PLANNING AN EXPERIMENT FOR MATHEMATICAL MODEL IDENTIFICATION

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An approach is proposed that permits obtaining an effective algorithm for solving questions of planning an experiment without involving analysis of the object sensitivity function.

Let a given model L_a containing a certain set of unknown quantities $a = \{a_k\}_{k=\overline{1,p}}$ be considered. With minimal error find those $\bar{a}$ for which it is known that the observation sample $u^\delta = \{u_i^\delta\}_{i=\overline{1,m}}$ has a prototype $\bar{u} = \{\bar{u}_i\}_{i-1,m}$:

$$u_i^\delta = \bar{u}_i + \varepsilon_i, \ i = \overline{1, m}, \tag{1}$$

that expresses a solution of the equation

$$L_a u = f, \tag{2}$$

in a given discrete set $\Theta = \{\Theta_i\}_{i=\overline{1,m}}$, where $\bar{u}_i = u|_{\Theta_i}$, under the condition that the observable elements u_i^δ deviated from the prototype $\bar{u}_i$ by the known quality

$$\|u_i^\delta - \bar{u}_i\| \leqslant \delta_i, \ i = \overline{1, m}, \tag{3}$$

where the norm of the observation space governing the mode of estimating the measurement error can be, say, the r.m.s.

$$\|u_i^\delta - \bar{u}_i\| = \sqrt{\sum_{i=1}^{m} (u_i^\delta - \bar{u}_i)^2}\ ,$$

the absolute

$$\|u_i^\delta - \bar{u}_i\| = \max_{1 \leqslant i \leqslant m} |u_i^\delta - \bar{u}_i|$$

or some other.

In the formulation presented for the abstract inverse problem, (1) expresses the simplest form of the observations. Meanwhile, utilization of its more general form when quantities are observed that are functions of the state u is allowed. The approach proposed below for planning the observation u^δ allows such a generalization.

Equation (2) describes the initial model that can be set in correspondence with the process being studied. It is assumed everywhere below that a unique and stable solution exists for the given a and f. No constraints are imposed on the form of the operator and any models utilized in practice with both lumped and distributed parameters are assumed in the consideration.

Condition (3) is one of the main conditions in determining the unknown properties of an object. According to it, the desired solution should assure closeness of the states observed and those computed by models to the accuracy of the measurement error. Let us turn attention to the fact that condition (3) will later not require the postulation of a measurement error distribution law as well as assignment of a mathematical expectation and covariational matrices to them.

Within the framework of the formulation made, let us answer the question of how to plan an experiment and construct an optimal observation plan in order to determine the desired

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properties of an object with the least possible identification errors when taking account of the action of a broad class of measurement interference and modeling errors.

The degree of generality taken for the original mathematical model of the object requires absolutely taking account of a number of features of the indirect representation of the dependence of the desired quantities on the initial data. From the viewpoint of questions on numerical realization in this case, the influence of the observation interference on the stability of the calculations, the absence of a sufficient sensitivity of the states function on the variations of the parameters being identified, and also expansion of the domain of allowable values of the desired quantities must be taken into account in this case. According to [1] determination of the object properties with the features noted taken into account should be performed by satisfying two demands. Firstly, the selection of the desired solution must be consistent with the error in the initial data, and secondly, execution of the constraint of the domain of allowable solutions of the corresponding inverse problem is certain. These demands can be satisfied in the most complete volume by using the regularization method [1]. In the modification [2] where formulation of the inverse problem in the form (1)-(3) is taken into account and the possibility of simultaneously finding several quantities at once is also considered, the desired values a in the operator L_a are determined as the solution of the variational problem

$$\hat{a} = \operatorname{Arg}\inf_{a \in A_L} \Omega[a], \quad A_L = \{a : L_a u = f, \ \|u_i^\delta - u_i\| \leqslant \delta_i, \ i = \overline{1, m}\}, \tag{4}$$

where $\Omega[a]$ is a continuous and nonnegative stabilizing functional to whose domain of definition the desired values of a belong.

Let us require execution of experiment planning in conformity with the mentioned features and let us examine the possibility of solving the planning problem by using the regularization method according to the scheme (4). The further exposition is determined completely by the following property of this scheme.

