OPTIMALLY PLANNED EXPERIMENTAL—COMPUTATIONAL DETERMINATION OF THERMAL CONDUCTIVITY OF SOLIDS IN TRANSIENT HEATING MODE

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UDC 536.21

A method is proposed for optimally planning an experiment to identify the thermal conductivity of solids with the mathematical apparatus of the sensitivity function.

A broad group of methods of determining the temperature dependence of the thermal conductivity $\lambda(t)$ of solids is based on solving inverse problems of transient heat conduction. One of the effective methods of solving these problems is parametric identification, in which the structure of the mathematical model describing the heat transfer in a given body is assumed to be reliably known except for the form of the $\lambda(t)$ relation and the latter can be approximated with a generalized polynomial in t [1]. The constant coefficients λ_j in this polynomial, combined into the vector $\lambda = [\lambda_j]_{j=1}^{r}$, are the object of parametric identification. The form of the generalized polynomial is chosen on the basis of a priori data on the characteristics of the sought function $\lambda(t)$. In these authors' view, it is preferable to use B-splines universal with respect to the form of the $\lambda(t)$ relation: an economical and highly accurate approximation approaching the values of that function as well as its derivatives of appropriate order. When using first-order splines, for instance, we have

$$\lambda(t) = \sum_{j=1}^{r} \lambda_j \,\mathrm{Sp}(t),$$
$$\mathrm{Sp}(t) = \begin{cases} 1 - |\xi| & \text{for } |\xi| \leqslant 1; \\ 0 & \text{for } |\xi| > 1, \end{cases} \qquad (1)$$

where $\xi = \frac{t}{\Delta} - j + 1$ is the dimensionless argument of the spline-function Sp(t) and Δ is a segment of the spline-approximation. In this case the coefficients λ_j are equal to the values of function $\lambda(t)$ at the approximation nodes.

An approximation with first-order splines of a typical temperature dependence of thermal conductivity $\lambda(t)$ and specific heat c(t), for Al_2O_3 ceramic over the 290-1370°K temperature range, has been constructed in Fig. 1 with six segments and Δ = 180°K.

The problem of parametric identification of $\lambda(t)$ reduces to optimal estimation $\hat{\lambda}$ of the vector of sought parameters λ from temperature readings $y_i(\tau) = t_i(\tau) + \varepsilon_i(\tau)$ at discrete points (i = 1, ..., m) of the given body, these readings containing a measurement noise $\varepsilon_i(\tau)$ and being combined into the measurement vector $Y(\tau) = [y_i(\tau)]_{i=1}^{m}$. For discrete instants of time $\tau_k = k\Delta\tau$ in $\Delta\tau$ steps we have $Y_k = Y(\tau_k) = [y_{ik}]_{i=1}^{m}$, $k = 1, \ldots, N$. The term "optimum estimates" is introduced as a reflection of the fact that from the results of measurement, which are always a random quantity, one can at any instant of time only estimate the sought vector of parameters but not determine its true values. Accordingly, estimates are regarded as optimum ones when they are good (unbiased, reliable, and sound).

Kharkov Institute of Aviation. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 45, No. 5, pp. 732-737, November, 1983. Original article submitted February 2, 1983.

0022-0841/83/4505-1227$07.50

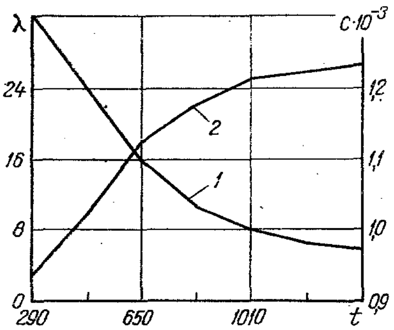

Fig. 1

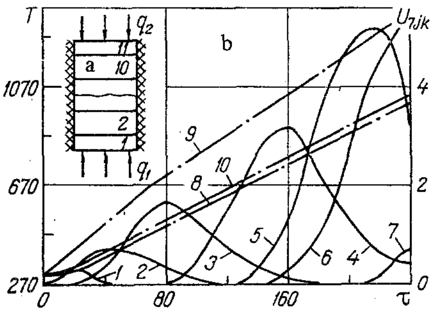

Fig. 2

Fig. 1. Approximation of temperature dependences λ(t) (curve 1) and c(t) (curve 2) with first-order B-splines: λ (W/m·K), c (J/kg·K), t (°K).

