and at the wall $x = x_w$; a prime above a function is ordinary differentiation; and independent variables as subscripts denote partial derivatives.

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PRACTICALLY ACHIEVABLE ACCURACY AND RELIABILITY OF THE SOLUTION OF INVERSE HEAT-CONDUCTION PROBLEMS

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We develop a method of solution of inverse heat-conduction problems which makes it possible to obtain a guaranteed minimum of reliable information in conditions of indeterminacy.

In practical analyses of data from model and natural thermal experiments, wide attention has been given to methods based on the solution inverse heat-conduction problems (IHCP) with the use of regularization [1]. It is known, however, that the regularization theory gives only a potential possibility to solve incorrectly posed problems. The regularization method itself has an asymptotically optimal character when the quality of the approximate solution is estimated from its behavior in comparison with the exact solution when the error of observations tends to zero. If the number of measurements is small and the noise is appreciable, the convergence of approximate solutions is of secondary importance, and the principal problem is to extract the maximum amount of reliable information from the available data, and to isolate fragments of solution which, under the existing indeterminacy, are observed reliably.

This formulation of the problem must be viewed alongside the fact that, in realistic conditions, there are always sufficiently large regions of competing interpretations of the input data (which are, objectively, of equal value) and any "optimum" solution chosen according to some principle, is capable of adequately reflecting only individual fragments of the true solution. It is difficult to analyze reliability of the local properties of the approximate solutions in terms of the classical estimates of accuracy constructed in terms of the metrics L_p. These facts stimulate the development of applied methods (adaptive [3], descriptive [4], local [5] and stepwise [6] regularizations) which make it possible to narrow down maximally the mass of the permissible solutions of the inverse problem by virtue of a more complete allowance for the restrictions on the properties of solutions and noise, and of a more special

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choice of the usual parameters in the computational schemes. These methods should be viewed on the background of the traditional forms of regularization oriented towards the minimum a priori information (for example, about the pair (δ, h): $\|u_\delta - u\| \leq \delta$, $\|A_h - A\| \leq h$ [2]) which are sufficient for the construction of stable approximations $z^{\delta,h}$ to the solution of the equation $Az = u$ (in mathematics, similar results are most valuable).

In the regularization theory, the former approach is developed in the theory of pattern recognition and in the determination of functional dependences from empirical data [7], in the theory of sensitivity of control systems [8], in several branches of geophysics [9, 10], and in other disciplines. This method is based on the principle that, in incorrectly posed problems with incomplete a priori information, it is often expedient to restrict oneself to a search for properties of the object under investigation which contradict no interpretation of the input data. Mathematical methods then make it possible to carry out a meaningful and comprehensive analysis of the multitude of formally permissible solutions of the inverse problem with the aim of finding the general properties of the object under study which are present in all the solutions and can be assumed to be a reliable information about the unknown solution. The optimum estimates of the model parameters are assigned the role of "reference" solution which can reduce the technological difficulties in the realization of the approach, and help to form more realistic criteria about the true limits of indeterminacy.

Below, we study the possibility of applying this concept to IHCP. The analysis is carried out using the example of a classical problem which requires to reconstruct the thermal regime $T(\xi, \tau_0)$ of an infinite, thermally insulated rod at time τ_0 from discrete measurements $\tilde{T}(x_i, \tau)$, $i = \overline{1, N}$ of the temperature at time $\tau > \tau_0$ which contain a random noise. Since the heat-conduction process is analogous to diffusion, this problem has found an important application in geochemistry [11] in the prognosis of the concentration profile $C(\xi, \tau_0)$ of a chemical element in undisturbed levels of mineral deposits using its distribution $\tilde{C}(x_i, \tau)$ in the diffusion halo.

We assume, for simplicity, $\tau_0 = 0$, and denote by subscript 0 the temperature at the initial moment of time. We then have, according to [12],

$$T(x, \tau) = \frac{1}{2\sqrt{\pi a \tau}} \int_{-\infty}^{\infty} T_0(\xi) \exp\left[-\frac{(\xi - x)^2}{4a\tau}\right] d\xi. \tag{1}$$

