Journal of Engineering Physics and Thermophysics, Vol. 65, No. 6, 1993

DETERMINATION OF THE TEMPERATURE AND DENSITY OF A HEAT FLUX FROM THE SOLUTION OF THE INVERSE HEAT CONDUCTION PROBLEM FOR A THERMALLY DESTRUCTIBLE MATERIAL

A. K. Alekseyev, A. Yu. Chistov, and B. A. Shvedov

UDC 536.5:541.12

The problem of determination of a heat flux density from the state of a material after heating is considered.

When construction elements and heat-protective coatings, consisting of polymer composites, are subjected to heating, they undergo thermal destruction, and their state after cessation of heating provides some information about the character of such heat action.

In the present work we consider how this information may be used to reconstruct the temperature dependence $T(t)$ at some point of a structure or to determine the specific heat flux $q(t)$ acting on a boundary. This may be done if there is a mathematical model of the thermal destruction process (the irreversible change of internal parameters of the material, viz., the density, the concentration of the constituents of the material, etc.). Such an approach is promising since it makes it possible to obtain a greater amount of information in full-scale tests by using of structural and heat-protective materials as heat indicators.

Below we illustrate use of information obtained from thermogravimetric analysis of material samples before and after heat loading.

We consider the simplest phenomenological model of a thermally destructible material [1]. According to [1], for thermogravimetric analysis of some thermally destructible materials the destruction process may be approximated by a sum of several reactions (stages) with different kinetic parameters. For the case of parallel independent stages the system of equations is as follows:

$$dG_i/dt = -A_i G_{0i} C_i^n \exp(-E_i/T(t)), \quad i = 1 \dots NST. \tag{1}$$

Prior to thermal loading $C_i = 1$, and after cooling

$$C_i = \exp\left(-\int_0^t \exp(\ln A_i - E_i/T(t))\, dt\right); \quad i = 1 \dots NST. \tag{2}$$

The problem is subdivided into three problems for determination of: 1) A_i, E_i, C_{0i} for the initial material (formulation of the mathematical model of material destruction); 2) C_i for the material after heating; 3) $T(t)$ in terms of C_i.

Problem 1 is solved analogously to [1, 2] (by successive subtraction of stages); problem 2 by optimization methods (for the given kinetic parameters the C_i values are chosen so as to provide the best approximation of the thermogravimetric curve of the material after heating).

To solve problems 1 and 2, we have composed a set of programs in Basic for an IBM PC AT and verified it for several materials. Subsequently, we analyze only problem 3, considering that we already have a model of the material (the values of the kinetic parameters) and the C_i values.

The system of equations for the concentrations of the stages after heating $T(t)$ has the form $(-\ln(C_i)/A_i = CK_i(tk))$:

Research Production Amalgamation "Énergiya." Moscow Forestry and Timber Processing Institute.
Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 65, No. 6, pp. 652-656, December, 1993.

$$CK_i(tk) = \int_0^{tk} \exp(-E_i/T(t))dt, \quad i = 1 \ldots NST. \tag{3}$$

We must find $T(t)$ by using the known CK_i, i.e., solve a nonlinear inverse problem (reconstruct the cause from its effect).

System of equations (3) has infinitely many solutions because the interchange of two sections of the curve does not change the value of the integral.

In order to single out the necessary solution we will use a priori information that contains the time interval tk (in order to eliminate the zeroth values) and requirements on smoothness and symmetry of the solution (to avoid the rearrangement symmetry). Knowing a sufficiently exact initial approximation $T(t)$, the problem may be linearized to give the system

$$CK_i(t) = \int_0^{t} K_i(T(\tau))\, \Delta T(\tau)d\tau, \quad i = 1 \ldots NST, \tag{4}$$

which is the discrete analog of the Fredholm equation of the first kind. Problems that are close in character arise in determining by satellite the temperature, moisture, and concentration of gases of the Earth or planets by their radiation spectrum [3-6].