Fig. 2. Schematic diagram of specimen (a); temperature at various points of specimen as function of time and change of sensitivity U_{7jk} (K/W/m·K) of temperature of block No. 7 to change in sought coefficients λ_j during heating process (b): 1) U_{71k}; 2) U_{72k}; ...; 7) U_{77k}; 8) and 9) boundary conditions of first kind; 10) temperature of block No. 7; T (K).

The most widely used universal method of determining $\hat{\lambda}$ is minimization of the quadratic discrepancy function

$$\Phi(\boldsymbol{\lambda}) = \sum_{k=1}^{N} [\mathbf{Y}_k - \hat{\mathbf{T}}_k(\boldsymbol{\lambda})]^T [\mathbf{Y}_k - \hat{\mathbf{T}}_k(\boldsymbol{\lambda})] = \sum_{k=1}^{N} \{[y_{1k} - \hat{t}_{1k}(\boldsymbol{\lambda})]^2 + \ldots + [y_{mk} - \hat{t}_{mk}(\boldsymbol{\lambda})]^2\},$$

with respect to **λ**, where components $\hat{y}_{jk}(\lambda)$ of the so-called prediction $\hat{\mathbf{T}}_k(\boldsymbol{\lambda}) = [\hat{t}_{jk}(\boldsymbol{\lambda})]_{j=1}^{m}$ of the measurement vector correspond to components of the latter and can be calculated as function of the sought parameters **λ** by any appropriate method according to the reference model of heat transfer.

Inasmuch as this procedure is an ingredient in the solution of the ill-conditioned original inverse heat-conduction problem, one can expect various difficulties all the way to the obtainment of ambiguous and/or unstable final results. In substance this has to do [2] with the peculiarities in the form of the function Φ(λ) in the space of sought parameters λ (existence of several global or local extrema, saddle points or other singularities, ambiguity, and flatness within the range of true λ values), which give rise to instability when the primary measurements are noisy. A way out of such a situation is, on the one hand, to use algorithms with regularizing properties [3] and, on the other hand, to control the form of function Φ(λ) during design of the experiment for the purpose of eliminating or mitigating those peculiarities [1].

The possibility of control derives from the fact that the function Φ(λ) depends on the characteristics of heat transfer in a given body and on the number r of sought coefficients in the approximation [1] as well as on all significant factors comprising the technology of the experiment: number m of points in the body and their locations at which the temperature is measured (structure of the measurement vector), quality of the recording equipment determined, in the first approximation, by the dispersion of noise σ^2 (assuming a normal noise), number N of measurements made throughout the entire interval τ_N, power and mode of heating (cooling), which determine the boundary conditions for the heat transfer.

Assemblage of these factors can be categorized as optimal planning of parametric identification of thermal conductivity. According to the earlier proposal [1], such a planning requires a test for uniqueness of the solution to the parametric identification problem, the condition for its uniqueness being the existence of a unique global minimum of function Φ(λ) corresponding to the true values of the sought parameters $\lambda = \lambda_0$. When alongside such a global minimum there are also several local ones, however, then there must be available a method of extremum search capable of revealing the global minimum among all the others. When negative results are obtained, then it becomes necessary to resort to variation of those factors.

Such an active planning includes an analysis of the influence of significant factors in the experiment on the maximum attainable accuracy of λ determination, this analysis requiring that an $(r \times r)$ matrix be constructed on the basis of a priori data on $\lambda(t)$ whose elements are functions describing the sensitivity of temperature readings to changes in the sought coefficients of the $\lambda(t)$ approximation (r denoting the number of sought coefficients):

$$A = \begin{bmatrix} \sum_{i=1}^{m} \sum_{k=1}^{N} U_{i1k}^2 & \cdots & \sum_{i=1}^{m} \sum_{k=1}^{N} U_{irk} U_{i1k} \\ \vdots & & \\ \sum_{i=1}^{m} \sum_{k=1}^{N} U_{irk} U_{i1k} & \cdots & \sum_{i=1}^{m} \sum_{k=1}^{N} U_{irk}^2 \end{bmatrix}. \quad (2)$$

Here $U_{ijk} = \frac{\partial}{\partial \lambda_j} t_{ik}(\Theta_0)$ is the sensitivity function of the i-th reading for sensitivity to change in the j-th sought parameter at the k-th instant of time ($i = 1, \ldots, m$; $j = 1, \ldots, r$; $k = 1, \ldots, N$), a universal numerical method of determining which will be now presented.