In the input data as an element of a finite-dimensional space (to avoid information incorrectness of the IHCP formulation), it is expedient to use also a finite-parametric description of the approximate solution of the inverse problem. This can be ensured by using, in the approximation of the unknown temperature, the model classes $\mathfrak{M}_n$ of functions of the type $T_0(\xi; A) = A_0 f_0(\xi) + \ldots + A_n f_n(\xi)$ which contain a finite number of free parameters A_j and have good approximative and computational properties. By this, we understand the following: the sequence of classes $\{\mathfrak{M}_n\}$ forms a chain of embedded sets $\mathfrak{M}_1 \subset \mathfrak{M}_2 \subset \ldots \subset \mathfrak{M}_m \subset \ldots$, which have, as a limit, the set $\mathfrak{M}$, which is dense in the space of continuous (or piecewise continuous) functions and, for any n, the problem can be solved in terms of elementary functions. These requirements are satisfied, for example, by sets of polynomials, sections of Fourier series and sums of exponentials for which, using the tabulated integrals [13], the direct problem can be solved in a close form. In particular, if

$$T_0(\xi) = A_0 + \sum_{j=1}^{n} A_j \exp(-j\xi), \tag{2}$$

then

$$T(x, \tau) = \sum_{j=0}^{n} A_j F_j(x, \tau), \quad F_j(x, \tau) = \exp(j^2 a \tau) \exp(-jx). \tag{3}$$

The problem of choosing n is to satisfy the incompatible requirements of a detailed description of the required dependence $T_0(\xi)$ while ensuring the stability of solution [6]. As in the application of the traditional methods of solution of IHCP to the present method, this problem is nontrivial. We therefore confine ourselves to recommendations [6]: the value of n should ensure that the temperature discrepancy is consistent with the level of error in the input information. The parametric dimensionality n of the problem should not exceed the number of measurements and should not lead to instability of the calculation as a result of the rounding errors in the results of computer calculations.

We consider a mixed formulation when, together with $T_0(\xi)$, one does not know the thermal diffusivity a. It should be noted that for a fixed a, the (theoretically) linear heat-conduction problem (given exact values of T(x) on the entire x axis) has, in the majority of cases, a unique solution. In the mixed formulation, however, the ambiguity manifests itself already in the narrow finite-parametric classes of solutions. For example, two different functions (2) transform into one function $T(x, \tau)$ if their coefficients $A_j^{(1)}$ and $A_j^{(2)}$ are related by

$$A_0^{(1)} = A_0^{(2)}, \quad A_j^{(1)} \exp(j^2 a_1 \tau) = A_j^{(2)} \exp(j^2 a_2 \tau), \quad j = \overline{1, n}, \tag{4}$$

where a_1 and a_2 are alternative values of thermal diffusivity. Nevertheless, the mixed formulation is meaningful if, together with the measured values $T(x_i, \tau)$, the value $\xi = \bar{\xi}$ of the required function is known (albeit in one point $T_0(\bar{\xi}) = \bar{T}$). (The attempt to estimate simultaneously several thermophysical parameters, and the use of reference values of the required functional dependences are discussed in [14] and [15], respectively.) The ambiguity is then considerably reduced. Indeed, let $T_0(\xi)$ be the solution of the form $A_0^{(0)} + A_1^{(0)} \exp(-\xi) + \ldots + A_n^{(0)} \exp(-n\xi)$ of Eq. (1) using an exactly specified function T(x) for an arbitrarily chosen value of $a = a_0$. In the general case $T_0(\bar{\xi}) \neq \bar{T}$ and the determined function is no longer a solution of IHCP with the restriction $T_0(\bar{\xi}) = \bar{T}$ which, with allowance for the constraints (4), leads to an algebraic equation with respect to the unkown a:

$$K_0 = \sum_{j=1}^{n} K_j u^{j^2} = 0, \quad u = \exp(-a\tau); \tag{5}$$

$$K_0 = A_0^{(0)} - \bar{T}, \quad K_j = A_j^{(0)} \exp(-j\bar{\xi}) \exp(j^2 a_0 \tau), \quad j = \overline{1, n}. \tag{6}$$

By finding its roots on the interval (0, 1), we find the (now finite) set of values $a_t = -\ln u_t/\tau$ of the coefficient a for which (and only for which) the mixed IHCP with one restriction has a solution.

We now go over to a direct exposition of the method of solution of IHCP. It includes: 1) The formation of a system of functionals M_s which will be used to express the result of analysis of the input data; 2) The formalization of a priori restrictions on the region $\mathscr{D}$ of the permissible solution of the inverse problem; 3) The formulation and solution of the optimization problems for the search of extremal values of the functionals M_s on the set $\mathscr{D}$.

