INVERSE PROBLEMS ASSOCIATED WITH THE CONTROL OF DIFFUSIONAL AND THERMAL PROCESSES

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UDC 539.219.3

Questions of the correctness of the formulation are considered for problems of controlling heat and mass transfer. The possibility of decisive choice of a control from a given class is elucidated. The efficiency of the regularizing operator for solving the problem is confirmed by mathematical experiments on a computer.

The effectiveness of the mathematical-modeling method for solving problems of the control of technological processes within the framework of a general variational formulation is well known [1-3]. In this formulation, the desired quantity is some controlling functional parameter (cause) ensuring a control result which is specified in advance (effect), and hence problems of this type belong to the class of inverse problems. This entails special attention to questions of the correctness of their formulation, and often this problem is solved at the algorithmic level using particular regularizing algorithms [4-6].

In the present work, on the basis of these concepts, some problems associated with nonlinear processes of high-temperature chemicothermal treatment of the samples in gas furnaces are discussed. Considering the problems of cementation and heating for subsequent treatment, in each case only one of these problems is mentioned, because of their mathematical similarity.

1. The cementation of steel samples, usually within the framework of a spatially one-dimensional model, is described by the conditions

$$\frac{\partial}{\partial x}\left(D(u)\frac{\partial u}{\partial x}\right)=\frac{\partial u}{\partial t},\quad (x,\ t)\in Q_{\hat{t}}\equiv\{(x,\ t):0<x<l,\ 0<t\leqslant\hat{t}\},$$
$$D(u)\frac{\partial u}{\partial x}\Big|_{x=0}=\beta(u)(u-w(t))|_{x=0},\quad D(u)\frac{\partial u}{\partial x}\Big|_{x=l}=0,\quad u|_{t=0}=u_0=\text{const},\tag{1}$$

where $u = u(x, t)$ is the carbon concentration in the sample material; u_0 is the initial concentration, corresponding to the grade of steel; $D(u)$ is the diffusion coefficient; $\beta(u)$ is the thermokinetic coefficient, characterizing the mass transfer at the sample boundary; $w(t)$ is the carbon potential of the furnace, regarded as a function of the time.

The problem of interest here is to choose $w(t)$, for known $D(u)$, $\beta(u)$, and u_0, such that the required cementation profile $\phi(x)$ is obtained at time $\hat{t}$:

$$u(x,\ \hat{t})=\hat{\varphi}(x).\tag{2}$$

Noting that the control class $w(t)\in W$, where W is some metric space, it is chosen in accordance with a priori information on the influence of particular controlling functions on the result. Here the behavior of $u(x, \hat{t})$ is determined by the problem in Eq. (1): $u(x, \hat{t})\in AW$, where A is a nonlinear operator implicitly specified by the conditions in Eq. (1). Since the resulting profile is also specified by those conditions, the two following possibilities exist:

a) $\hat{\phi}$ is the profile actually achievable with the given $W: \hat{\phi}\in AW$; then the problem is equivalent to the operator equation

$$Aw=\varphi,\ w\in W,\ \varphi=\hat{\varphi}\in\Phi,\tag{3}$$

Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 53, No. 5, pp. 835-842, November, 1987. Original article submitted March 24, 1987.

0022-0841/87/5305-1329 $12.50

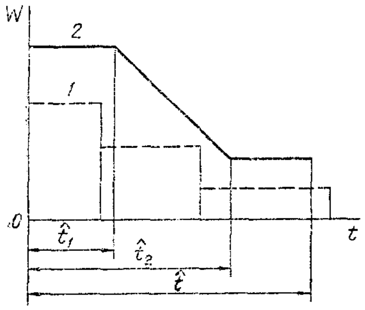

Fig. 1

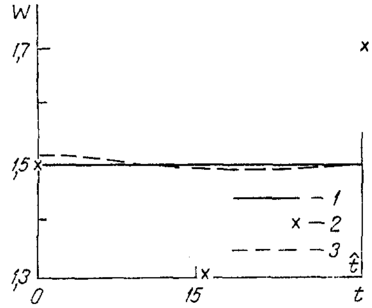

Fig. 2

Fig. 1. Types of control: a) step; b) continuous.

Fig. 2. Model of constant (over time) control: 1) specified; 2) initial approximation; 3) solution of the problem when $\alpha = 10^{-6}$; $T = 930°C$, $u_0 = 0.15\%$ C; $\hat{t} = 30$ h.

where Φ is a metric space coinciding in this case with AW;

b) $\hat{\phi}$ is only the desirable cementation profile, but is unachievable with W: $\hat{\phi}\bar{\in}AW$; then Eq. (3) has no solution, and hence the formulation is incorrect.