If the change in the temperature $T(t)$ is not arbitrary but is determined by some heat transfer and heat conduction problems, then some of the solutions of system of equations (3) may be realized only for nonphysical values of the heat flux, thus permitting regularization of problem 3 by solving the inverse heat conduction problem. As a result, we arrive at a problem that differs from those described in [7, 8] and is close to problems of optimal control.

We now consider a thin plate made of a material that is destroyed on heating according to some known law (this is the kinetic equation of a first-order reaction):

$$C(T)\, G(t)\, dT(t)/dt = q(t) - \varepsilon\sigma T^4(t), \tag{5}$$

$$G(t) = G_0 \exp\left(-A \int_0^{t} \exp(-E/T(t))\, dt\right), \tag{6}$$

$$t \in [0,\ tk]; \quad T(0) = T_0.$$

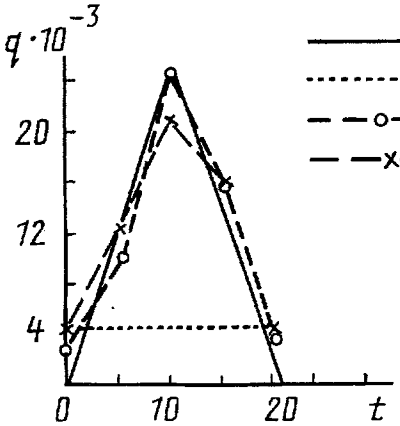
We assume that $G(tk) = GK$ is known from experiment, and it is necessary to determine $q(t)$. We will seek the heat flux in the form $q(t) = \bar{q}q_0(t)$, where $q_0(t)$ is the a function given a priori; $\bar{q}$ is a parameter (a relative heat flux). We seek a $\bar{q}$ that minimizes the discrepancy $(GK\text{-}G(tk, \bar{q}))^2$.

If the rather natural assumption that with an increase in the heat flux and the temperature the final mass of the material decreases ($dG(tk, \bar{q})/d\bar{q} < 0$) is fulfilled, then a solution exists and it is unique. Thus, a thermally destructible material may be used for determination of the relative heat flux similarly to heat-sensitive paints or irradiated crystals [9].

We now consider a material whose thermal destruction is described by several parallel independent reactions:

$$G_i(t) = G_{0i} \exp\left(-A_i \int_0^{t} \exp(-E_i/T(t))\, dt\right), \quad i = 1 \ldots NST, \tag{7}$$

$$G(t) = \Sigma G_i(t) \quad \text{or} \quad G(t) = \text{const}.$$



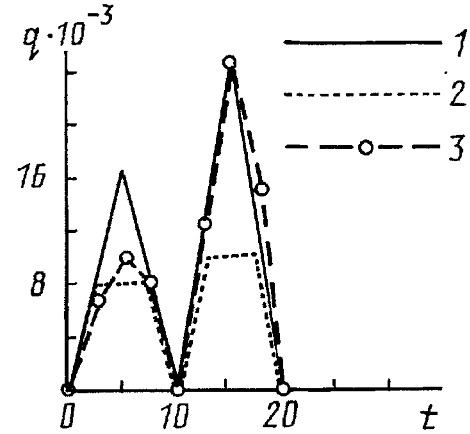


Fig. 1. Reconstruction of the heat flux density $q(t)$: 1) exact solution; 2) initial approximation; 3, 4) solutions with exact and disturbed initial data, respectively. q, W/m^2; t, sec.

Fig. 2. Reconstruction of the heat flux density (nine points) $q(t)$: 1) exact solution; 2) initial approximation; 3) solution by the suggested method.