We expand on the contents of each point with application to the problem (1). We start with the first one. It is widely accepted that, in the analysis of any algorithms of the solution of inverse problems, it is necessary to try to adapt the algorithm exclusively to the solution of the target problem and not more than that (this is not so much a problem of the method as a requirement that the obtained solution is informationally meaningful). Accordingly, it is necessary to specify first the properties (characteristics) of the exact solution which were focused on in the physical experiment. In problems of the type (1), this can be local characteristics (the number, position and values of the extrema of the function $T_0(\xi)$), as well as integral characteristics (linear storage of matter on the segment (α, β) at moment τ_0 in the inverse diffusion problem equivalent to (1)). In particular, one can discuss the integral estimates of the parameters A_j, which approximate the functions $T_0(\xi; A)$ (a similar problem was considered in [16] within the regularization framework).

One of the advantages of the approach oriented towards the analysis of the set of permissible solutions is the fact that it can be easily adapted to different aims followed by the interpreter in the solution of the inverse problem. We shall illustrate this by a nontypical formulation of the inverse problem which is not associated with the estimate of the solution in terms of classical metrics. Suppose that the target problem is a description of the set Ω of points $\xi \in (\alpha, \beta)$ where the values of an unknown function $T_0(\xi)$ exceed a given $T^{(0)}$. This formulation is interesting, incidentally, for geochemical applications where one chooses $C^{(0)}$ as the minimum anomalous concentration of an industrial deposit, and the problem reduces to the prediction of perspective segments within the region under study. The scattering parameter $\sigma = \sqrt{2D\tau}$ is usually not known exactly (it is difficult to estimate the time from the beginning of the process). However, the reference values of $C_0(\bar{\xi}_k) = \bar{C}_k$ for an unknown concentration profile can be established by testing the uncovered natural or artificial native rocks.

We shall now attempt to formulate the target problem in terms of functionals. If $\Omega = \{\xi \in (\alpha, \beta): T_0(\xi) > T^{(0)}\}$ is a meaningful characteristic of the solution of IHCP, the following three sets will be meaningful characteristics of any family of possible solutions of the inverse problem: Ω_1 set of points $\xi \in (\alpha, \beta)$ in which the value of each of the permissible approximate solutions $T_0(\xi)$ exceeds a given $T^{(0)}$; the set Ω_2 of points $\xi \in (\alpha, \beta)$ for which, among the permissible solutions, there are both functions with the value $T_0(\xi) \geq T^{(0)}$ as well as functions with the value $T_0(\xi) < T^{(0)}$; and the set Ω_3 of points $\xi \in (\alpha, \beta)$ where all the permissible solutions take the values $T_0(\xi) < T^{(0)}$. If these sets are constructed, the analysis of the data $\{\tilde{T}(x_i)\}$ allows the following interpretation: for an incomplete a priori information, it is impossible to construct the region Ω but one can assert that a) $\Omega_1 \subset \Omega$, i.e., it is certain to identify some subset of Ω; b) $\Omega_3 \cap \Omega = \varnothing$, it is reliably established that segment Ω_3 is of no interest from the viewpoint of the target problem; c) Ω_2 is a uncertainty region in whose every point ξ one can expect, for the unknown function $T_0(\xi)$, both $T_0(\xi) \geq T^{(0)}$ (because the points $\xi \in \Omega \setminus \Omega_1$ have not been identified) as well as $T_0(\xi) < T^{(0)}$.

In the general case, the sets Ω_m, m = 1, 2, 3 are sets of nonintersecting segments, and the required functionals M_s can be the coordinates of their ends.

The second point of the method is the set of permissible approximate solutions $T_0(\xi) = A_0 f_0(\xi) + \ldots + A_n f_n(\xi)$ of the inverse problem which are obtained for some possible values $\underline{a}$. This is determined by the composition of the input data. We assume that besides the values $\tilde{T}(x_i)$ we know: the estimate ε of the absolute error of the measurements (one could take also the pointwise estimates for each x_i); the boundaries $(\underline{a}_{min}, \underline{a}_{max})$ for the unknown thermal diffusivity; the values $\bar{T}_k = T_0(\bar{\xi}_k)$, given with some error ε_1, of the required function in points $\bar{\xi}_k$, $k = \overline{1, K}$ (since one can use two different registration schemes we have, in general, $\varepsilon_1 \neq \varepsilon$). The set of allowed solutions of the inverse problem will be composed of all coefficients A_j of function $T_0(\xi; A)$ and values a which satisfy the inequalities