In the latter case, only some approximation to the desirable result may be expected, and it is natural to call the solution of the following variational problem the optimal approximation

$$\tilde{w} = \arg\inf_W \rho_\Phi(Aw,\ \hat{\varphi}), \tag{4}$$

which is known to exist in view of the continuity of A.* The quantity $\tilde{\delta} = \rho\Phi(A\tilde{w},\ \phi)$ here gives the smallest possible (on W) deviation of the optimal profile from the desirable profile. This means that, with δ specified in advance ($\delta < \tilde{\delta}$), the problem of choosing $\tilde{w}$ from the condition $\rho_\Phi(Aw,\ \phi) \leq \delta$ is also found to be incorrectly formulated, since its solution with W is nonexistent, and in this case it appears that the formulation is not valid [1].

Note that, within the framework of any stable algorithm, the solution in Eq. (4) may be interpreted as the solution of Eq. (3) when $\phi = \tilde{\phi}$, where $\tilde{\phi} = \arg\inf_{AW} \rho_\Phi(\phi,\ \hat{\phi}) \equiv \Pi p_{AW}\hat{\phi}$ [7]. Therefore, the problem of the uniqueness of the solution of Eq. (3) with the specified $\phi\in AW$ is of equal interest in both cases. Its positive solution is not only of theoretical importance with respect to the correctness of formulation of the problem in Eq. (3) [1], but also raises the question of the choice of $\tilde{w}$ from W, one of which may be "more convenient" than another, for example, for technical reasons.

2. Analysis of the uniqueness is now undertaken for a formulation of the problem somewhat different from Eq. (3). Specifically, the initial data of the control problem are taken to be the concentration field $\{u\}_\varepsilon$ in a time band that is as narrow as desired $\bar{Q}_\varepsilon \equiv \{(x,\ t):\ 0 \leq x \leq \ell,\ \hat{t} - \varepsilon \leq t \leq \hat{t}\}$.

The requirement of analyticity of the functions $\beta(u)$, $D(u)$ when $u\in[u_0,\ u_m]$ where $u_m = \max_{Q_{\hat{t}}} u(x,\ t)$, and also of $w(t)$ when $t\in[0,\ \hat{t}]$, is called condition (α). Note that, for $D(u)$ and $\beta(u)$, this condition does not limit the class of real models too much.

<u>LEMMA</u>. With the condition (α), the specified $\{u\}$, with a fixed $\varepsilon > 0$ that is as small as desired, corresponds to the unique function $\mu(t) = u(0,\ t)$, the boundary conditions of concentration variation over time when $t\in[0,\ \hat{t}]$.

In fact, with condition (α), the unique solution of Eq. (1) is an analytic function [8], and hence $u(0,\ t)$ is analytic when $t\in[0,\ \hat{t}]$. At the same time, for $\forall\varepsilon > 0$, the specified $\mu(t) \equiv u(0,\ t)$ when $t\in[\hat{t} - \varepsilon,\ \hat{t}]$ is also analytic. It has the unique analytic continuation $\mu(t)$ (for example, over the complex plane $z = t + i\sigma$ [9]) on the segment $[0,\ \hat{t}]$, which proves the above assertion.

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* The formulation in Eq. (4) is also necessary for problems of interpretation (discrimination) [1], when the right-hand side of the corresponding Eq. (3) is burdened with errors, so that $\phi\bar{\in}RW$.

The conditions on the coefficients of Eq. (1) are refined by requirement (β): $D(u)$, $\beta(u) > 0$ when $u \in [u_0, u_m]$.

The condition that $u(0, t) = \mu(t)$ with known $\mu(t)$ is considered as an addition to Eq. (1). It may be expected that this set of conditions uniquely determines a pair of functions: $(u(x, t), w(t))$; this is equivalent to unique solution of the problem: $\mu(t) \to w(t)$. In fact, the following theorem holds.

THEOREM. With conditions (α) and (β), the specified $\mu(t)$ corresponds to a unique controlling function $w(t)$, $t \in [0, \hat{t}]$.

This theorem is proved by the method of integral identities proposed for an analogous purpose in [10].

For any $\phi(x, t) \in C^{2,1}(\overline{Q}_\tau)$, $\overline{Q}_\tau \equiv \{(x, t): 0 \leq x \leq \ell, 0 \leq t \leq \tau\}$, at any $\tau: 0 < \tau \leq \hat{t}$, the following identity holds

$$L(u, w) \equiv \iint_{\overline{Q}_\tau} [(Du_x)_x - u_t]\varphi d\sigma = \iint_{\overline{Q}_\tau} (b_{xx} - u_t)\varphi d\sigma = 0, \tag{5}$$

where $b = b(u) = \int_{u_0}^{u} D(s)ds$, so that $b_x = D(u)u_x$.