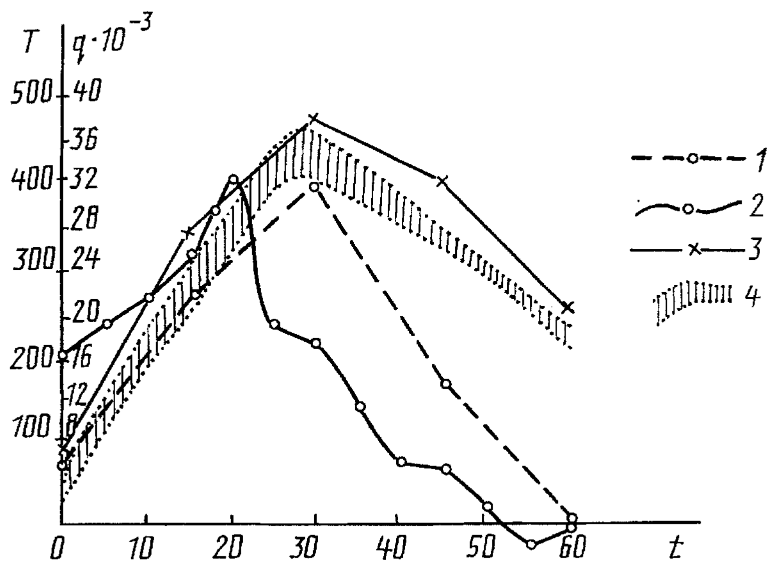


Fig. 3. Reconstruction of the heat flux density $q(t)$ and temperature: 1) heat flux density (calculation); 2) heat flux density (experiment); 3) temperature (calculation); 4) temperature (experiment). T, °C.

For $G(t)$ = const this system may be interpreted as one describing several materials that undergo destruction by a single-stage mechanism and are deposited onto a nondestructive substrate, i.e., some analog of heat-sensitive paints on a thin shell.

We know the values of $GK_i = G_i(tk)$ obtained on heating by an unknown heat flux $q(t)$, which must be determined. We use the a priori information (tk is known, $q(0) = q(tk) = 0$, the time network matches with the solution). Since the given system is rather complicated, we have performed computations to investigate the existence and the uniqueness of the solution. We have sought the vector q_j ($j = 1, \ldots, NTP$) that represents parametrically some function ($q_j = q(t_j)$) as the vector minimizing the discrepancy $\Sigma\ (GK_i - G_i\ (tk,\ q_j))^2$. In seeking a minimum, we used the method of conjugate gradients [5]. Derivatives of the functional of the discrepancy were obtained by performing the difference approximation with respect to the parameters q_j. Computations were made on a BESM-6 LSI computer for approximately 1 h. The values of $q(t)$ between the nodes were found by linear interpolation. Figure 1 shows the data of a model computation of heat flux reconstruction at $NTP = 5$, the result being satisfactory.

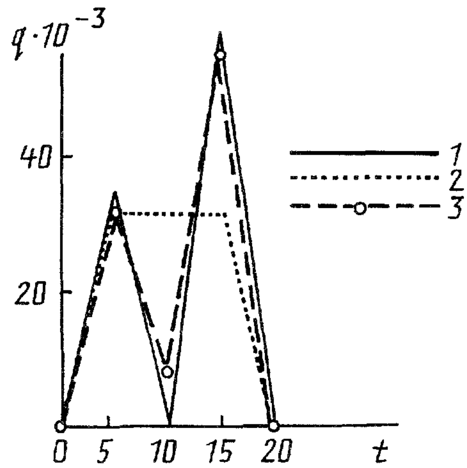


Fig. 4. Reconstruction of the heat flux density (a thick plate, five points) $q(t)$: 1) exact solution; 2) initial approximation; 3) solution by the suggested method.

In the same figure, the results of GK_i computation with a random error of ±10% are given. The solution is rather stable to this error. Figure 2 shows the results of reconstruction of a heat flux with two maxima. There are also solutions with nonzero discrepancy in which gradient methods are no longer valid, indicating the probability of local minima. It is pertinent to note here that the discrepancy has a pronounced "ravine" character (depending on the direction of change q, the increment of the discrepancy may differ by many orders of magnitude). A reliable method (but unfortunately one requiring a long computation time) is that of random search, which allows several solutions to be obtained at once.