$$|\tilde{T}(x_i) = \sum_{j=0}^{n} A_j F_j(x_i, a)| \leqslant \varepsilon, \quad i = \overline{1, N}, \tag{7}$$

$$\left|\sum_{j=0}^{n} A_j f_j(\bar{\xi}_k) - \bar{T}_k\right| \leqslant \varepsilon_1, \quad k = \overline{1, K}, \tag{8}$$

$$a_{\min} \leqslant a \leqslant a_{\max}. \tag{9}$$

It remains to specify the method of construction in terms of the sets Ω_1, Ω_2 and Ω_3. The interval (α, β) is covered by a grid $\{\xi^{(\ell)}\}$, $\ell = \overline{1, L}$ with a sufficiently small step h, and the points $\xi^{(\ell)}$ are classified as points from one of the sets Ω_1, Ω_2 and Ω_3. To this end, for each ℓ we formulate two mathematical programming problems: to minimize (maximize) the linear functional

$$T_0(\xi^{(l)}) = f_0(\xi^{(l)}) A_0 + f_1(\xi^{(l)}) A_1 + \ldots + f_n(\xi^{(l)}) A_n \tag{10}$$

on the set of vectors $(A_0, A_1, \ldots, A_n; \underline{a})$ which satisfy (7)-(9).

Let $T_\ell^{(\min)}$, $T_\ell^{(\max)}$ be the solutions of these problems for instantaneous ℓ. Three cases are possible:

1) if $T_l^{(\min)} > T^{(0)}$, then $\xi^{(l)} \in \Omega_1$;
2) if $T_l^{(\max)} > T^{(0)}$, but $T_l^{(\min)} < T^{(0)}$, then $\xi^{(l)} \in \Omega_2$;
3) if $T_l^{(\max)} < T^{(0)}$, then $\xi^{(l)} \in \Omega_3$.

The union of points $\xi^{(\ell)}$ which correspond to one case is a pointwise approximation of the required solution $\langle\Omega_1, \Omega_2, \Omega_3\rangle$.

It is apparent that the identification of the points $\xi^{(\ell)}$ which coincide with any of the reference points $\bar{\xi}_k$ from the restriction (8) can be simplified. One more remark. The search for the extrema of the function (10) is complicated considerably by the restriction (7) which is nonlinear with respect to $\underline{a}$. It is expedient to linearize the problem. The interval $(\underline{a}_{min}, \underline{a}_{max})$ will be covered by the grid $\{\underline{a}_q\}$, $q = \overline{1, Q}$ and the extrema of the functions (1) will be defined for each pair $(\xi^{(\ell)}, \underline{a}_q)$ but within the linear constraints (7) and (8). The point $\xi^{(\ell)}$ will be referred to Ω_1 or Ω_3 only when the cases 1) and 3) take place for all $\underline{a}_q$, $q = \overline{1, Q}$.

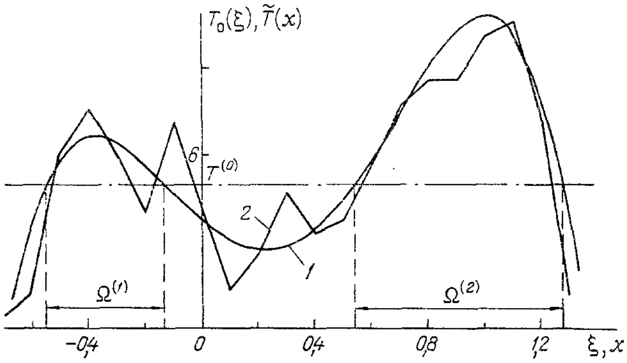

Fig. 1. Graphs of the functions 1) $T_0(\xi)$, 2) $\tilde{T}(x)$; $\Omega^{(1)}$, $\Omega^{(2)}$ are the segments which make up the unknown region Ω.