THEOREM. If the element $\hat{a}$ is a solution of the problem (4), then

$$\|u_i^\delta - u_i|_{\hat{a}}\| = \delta_i, \quad i = \overline{1, m}.$$

The theorem presented, whose proof is performed analogously to [3], shows that if a known vector $\bar{a}$ with respect to which the identification error $\nu = \|\bar{a} - a\|$ must be minimized is considered, then the magnitudes of these latter can be determined as the solution of the operator equations

$$\|u_i^\delta - u_i|_{a(\nu)}\| = \delta_i, \quad i = \overline{1, m}, \tag{5}$$

where the functions $u_i|_{a}(\nu)$ are found from (2) at given observation points Θ_i under the condition that the stabilizing functional $\Omega[a]$ is minimized by the values $a^{(\nu)}$ in a set whose element differs from the etalon by not more than the quantity ν:

$$a^{(\nu)} = \operatorname{Arg}\inf_{a \in A^{(\nu)}} \Omega[a], \quad A^{(\nu)} = \{a : \|\bar{a} - a\| \leqslant \nu\}. \tag{6}$$

The formulation (5) and (6) is equivalent to the problem (4) under the additional condition $\|\bar{a} = a\| \leq \nu$. If the problem (4) is solved without this condition, but then a norm of the deviation from the etalon $\bar{a}$ is found, then for convex $\Omega[a]$ and strictly normalized observation spaces there always exists a single element $\hat{a} \equiv a^{(\nu)}$. The quantity ν is here related uniquely with the found value $\hat{a}$ while the additional condition expresses the finite error of identification that does not influence the solution itself of the problem (4).

Then if a single element of the form (6) corresponds to a given ν from the domain of definition of the problem (5), then the former is also a solution of (4) for a certain observation point of the state function of the model (2) $a^{(\nu)} \equiv \hat{a}$. Therefore, by selecting some element $a^{(\nu)}$, a ν can always be found that will satisfy (5) at a given observation point. If the values of ν are determined in a certain set of allowable measurement points, then in the long run a distribution can be obtained of the identification error as a function of the observation point location. Hence, the required optimal points are found that assure identification with the greatest possible accuracy.

Therefore, planning an experiment that proposes execution on the basis of the construction of locally optimal planes in the formulation (5) and (6) reduces to determining the error ν in a set of parameters of interest in the model under consideration. In such an approach the final optimal plan, the most informative actions on an object, the fiducial estimate intervals, the guaranteed identification accuracy, etc., can be determined by analyzing the behavior of the minimum of the identification error ν in the variations of a that are set up by a certain set $\bar{A}$ of assumed properties of the object of investigation as well as during changes of other model parameters of interest from the planning viewpoint in given intervals.

Let us mention the general possibilities of experiment planning that are allowed by the formulation (5) and (6).

Firstly, it is necessary to note that the so-called guaranteed approach within whose framework postulation of the distribution law for the measurement errors, their mathematical expectation, and the covariational matrices is not required is expressed in this case. This means that the solutions of the planning problem can be obtained under the most general assumptions about the kinds of measurement interference, including even systematic errors. Furthermore, the formulation can be used for planning experiments associated with the determination of any kinds of desired quantities including for reverse boundary, coefficient, geometric, and any other problems. Its utilization is independent of the initial model (2) where both multidimensional and different nonlinear equations can be there as well as models with lumped and distributed parameters. Finding the fiduciary identification intervals of several unknown quantities, by which the conditions for conservation of a mutually one-to-one correspondence are not spoiled, is possible.

The domain of allowable solutions and the a priori information about the desired quantities can be given under the most general assumptions about their functional properties. In the case of incomplete a priori information, a constraint on the retrieval of the desired properties from the condition of consistency of none of the interpretations of the available sets of input data is assumed. Regularization of the domain of allowable solutions is performed with the greatest possible degree that is determined by the selected method of approximating the desired quantities. Taking account of any quantitative and qualitative a priori information about the desired quantities and state functions is possible. Agreement with the observations is realized separately at each measurement point. An important feature of the approach proposed is the fact that in contrast to planning methods based on analysis of the sensitivity function, it permits not only finding the observation plane optimal in accuracy but also the setting up of the identifications allowable for this error.

The formulation (5) and (6) expresses a constitutive approach, whose numerical realization is oriented towards a standard mathematical and programmed support. Such an orientation permits a significant reduction in the labor-intensive development of appropriate planning algorithms.

The proposed locally optimal planning within the framework of the formulation (5) and (6) reduces to solving three self-consistent subproblems. The first is the minimization of a convex stabilizing functional in a set with a limited measure of the deviation from the etalon. The second is determination of the object state from its known properties as well as by given external and boundary actions. The third is solution of a system of nonlinear equations and reduces in the case of one desired quantity to the solution of one equation if the initial data are not overdetermined.

