions:

$$J_3^2 \equiv \iint_G \left[c \frac{\partial u}{\partial \tau} - \frac{\partial}{\partial \xi}\left(\lambda \frac{\partial u}{\partial \xi}\right)\right]^2 dG = 0, \ (c, \lambda) \in M. \tag{10}$$

We note that, in contrast from the case considered of pure materials, the function $v(\xi, \tau)$ is assumed to belong only to the class $C(\overline{G})$. The solution of the problem, of Eq. (9) and (10), can be constructed by the methods of unconditional minimization [4]. We introduce the new functional

$$J(\delta) = \delta_2^2 + \delta J_3^2,$$

here, δ is a positive scalar parameter.

Suppose that $\{\delta_n\}$ is an increasing succession of positive numbers, $\delta_n \nearrow +\infty$. We denote by $\{c_n, \lambda_n, u_n\}$ the triplet of functions providing the minimum to the functional $J(\delta)$ when $\delta = \delta_n$ [$(c_n, \lambda_n) \in M$, $u_n \in C^{2,1}(\overline{G})$]. The solution of the problem of Eq. (9) and (10) at an arbitrary extremum is constructed as

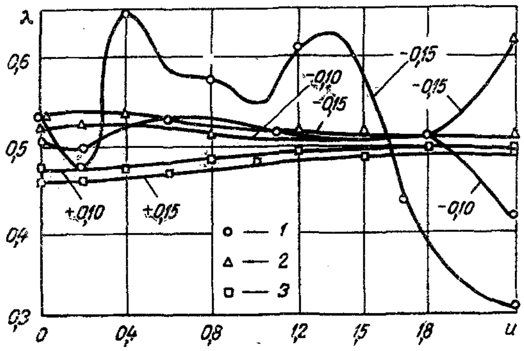

Fig. 2. Function λ(u) for different values of ε: 1-3) same as in Fig. 1.

the limit of $\{c_n, \lambda_n, u_n\}$ when $n \to \infty$ [4]. The functional $J_n = J(\delta_n)$ is minimized by the method of quickest descent in the space

$$F \equiv C^{2,1}(\bar{G}) \times C(\bar{I}_1) \times C^1(\bar{I}_1).$$

We note some special features of this procedure. Suppose that $\{c^1, \lambda^1, u^1\}$ is the first approximation of the extremal I_n. Variation of I_n relative to the function u at the point $\{c^1, \lambda^1, u^1\}$ is written in the standard way, by defining the gradient of the functional J_n in the space $C^{2,1}(\bar{G})$:

$$\delta J_n = 2\iint_G z_1 \delta u dG + 2\delta_n \oint_\Gamma \left[z_2 - \frac{\partial}{\partial \Gamma}(P_1\lambda^1)\right] d\Gamma \delta u,$$

where

$$z_1 = z - \delta_n \left[\frac{\partial}{\partial \tau}(P_1 c^1) + \frac{\partial}{\partial \xi}\left(2P_1 \frac{\partial \lambda^1}{\partial \xi}\right)\right] - \delta_n \frac{\partial^2}{\partial \xi^2}(P_1\lambda^1),$$

$$z_2 = 2P_1 \frac{\partial \lambda^1}{\partial \xi}\frac{\partial \xi}{\partial \Gamma} - \frac{\partial}{\partial \xi}(P_1\lambda^1)\frac{\partial \xi}{\partial \Gamma} + P_1 c^1 \frac{\partial \tau}{\partial \Gamma}, \quad z = u^1 - v + \delta_n P_1 \left[\frac{\partial c^1}{\partial \tau} - \frac{\partial^2 \lambda^1}{\partial \xi^2}\right],$$

$$P_1 = c^1 \frac{\partial u^1}{\partial \tau} - \frac{\partial}{\partial \xi}\left(\lambda^1 \frac{\partial u^1}{\partial \xi}\right), \quad u = u^1 + h\delta u.$$

Descent in the direction of the gradient δu for fixed functions $c^1(u)$ and $\lambda^1(u)$ is accomplished by a stepped change of the scalar parameter h. As concerns the minimization of I_n in the space $C(\bar{I}_1) \times C^1(\bar{I}_1)$ with the fixed function u^1, this procedure coincides in accuracy with that described above for the case of pure materials. The difference consists in that the role of v is played here by u^1 and the minimum, generally speaking, will not be zero (it will tend to zero when $n \to \infty$).