TABLE 1. Results of Solution of IHCP for Different Quality of the Input Data and Different Volume of the a priori Information

Δ	I				II			
	$\Omega_1^{(1)}$	$\Omega_1^{(2)}$	ν_1	ν_2	$\Omega_1^{(1)}$	$\Omega_1^{(2)}$	ν_1	ν_2
0,5	(—0,48; —0,2)	(0,6 ; 1,24)	0,8	0,12	(—0,52; —0,16)	(0,6 ; 1,24)	0,87	0,10
1,0	(—0,46; —0,22)	(0,66; 1,22)	0,7	0,25	(—0,50; —0,18)	(0,62; 1,22)	0,8	0,22
2,0	(—0,40; —0,3)	(0,70; 1,12)	0,45	0,52	(—0,44; —0,24)	(0,70; 1,20)	0,61	0,44
4,0	$\varnothing$	(0,86; 1,08)	0,19	0,86	(—0,32; —0,28)	(0,80; 1,18)	0,37	0,78
8,0	$\varnothing$	(0,90; 0,96)	0,06	0,91	$\varnothing$	(0,88; 1,0)	0,11	0,84

We consider a methodological example. The true temperature distribution $T_0(\xi)$ (Fig. 1) is a fourth-degree polynomial with the range of definition $(\alpha, \beta) = (-0.7; 1.3)$. The observations $\tilde{T}(x_i)$ were modelled by the superposition of a normal random noise onto the values of $T(x_i)$, $i = \overline{1, 25}$ calculated from (1) for $\underline{a} = 1$ and $\tau = 10^{-2}$. We assumed that $T^{(0)} = 5$ (in relative units). Then (see Fig. 1), the unknown region Ω consists of two segments $\Omega^{(1)} = (-0.55; -0.13)$ and $\Omega^{(2)} = (0.54; 1.27)$.

We carried out a series of calculations (Table 1) for five root-mean-square values Δ of the noise in $\tilde{T}(x_i)$. In each variant, we studied the cases when, in point $\xi = 0$, an a priori value of the unknown function is given (II), and when the investigator does not have this information (I). The thermal diffusivity was, for simplicity, assumed known. Besides the coordinates of the segments $\Omega^{(1)}$ and $\Omega^{(2)}$ which make up the set of points ξ in which, from the available limited information one can guarantee that the unknown values $T_0(\xi) > T^{(0)}$, Table 1 contains the normalized indices ν_1 and ν_2 of quality of the solution of the inverse problem. These indices are the ratios of the lengths of the segments which make up the sets Ω_1 and Ω_2, respectively, to the sum of the lengths of segments $\Omega^{(1)}$ and $\Omega^{(2)}$ and to the length of the interval (α, β) (it is clear that, in the ideal case when there is no noise and the function $T_0(\xi)$ is reconstructed unambiguously, $\Omega_1 = \Omega$, $\Omega_2 = \phi$, $\nu_1 = 1$, $\nu_2 = 0$, and in the worst case $\Omega_1 = \phi$, $\Omega_2 = (\alpha, \beta)$, $\nu_1 = 0$, $\nu_2 = 1$). In the terms of the sets Ω_1, Ω_2, Ω_3, the solution reduces to the search for the extremal properties of the individual functions $T_0(\xi)$ from the permissible set of solutions of IHCP. Therefore, all approaches which were developed in the theory of solution of incorrectly posed problems to ensure a high stability of the results assist also to the growth of the indices of quality ν_1, ν_2. In the present example, in particular, a very high quality of the results of interpretation is, in many ways, predetermined by the a priori specification of the degree n of the polynomial which describes the true temperature distribution. In the direct methods of solution of IHCP, the variation of the parameter n corresponds to one of the possible methods with self-regulation [6]. However, the class of retrospective IHCP whose solution does not contain the time τ explicity is narrow. In the realization of the suggested approach in formulations where numerical methods of construction of individual permissible solutions of IHCP cannot be avoided, an important factor in the increase of the quality ν_1, ν_2 of the solution $\langle\Omega_1, \Omega_2, \Omega_3\rangle$ becomes the use of the principle of step regularization [6] for a given computation step $\Delta\tau$.

The solution of a concrete example shows clearly the particular features which are characteristic for the developed method as a whole. We note, in particular, the following fact. In the usual approach, the unique solution of the inverse problem is affected strongly by a random factor (the nature of the concrete realization of noise in the measurements): the accuracy of the solution constructed from very broad information can, in principle, be lower than the accuracy of a solution obtained from fewer data. It is the characteristic feature of methods adapted for the extraction of a guaranteed minimum of reliable information that the information content of the results of interpretation of the input data depends monotonically on their quality. This fact makes it possible to solve, in the regime of imitation modelling, such problems as the estimate of threshold conditions (critical accuracy of measurements whose analysis makes it possible, in addition, to extract information of the necessary quality), planning of a thermophysical experiment (for example, to choose if it is preferable to improve the accuracy of the measuring apparatus or to increase the volume of measurements).