From the viewpoint of their numerical realization the listed subproblems have the following singularities. A broad class of functionals $\Omega[a]$ minimizable according to (6) after parametrization of the desired quantities $a_k = \{\alpha_k^{(\ell)}, S_k^{(\ell)}\}_{k=\overline{1,p}}^{\ell=\overline{1,N}}$ is reduced to quadratic functions in the unknown approximation coefficients $\alpha_k^{(\ell)}$ according to the basis functions $S_k^{(\ell)}$. In addition the measure of the deviation of the desired functions from the etalon $\bar{a}$ can be selected in the form of a norm differentiable with respect to the desired coefficient $\alpha_k^{(\ell)}$. In this connection it turns out to be possible to construct effective and fast-response algorithms to solve the first subproblem.

In the second case it is assumed that the domains of definition and the values of the operator L_a satisfy requirements that assure a unique and stable solution of (2) for any $a \in A$. It is also considered that the model under examination is identifiable by the desired quantities. All these conditions are known for a broad class of mathematical models, and many algorithms for the solution of equations of the form (2) have been worked out up to the level of standard subprograms.

Generally speaking, the solution of the third subproblem can be ambiguous, as will be shown in the examples presented below. In such cases among the elements $a^{(\nu)}$ that satisfy (5) those values should be selected to which the least magnitude of the stabilizing functional $\Omega[a]$ corresponds.

Algorithmically the proposed approach of locally optimal planning is an iteration process in the general case, that includes execution of the following typical actions. Firstly, the sampling of the observations $\{u_i^\delta\}_{i=\overline{1,m}}$ is simulated. Then for given $\{\nu_k\}_{k=\overline{1,p}}$, the $\{a_k^{(\nu)}\}_{k=\overline{1,p}}$ are sought to satisfy (6). Furthermore, the state of the object is determined from (2), after which it is compared with the observations $\{u_i^\delta\}_{i=\overline{1,m}}$. All the operations are repeated until values $\{\nu_k\}_{k=\overline{1,p}}$ are found that result in satisfaction of the conditions for the agreement of (5) with a given degree of accuracy.

In addition the possibility of obtaining analytic solutions is also assumed, i.e., in a number of cases exact final expressions of the optimal plans and their corresponding minimally allowable identification errors can be found.

Let us display the practical possibilities of the approach described as well as its fundamental realization features by examples of certain planning problems that have known solutions. The problems being examined below permit a complete representation to be obtained of the circle of questions that are included within the framework of the formulation (5) and (6).

Let be considered a given mathematical model

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + a \sin \pi x, \ 0 < x < 1, \ t > 0; \tag{7}$$

$$u|_{t=0} = 0, \ u|_{x=0} = 0, \ u|_{x=1} = 0,$$

with an unknown coefficient a = const to be determined. An optimal observation plan is constructed for it in [4] with measurements performed according to the law

$$u_i^\delta(t) = \bar{u}(x_i, \ t) + \varepsilon_i e(t), \quad i = \overline{1, m},$$

where ε_i are arbitrary random numbers, e(t) is a given nonrandom function simulating the measurement trend, say, and $\{x_i\}_{i=\overline{1,m}}$ are the observation points.

Let us determine the coordinates of the optimal observation points and let us also establish the properties of the identification estimates by using the proposed approach.

In conformity with (6) and also the recommendations in [2], let us introduce the following minimization subproblem

$$\min_{a \in R^1} \max |a|,$$

$$|\bar{a} - a| \leqslant \nu.$$

It has the solution $a^{(\nu)} = \bar{a} - \nu$. In the case m = 1 adequate for the determination of one coefficient a, (5) has the following final expression

$$\max_{x,t} \left| \nu \frac{1 - \exp(-\pi^2 t)}{\pi^2} \sin \pi x + \varepsilon e(t) \right| = \max_{x,t} |\varepsilon e(t)|. \tag{8}$$

Among all the values of ν determined by (8) for given ε, e, and x, the least turns out to be in the case when the function $[1 - \exp(-\pi^2 t)] \sin \pi x$ achieves its maximum in the domain $Q = \{(x, t): \ 0 < x < 1, \ t > 0\}$. We hence obtain that for any functions e(t), interference ε, and $t > 0$ measurements at the point $x_{opt} = 0.5$ assure identification of the coefficient of the model (7) with a minimal error. An analogous result is also obtained in [4] where the optimal plan was constructed by using the criterion of D-optimality. Let us note here that the method utilized here permitted the desired solution to be obtained under more general assumptions about the properties of the measurement interference that those made in [4].