From known A and dispersion σ^2 of the measurement noise can be constructed the $(r \times r)$ matrix of errors of optimum estimates $\hat{\lambda}$ [1]

$$P(\hat{\Theta}) = \sigma^2 A^{-1}. \quad (3)$$

The maximum accuracy of $\hat{\lambda}$ determination is related to the quadratic form $\lambda_0^T A \lambda_0$ describing a multidimensional ellipsoid in the vicinity of λ_0 which represents the joint confidence region [4]. In this region lie, with a known confidence coefficient which depends on σ^2 and N, the estimates $\hat{\lambda}$ as results of identification. The shape of this region is qualitatively characterized by the A-matrix eigenvalues and eigenvectors. By projecting this multidimensional ellipsoid onto the coordinate axes in the λ-space, one obtains the confidence limits of the estimates [4].

In the first approximation this analysis is confined to consideration of the matrix $P(\hat{\lambda})$, its diagonal elements representing the dispersion $\sigma^2_{\lambda_j}$ of the estimates of the sought parameters λ_j and its other elements representing the correlations between those estimates.

In this way, the basic stage in planning the determination is selection of the aforementioned factors of the experiment following a quantitative analysis of the $P(\hat{\lambda})$-matrix or of the region of joint confidence, the shape of that region being determined by the A-matrix. The planning can be executed by known methods in theory of optimal planning [5] as well as in the dialog mode by direct scanning of possible variants of experimentation.

We will demonstrate the proposed method on the specific optimal planning of identification, over the 290-1370°K temperature range, of thermal conductivity $\lambda(t)$ of a high-temperature ceramic with properties close to those of Al_2O_3. Heat transfer in a cylindrical specimen 18 mm long and 18 mm in diameter is in the experimental setup effected by feeding a thermal flux q_1 from a flat graphite heater to one base of that cylinder and extracting a thermal flux q_2 from its other base through guard rings made of the same material, with additional heating along the sides. The magnitudes of the thermal fluxes q_1 and q_2 as well as their variation in time can be stipulated as necessary. As boundary conditions, during the experiment are measured the temperatures of the base surfaces as well as the temperature at

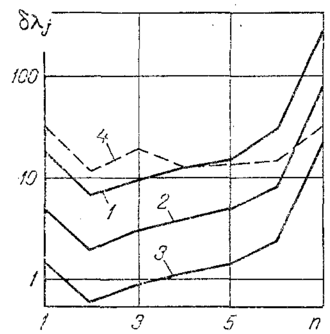

Fig. 3

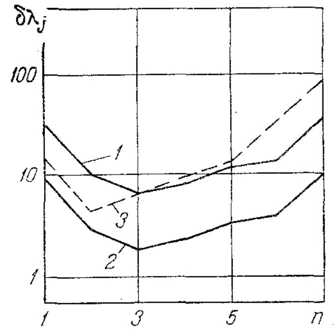

Fig. 4

Fig. 3. Dependence of rms relative errors $\delta\lambda_j$ (%) on some factors of experiment with single temperature probe: 1) $\sigma^2 = 100°K^2$, 2) $\sigma^2 = 10°K^2$, 3) $\sigma^2 = 1°K^2$ for block No. 3; 4) $\sigma^2 = 10°K^2$ for block No. 5; N = 120, $q_1 = 3 \cdot 10^5$ W/m², n is order of spline coefficients.

Fig. 4. Dependence of rms relative errors $\delta\lambda_j$ (%) on some factors of experiment with two temperature probes: 1) $\sigma^2 = 100°K^2$, 2) $\sigma^2 = 10°K^2$ for blocks No. 3 and No. 6 with N = 60 and $q_1 = 3 \cdot 10^5$ W/m²; 3) $\sigma^2 = 10°K^2$ for blocks No. 3 and No. 6 with N = 60 and $q_1 = 1.3 \cdot 10^6 (1 - e^{-p\tau})$ W/m² ($p = 18 \cdot 10^{-3}$).

one point or several points along the lateral surface. The experimental specimen is shown schematically in Fig. 2a.