Note that the solutions are stable to small changes in $q(t)$. This means that regularization of the problem may be accomplished with the aid of a sufficiently accurate initial approximation.

Figure 3 illustrates reconstruction of the heat flux and the temperature of a thin (0.5 - mm) composite polymer shell in comparison with experimental data.

We extend the problem to a plate with a one-dimensional temperature distribution over depth. Assume that the concentrations of the components at several ($NT \geq 1$) depths are known:

$$G(t, x)\, C(T) \frac{\partial T(x, t)}{\partial t} - \frac{\partial}{\partial x} \left[\lambda(T) \frac{\partial T(t, x)}{\partial x} \right] = 0, \tag{8}$$

$$G_i(t, x) = G_{0i} \exp \left[- A_i \int_0^t \exp(- E_i / T(t, x))\, dt \right], \quad i = 1 \ldots NST,$$

$$G(t, x) = \Sigma G_i(t, x); \quad \frac{\partial T(t, X_m)}{\partial x} = (q(t) - \varepsilon \sigma T^4(t, X_m)) / \lambda(T), \tag{9}$$

$$\frac{\partial T(t, X_m)}{\partial x} = 0; \quad t \in (0, tk); \quad x \in (0, X_m); \quad T(0, x) = T_0(x); \quad G_i(tk, x_j) = GK_{ij}.$$

The values of CK_{ij} are determined from thermogravimetric analysis of the sample after testing. It is necessary to determine the heat flux $q(t)$ acting at the boundary $x = X_m$.

At $NT = 1$ the problem differs slightly from problem (7) but at $NT = 2$ this difference becomes substantial. If the layers where "measurements" are made are sufficiently far from each other in the sense of noncoincidence of CK_{ij} values and there is no degeneracy ($CK_{ij} \neq 0,\ 1$), then the possibility of permutations and addition of zeroth terms is eliminated.

Because of the complexity of the analysis we investigated the problem numerically for the most part. In the calculations, we sought the vector q_j, representing parametrization of the desired function $q(t)$: $q_j = q(tk)$, as the vector minimizing the discrepancy $\sum_{i,j} [G(tk, x_j) - GK_{ij}]^2$.

The computations have shown that the functional of the discrepancy has many local minima and a distinct "ravine" profile. We adopted the methods of conjugate gradients [7] and random search. Problem (9) was solved by A. A. Samarskii's integrointerpolation method. In each step the direct heat conduction and the thermal destruction problems were computed. Next, we calculated the discrepancy and selected a heat flux for its minimization.

As the computations have shown, gradient methods are effective only with a relatively good initial approximation, which is explained by the presence of local minima.

The random search method may be used with any initial approximation but it is limited in the number of parameters to be optimized since they require a long computation time (computation on a BESM-6 LSI computer takes several hours).

On the whole, the numerical experiments have confirmed that the proposed system of equations may be regularized by using a priori information on the heat flux (heat load duration, number of maxima, $q(0) = q(tk) = 0$)) (see Fig. 4).

Thus, use of data of thermogravimetric analysis makes it possible, provided a mathematical model of thermal destruction and a priori information on heat flux action are available, to reconstruct the time dependence of the heat flux density in a composite polymer material.

NOTATION

G, sample weight; G_i, weight of the i-th stage ($\Sigma G_i = G$); C_i, concentration of the stage ($0 \leq C_i \leq 1$); E_i, reduced activation energy (K); n, degree of the reaction (in the given case $n = 1$); A_i, preexponential factor (1/sec); t, time; x, coordinate; T, temperature; $q(t)$, heat flux density; $C(T)$, specific heat; λ, thermal conductivity; σ, Stefan-Boltzmann constant; ε, emissivity factor; NST, number of stages; NTP, number of points in time.

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