Analysis of the solutions of (8) for specific functions e(t) permits determination of further properties of the identification errors as well as the allowable error estimates of the values of the desired coefficient required in conformity with the guaranteed approach. As an illustration, let us take the function $e = T - 2t$, $T \neq 0$ describing the conditional trend with constant rate in the segment $0 < t < T$. In this case (9) has several roots including the value $\nu = 0$ also. It follows from the condition of the minimum of the stabilizing functional $\Omega = \max|a|$ introduced for the identifiable coefficient that the root having the greatest absolute value should be that desired. It can be shown that such a root always exists for (8) while for $\varepsilon > 0$ it has the value $\nu = 2\varepsilon/\sin\pi x$. Then the desired coefficient having the minimal identification error in observations with the mentioned measurement interference characteristics is expressed by the quality $a^{(\nu)} = \bar{a} - 2\varepsilon$.

Another case, when $\varepsilon < 0$, is more preferable since a small identification error is associated with it. In this sense the value $\nu_{min} = 2|\varepsilon|$ can be the majorant to obtain further properties of the error ν. In particular, a dependence of the allowable absolute error of measurement $\Delta = \max|u^{\delta} - u|$ on the guaranteed identification error can be established: $\Delta_{all.} = 2T\nu_{guarant.}$, or in relative quantities $\delta_{all.} = 2\pi^2 T/[1 - \exp(\pi^2 T)]\mu_{guarant.}$, where $\delta = \max|u^{\delta} - \bar{u}|/\max|\bar{u}|$, $\mu = |\bar{a} - a|/\bar{a}$. It is hence seen that identification of the model (7) to identical accuracy but for different lengths of the observation interval requires that the greater the value of T the smaller the measurement accuracy, and vice-versa. For $T > 0.5$ determination of the coefficient a is guaranteed with both an absolute and relative error that does not exceed the magnitude of the measurement error.

Now we turn to examination of the problem associated with determining the coefficient of the highest derivative of the state fucntion. We assume that the value a = const must be found in the mathematical model

$$\frac{\partial u}{\partial t} = a\frac{\partial^2 u}{\partial x^2},\ 0 < x < \infty,\ t > 0;$$
$$u|_{t=0} = u_0(x),\ u|_{x=0} = 0. \tag{9}$$

It is known in this case [4] that if the initial distribution has the form $u_0(x) = \sin k_0\pi x$ where $k_0 \geq 1$ is an integer and the observations are performed in the half-interval $0 < x < 1$, then points with the coordinates $x_{opt}^{(k)} = ((2k - 1)/2)/k_0$, $k = \overline{0, k_0 - 1}$ are optimal.

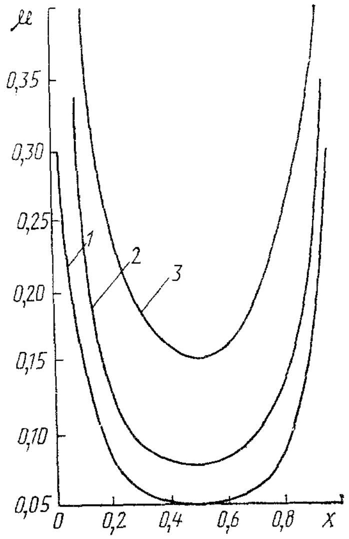
Reasoning analogous to that presented above permits obtaining the following consistency condition

$$\max_{x,t}|\exp(-k^2\pi^2\bar{a}t)[1 - \exp(k_0^2\pi^2\nu t)]\sin k_0\pi x + \varepsilon| = \max_{x,t}|\varepsilon|.$$

It shows that for any $\bar{a}$ and ε the minimal identification errors are achieved where the function $|\sin k_0\pi x|$ has a maximum. Hence, we find the mentioned points $x_{opt}^{(k)}$. Exactly as above, the optimal observation coordinates are obtained under the most general assumptions relative to the values of a and the properties of the interference ε.

Numerical modeling of the measurement interference ε permits development of the investigation of the identification error properties for the model under examination. Results obtained during simulation of measurement interference with a normal distribution law and zero mathematical expectation are presented in Figs. 1 and 2 for the case m = 1.