The object of planning the given experiment is the ensemble of the following factors: laws of heating q_1 and q_2, number and locations of temperature probes along the specimen, interval τ_N of recording of signals from a temperature probe (or number of measurements N), and accuracy of recording channels characterized by the dispersion σ^2 of noise. Bases for planning are, in addition to the just described fundamental thermal scheme of the experiment, also a priori stipulated functions λ(t) and c(t), with their spline-approximations in six segments appropriately indicated. It is noteworthy that, according to studies made by these authors, the fundamental conclusions and the results of planning do not depend, for all practical purposes, on the degree of accuracy with which λ(t) has been stipulated. Function c(t) in the experiment is, at the same time, assumed to be known.

Under consideration were two realistic variants of stipulating the boundary conditions: (I) $q_1 = q_{01}[1 - \exp(-p\tau)]$ and $q_2 = 0$; (II) $q_1 = q_{02}$ and $q_2 = 0$. The quantities q_{01}, q_{02}, and p had been selected so as to ensure heating of the specimen up to 1300-1400°K within approximately the same time of 250 sec in each case.

For determining the boundary conditions of the first kind and constructing the sensitivity function were used numerical means of solving the original equation by the method of elimination with the number of blocks equal to 11. The sensitivity function U_{ijk} was evaluated according to the relation

$$U_{ijk} = \frac{1}{\Delta\lambda_j} [t_{ik}(\lambda_{10}, \ldots, \lambda_{j0} + \Delta\lambda_j, \ldots, \lambda_{r0}) - t_{ik}(\lambda_{10}, \ldots, \lambda_j, \ldots, \lambda_{r0})]. \quad (4)$$

The evaluation consisted of calculating the temperature trend in the i-th block at the hypothetical location of the temperature probe corresponding to the true λ_{j0}. Then an increment $\Delta\lambda_j$ of λ_j was stipulated and the temperature trend was again calculated. The difference between both trends was referred to the value of λ_j, which yielded N values of U_{ijk} in time (k = 1, ..., N).

In the calculations made by these authors $\Delta\lambda_j$ was made equal to 1-3% of λ_j. The graph in Fig. 2b depicts boundary conditions of the first kind and the sensitivity function U_{7jk} for the temperature t_{7k} of block No. 7 in variant II ($q_{02} = 3 \cdot 10^5$ W/m²).

In describing the optimal planning of this experiment we will analyze only the results pertaining to the dispersion $\sigma^2_{\lambda_j}$ of λ_j estimates, i.e., the diagonal elements of the $P(\hat{\lambda}_j)$-matrix, which had been constructed by a certain numerical method of inverting the A-matrix with respect to U_{ijk}. In the process were evaluated the rms relative errors of determination of the sought parameters, the calculations being made according to the relation

$$\delta\lambda_j = \frac{\sigma\lambda_j}{\lambda_j} \cdot 100\ [\%]. \tag{5}$$

Optimization of the errors $\delta\lambda_j$ has yielded the ensemble of all earlier-enumerated factors in the experiment. Let us show here some quantitative fragments of the planning procedure which will reveal its mechanism.

The graph in Fig. 3 depicts values of $\delta\lambda_j$ for various values of σ^2 pertaining to one temperature probe installed in block No. 3. It is evident here that the errors increase by 1-2 orders of magnitude (the rms error increasing from ± 1°K to ± 10°K) as the noise level in the original readings rises.

A comparison of curves 2 and 4 in Fig. 3 reveals that the errors depend heavily on where the temperature probe is located along the specimen. In both variants, moreover, this dependence is most significant for the first few coefficients λ_1-λ_5 of splines.

Addition of another temperature probe greatly reduces the errors, as revealed by a comparison of curves 1 and 2 in Figs. 3 and 4 (with temperature probes in blocks No. 3 and No. 6). It appears that using one temperature probe in block No. 5 for N = 120 measurements with $\sigma^2 = 10$°K² ensures approximately the same accuracy as using two temperature probes in blocks No. 3 and No. 6, respectively, with much less severe requirements imposed on the information ($\sigma^2 = 100$°K² and N = 60).

A comparison of curves 2 and 4 in Fig. 4 reveals also that variant II of heating the specimen is preferable to variant I, especially for determination of the coefficients λ_1-λ_5.

We have thus described a method of optimally planning an experiment for parametric identification of thermal conductivity. This method makes it possible, on the basis of a priori information, to assemble the values of all significant factors in the experiment. For illustration we have shown the main results of optimally planning the identification of thermal conductivity of a high-temperature ceramic through approximation of $\lambda(t)$ with first-order B-slines.

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