3. Errors in the Specification of the Temperature Fields. Let us consider the following specific problem, namely, that it is necessary to find the thermal conductivity of a material λ(u) for a specified temperature field

$$u(\xi, \tau) = \tau + \xi^2(1 + \varepsilon\tau), \quad (\xi, \tau) \in (0, 1) \times (0, 1). \tag{11}$$

The specific heat c is assumed to be constant ($c \equiv 1$). The problem has an obvious solution in the class of pure materials when $\varepsilon = 0$: $\lambda \equiv 0.5$. In the sense of the definitions introduced above, this means that the temperature field $u(\xi, \tau)$ when $\varepsilon = 0$ belongs to a form k(M) of the set M:

$$u(\xi, \tau, \varepsilon)|_{\varepsilon=0} = K[(1;\ 0.5)].$$

By the method of reduction to the system of linear equations (8), the function λ(u) has been found in the form of a cubic spline for certain values of the parameter ε in the neighborhood of zero. Simultaneously, the value of the functionals of the mean-square and homogeneous convergence has been calculated:

$$\delta_1 = \max_{(\xi,\tau)\in\bar{G}} |P[u]|, \quad \delta_2 = \left(\iint_G P^2[u]\, dG\right)^{1/2}.$$

The results of the numerical solution are shown in Figs. 1 and 2. In addition to the parameter ε, the number of points $N_\xi \times N_\tau$ was also varied in the square $(0.1) \times (0.1)$, in which the specified field $u(\xi, \tau)$ is assumed to be. The calculations were carried out for three values of $N_\xi \times N_\tau$: $N_\xi \times N_\tau = 6 \times 10$, 21×21 and 51×21. All the derivatives of $u(\xi, \tau)$, participating in P[u], were calculated exactly by differentiations of Eq. (11). The integrals $H_p^{i,k}$, occurring in the coefficients of system (8), were replaced by integral sums of the type:

$$H_p^{i,k} \approx \sum_{m,n} h^{p,i}(\xi_m, \tau_n) h^{p,k}(\xi_m, \tau_n) \Delta G(m, n),$$

$$(\xi_m, \tau_n) \in G_p, \quad 4\Delta G(m, n) = (\xi_{m+1} - \xi_{m-1})(\tau_{n+1} - \tau_{n-1}). \tag{12}$$

Figure 1 shows the functions $\delta_1(\varepsilon)$ and $\delta_2(\varepsilon)$ for different numbers of $N_\xi \times N_\tau$. The solutions of $\lambda(u)$ for $\varepsilon = \pm 0.1$ and ± 0.15 and three values of $N_\xi \times N_\tau$ are plotted in the form of graphs in Fig. 2. The nonvanishing of the functional $\delta_1(\varepsilon)$ and $\delta_2(\varepsilon)$ shows that when $\varepsilon \neq 0$, the temperature field $u(\xi, \tau)$ cannot be observed in pure materials with $c \equiv$ const (this limitation is important). The behavior of $\lambda(u, \varepsilon)$ in terms of the integral sums (12) is found to be a strong function of the number of points at which the field $u(\xi, \tau)$ is specified and its derivatives. This example shows that extrapolation of the thermophysical properties in a class of pure materials [minimization of the functional (6)], even with small perturbations of the field $v(\xi, \tau)$, is very indeterminate. Bearing in mind that the experimental measurements always are characterized by some or other errors and the derivatives $du/d\tau$, $du/d\xi$ and $d^2u/d\xi^2$ can be obtained only by numerical differentiation, introducing additional errors in the specification of the starting data for solving the reverse problem, the conclusion can be drawn that the application of the method of the solutions to a class of pure materials [minimization of the functional (6)] in practical problems must reveal considerable difficulties. On the other hand, if the field $v(\xi, \tau) \in K(M)$, then minimization of Eq. (9) with the condition (10) leads to the solution (c, λ), providing a zero value to both functionals, i.e., the solution to a class of pure materials.

NOTATION

ξ, space coordinate; τ, time coordinate; $u(\xi, \tau)$, temperature at the point (ξ, τ); c, specific heat; λ, thermal conductivity as a function of temperature; $C(\bar{I}_1)$, space of the continuous functions on I_1; $C^1(\bar{I}_1)$, space of the continuous functions on $\bar{I}_1$, together with the first derivative; $C^{2,1}(\bar{G})$, space of functions $u(\xi, \tau)$, continuous on $\bar{G}$, together with second order derivatives in ξ and first order derivatives in τ; ε, scalar parameter, defining the measure of perturbation of the exact solution of $u(\xi, \tau) \in K(M)$.

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