The found relative error function $\mu(x)$ (Fig. 1) shows the nature of the influence of accuracy of the identification of the desired parameter a on the change of the observation point coordinates. Obtaining functions of such form together with determination of the location of the optimal measurement points and finding the fiduciary interval of the accuracy of the inverse problems solutions is intended for analysis of changes in the identification error in the case of deviation of the observations from the optimal plan.



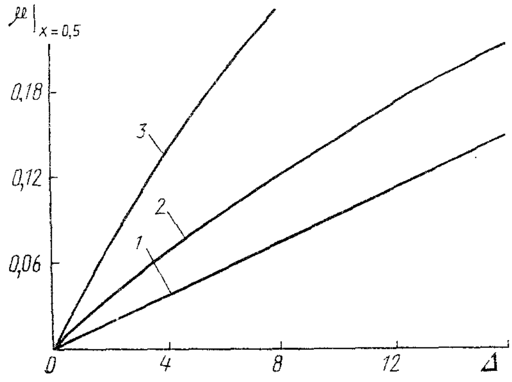


Fig. 1

Fig. 2

Fig. 1. Relative identification error for the model (9) during simulation of the measurement interference with a 5% level of observation errors: 1) $\bar{a}$ = 0.1; 2) 1; 3) 10.

Fig. 2. Minimal relative identification error of the model (9) as a function of the measurement interference level: values of 1-3 are the same as in Fig. 1. Δ, %.

Let us note that a further study of the behavior of the function μ(x) during simulation of the operation of any other observation interference of practical interest, including systematic errors, also permits finding the fiduciary intervals of identification error and performing an appropriate analysis of the accuracy of the inverse problem solution in any direction of interest.

The dependence $\mu_{min}(\delta)$ (Fig. 2) expresses the value of the allowable interference level and the associated guaranteed identification error. As is seen, obtaining the desired coefficient with an error not exceeding the measurement error is guaranteed for $\bar{a}$ < 0.1 in the case under consideration.

The identification accuracy of the model (9) as a function of the volumes of the observation samples n = 50, 100, 500, 1000 was, respectively, $|\bar{a} - a^{(\nu)}|/\bar{a}$ = 0.08157; 0.08126; 0.04; 10^{-12}. The results obtained reflect the known property of consistency of the estimates obtained. Let us note that the assumption of noncorrelativity of the measurement errors and the normality of their distribution law turns out to be essential here. There is no monotonic improvement in the estimates as the sample volume increases during deviation from these assumptions and a certain optimal value of the number of measurements n exists. Developing the investigation in this direction, the best measurement times can be found that will assure minimality of the identification error for a given number n.

We now show the possibility of the proposed approach when it does not seem possible to obtain (5) in the form of explicit expressions relative to the desired errors ν. In such cases the construction of the optimal observation plan is based completely on a numerical analysis that can also be performed successfully within the framework of the formulation (5) and (6), as in the analytic methods applied above.

Let a given model be considered

$$c\rho\frac{\partial u}{\partial t}=\frac{\partial}{\partial x}\left(\lambda\frac{\partial u}{\partial x}\right),\ x_0<x<x_k,\ 0<t<T;$$
$$u|_{t=0}=u_0(x),\ x_0<x<x_k; \qquad (10)$$
$$-\lambda\frac{\partial u}{\partial x}\Big|_{x=x_0}=q_1(t),\ \lambda\frac{\partial u}{\partial x}\Big|_{x=x_k}=q_2(t),\ t>0.$$

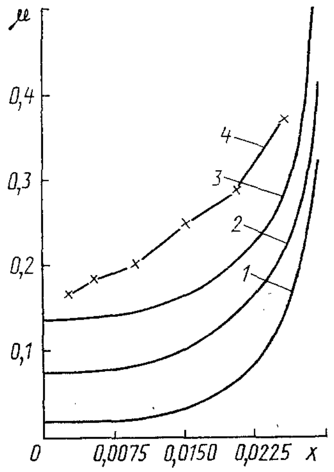


Fig. 3. Relative identification error of the model (10); 1) Δ = 1%; 2) 5; 3) 10; 4) results of [7]. x, m.

Let us examine the observation planning problem for it $\{u_{ij}{}^{\delta}\}_{i=\overline{1,m}}^{j=\overline{1,n}}$ given in the domain $Q = \{(x, t): x_0 < x < x_k, 0 < t < T\}$ for the determination of the heat flux $q_1(t)$, say.