We consider in more detail the necessity of a preliminary study of the conditions of uniqueness and stability of solutions of the inverse problem. We consider a simple situation when the true solution $T_0(\xi)$ is a function of the type (2) and the parameter $\underline{a}$ is known but lies within the limits $(\underline{a}_{min}, \underline{a}_{max})$. From a formal viewpoint, the theoretical inverse problem is posed incorrectly. In practice, if the interval $(\underline{a}_{min}, \underline{a}_{max})$ is sufficiently narrow, the error of solution of the inverse problem using approximate data is affected most significantly not by the ambiguity factor (it follows from (4) that the approximate solutions do not converge with respect to $\underline{a}$), but by the noise level in the measurements of $\tilde{T}(x_i)$. Let us now suppose that $\underline{a}$ is known. The stability (as one of the conditions of correct formulation) is then ensured, but it does not always give a guarantee to obtain an approximate solution with a given quality. The classical concepts (existence, uniqueness, and stability of solution) arose from the requirement for the cognizability of realistic objects from their indirct manifestations. In applied problems where idealization of the input data is impermissible, it is necessary to express quantitatively (in terms of normalized indices) the effect of particular instability parameters on the quality of the final result of mathematical processing of experimental data, in addition to the analysis of fundamental properties of uniqueness and stability of the solutions of IHCP.

Lastly, about the synthesis of algorithms based on the concepts of analysis of the set of permissible solutions and regularization. We turn to the structure of restrictions (7) on the allowed parameters. All the evidence about the noise is expressed here in terms of one value ε since the information can easily be formalized in the form of a convenient system of linear inequalities. In reality, the evidence about the noise is often less complete and the advantage of the regularization method is that they can be allowed for without particular mathematical difficulties. This is reflected in the high filtering properties of the method when the residual deviation ε_0 between unknown true function $T(x)$ and the optimum approximation $T^{(opt)}(x)$ is considerably smaller than the intensity ε of the noise (as a rule, by factor 5-10 or more). This makes it possible to take the smoothed-out curve $T^{(opt)}(x)$ as the basis rather than $\tilde{T}(x)$ (as a reference), and to replace the restrictions (7) by the more stringent $|T^{opt}(x_i) - A_0F_0(x_i, \tau) - \ldots - A_nF_n(x_i, \tau)| \leq \varepsilon_0$. The set of allowed solutions is then narrowed down and the quality of the solution ν is increased.

In conclusion, we discuss briefly the position which the developed approach may take among other methods of solution of incorrectly posed IHCP which are successfully used at present. The aim of these methods is to increase the information content of the investigations and to search for new methods of processing and analysis of the measured data which make it possible to make the required results more reliable [6]. New opportunities of the developed approach arise because the results of interpretation of the input data are represented in a different form than it is done conventionally. In addition to the optimum approximation $T_0^*(\xi)$ for the unknown function $T_0(\xi)$ and the estimate of proximity of $T_0^*(\xi)$ to in terms of one of the classical metrics which can be obtained by the traditional methods of solution of IHCP, one can now give guaranteed evidence (under indeterminacy conditions) about the object under study, and estimate the quality of the input data (independently of the method which is used in their subsequent analysis). This indicates that the results of solution of IHCP in terms of reliable information about the object under investigation can be used as distinct estimates of the information content of the approximate solutions obtained using the known methods of interpretation of data of a thermal experiment. In the retrospective formulation of IHCP, the developed method makes it possible to observe fragments of any of the allowed solutions which are of interest to the investigator and which describe adequately the unknown true temperature distribution $T_0(\xi)$.

NOTATION

$\underline{a}$ and D, thermal diffusivity and the diffusion coefficient; σ, scattering parameter; $T_0(\xi)$ $(C_0(\xi))$, $T(x)$ $(C(x))$, initial and instantaneous temperature (concentration) profiles; τ, time; x and ξ, coordinates; A_j, coefficients of the temperature distribution function; ε, norm of the error of measurements; $\tilde{T}$, reference value of the function $T_0(\xi)$; Ω, Ω_1, Ω_2, Ω_3, regions which are used to determine the solution of the inverse problem.

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