In conformity with (6) we introduce the following extremal subproblem

$$q_1^{(\nu)} = \mathrm{Arg} \inf_{q_1 \in A^{(\nu)}} \Omega[q_1] , A^{(\nu)} = \left\{q_1 : \int_0^t (\bar{q}_1 - q_1)^2 \, dt \leqslant \nu\right\}, \tag{11}$$

where $A^{(\nu)}$ is the domain of allowable solutions defined, say, as the class of triply differentiable functions, Ω is the stabilizing functional selected according to the recommendations in [5, 6], and $\bar{q}_1$ is the standard solution.

The desired value of the error ν allowable at a given observation point x_i is determined by the solution of the system

$$\max_{1 \leqslant j \leqslant n} |u_{ij}^{\delta} - u(x_i, t_j)|_{q_1^{(\nu)}}| = \delta_i, \ i = \overline{1, m}. \tag{12}$$

This latter can be represented as

$$\nu = \mathrm{Arg} \min_{\nu} \sum_{i=1}^{m} [\max_{1 \leqslant j \leqslant n} |u_{ij}^{\delta} - u(x_i, t_j)|_{q_1^{(\nu)}}| - \delta_{ij}]^2.$$

By using the formulation (11) and (12) the model case considered earlier in [7] was investigated. Assignment of the standard value $\bar{q}_1$, approximation of the desired function q_1 as well as determination of the identification accuracy were all done in conformity with the work mentioned.

The dependence found for the relative error on the observation point coordinates is shown in Fig. 3 for m = 1 for different values of the relative measurement errors. The observation interference was simulated by a pseudorandom number sensor with a normal distribution law and zero mathematical expectation.

The results obtained reflect the fundamental asymptotic properties of the error in identification by the regularization method according to the scheme of particular consistency when the measurement interference level tends to zero. Let us turn attention to the error in determining the flux obtained in [7] that even for $\delta = 0$ exceeds the error allowed by the scheme (4) when $\delta \neq 0$. As the results obtained earlier [5, 6], this comparison shows that a number of algorithms allow significant identification errors, despite the realizable constraints on the domain of allowable solutions and the satisfaction of the consistency conditions with errors of the initial data.

This latter indicates that if the limitation of the domain of allowable solutions can generally assure the stability of the solution of an incorrectly posed problem, then execution of a sufficient degree of regularization, which should certainly be consistent with the selected method of parametrization of the desired quantities, is necessary to obtain satisfactory accuracy. In the opposite case the solution can be stable and consistent with errors in the initial data but have unsatisfactory accuracy (Fig. 3) or have nothing in common with its true form [5, 6].

Summarizing the investigation conducted, we note the following fundamental results. The proposed experiment planning approach permits taking account of features of the implicit representation of the relation between the observable and the desired quantities when the appearance of a weak state function sensitivity turns out to be essential and expansion of the domain of allowable solutions of the corresponding inverse problem occurs. The method based on it permits carrying out a multilateral study of the identification accuracy as well as solving a broad circle of practical questions under the condition of operation of the most diverse measurement interference and modeling.

It is shown that both an analytic and an effective numerical determination of observation plans optimal in accuracy, finding the ultimate identification error estimates and their fiduciary intervals, investigation of the action of different kinds of interference including systematic errors, the build-up of the interference level necessary to obtain guaranteed identification errors, and the exposure of the most informative observation domains are possible.

In conclusion, we emphasize once again that the ultimate estimates obtained for the identification accuracy are possible only for a suitable constraint on the domain of allowable solutions of the problem under consideration. All this makes study of the question of methods of limiting a given domain of allowable solutions and the corresponding identification error urgent in the theory of incorrectly posed problems. Obtaining recommendations relative to the necessary degree of contraction for the most typical methods of parametrizing the desired quantities is especially important in those cases when it is impossible to do it explicitly, as in the regularization method, say.

NOTATION

u, object state function: f, external actions on the object; L_a, model that can be set in conformity with the object being studied; a, desired quantities characterizing the object properties; p, their number; u^δ, observations; $\bar{u}$, observation prototype; Θ_i, observation points; m, number of observations; n, number of measurements at a given observation point; x_0, x_k, observation domain boundaries; ε, measurement interference; δ, guaranteed measurement error; Δ, absolute measurement error; ν, identification error; μ, relative identification error; A, domain of allowable solutions of the inverse problem; Ω, stabilizing functional; c, specific heat; λ, heat conductivity; u_0, initial distribution; $q_{1,2}$, boundary heat fluxes; and $\bar{a}$, standard value of the desired quantity.

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