Suppose that there are two pairs of functions $(u_s(x, t), w_s(t))$, $s = 1, 2$ satisfying the conditions in Eq. (1) and the additional boundary condition. Then, integration by parts, taking account of the conditions in Eq. (1), leads, after simple identity transformations, to the result

$$0 = L(u_1, w_1) - L(u_2, w_2) = -\int_0^\tau \{(b_{1x} - b_{2x})\varphi|_{x=0} + (b_1 - b_2)\varphi_x|_{x=l}\} dt -$$

$$- \int_0^l (u_1 - u_2)\varphi|_{t=\tau} dx + \iint_{\overline{Q}_\tau} (u_1 - u_2)(\varphi_t + p\varphi_{xx}) d\sigma,$$

where $p = (b_1 - b_2)/(u_1 - u_2)$ when $u_1 \neq u_2$ and $p \equiv D(u_2)/u_2$ when $u_1 = u_2$, $p > 0$. Next ϕ is chosen from the conditions $\phi_t + p\phi_{xx} = 0$, $(x, t) \in Q_\tau$; $\phi_x(\ell, t) = 0$; $\phi(0, t) = \chi(t) \geq 0 (\chi(t) \not\equiv 0)$, $\phi(x, \tau) = 0$.

As shown in [8, 10], the solution of this problem exists for any continuous χ. Then, the preceding identity may be written in the form

$$0 = \int_0^\tau \{D(u_1)u'_{1x} - D(u_2)u'_{2x}\}|_{x=0}\chi(t) dt = \int_0^\tau \{\beta(\mu)(\mu - w_1) - \beta(\mu)(\mu - w_2)\} \chi dt \equiv \int_0^\tau \varkappa(t)\chi(t) dt.$$

Hence, since τ and $\chi(t)$ are arbitrary, it follows that $\kappa(t) = 0$ almost everywhere in $[0, \hat{t}]$, and then, with condition (α), $\kappa(t) \equiv 0$ and hence $\beta(\mu(t))(w_2(t) - w_1(t)) \equiv 0$. Since $\beta(u)$ is positive, it follows that: $w_2(t) = w_1(t)$, which proves the theorem.

COROLLARY. With conditions (α) and (β), for any fixed $\varepsilon > 0$ that is as small as desired, the given $\{u\}_\varepsilon$ corresponds to a unique function $w(t)$.

Note that, in order to prove the preceding theorem, it is sufficient to require, instead of (α), that

$$D(u) \in C^1[u_0, u_m], \ \beta(u) \in C^0[u_0, u_m], \ \mu(t) \in C^0[0, \hat{t}].$$

At the same time, it is obvious that, with analogous conditions regarding the thermal conductivity $k(u)$ and volume specific heat $c(u)$, the results transfer to the corresponding problem of controlling heating.

Of course, the above analysis does not give an exhaustive solution of the uniqueness problem, but the result established gives an idea of the possibility of obtaining a unique solution of the problem which is of interest here, where the initial information is the depth of the cementation profile. This permits practical confidence that, in the case of unique $\Pi p_{AW}\ \hat{\phi}$ (the general conditions for which were studied in [7] for interpretation problems), any stable algorithm for solving Eq. (4) leads to the same result.

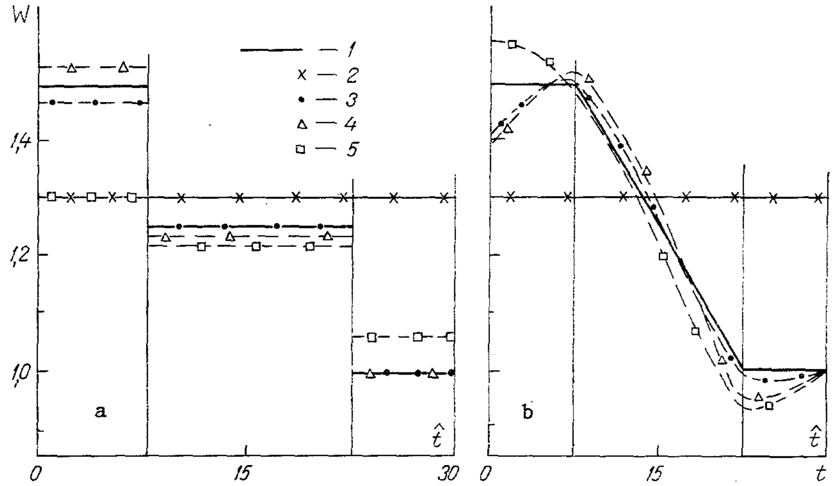

Fig. 3. Model of step (a) and continuous (b) controls: 1) specified; 2) initial approximation; solution of the problem with inaccurate data: 3) $\delta = 10^{-3}$, $\alpha = 10^{-4}$; 4) $\delta = 10^{-2}$, $\alpha = 10^{-4}$; 5) $\delta = 10^{-1}$, $\alpha = 10^{-2}$ (a), 10^{-3} (b). T = 930°C, u_0 = 0.15% C, $\hat{t}$ = 30 h.

3. The stability of the problem in Eq. (4) is understood in the sense of convergence of any minimizing sequence $\{w_n\}$ [1] in the metric of some enveloping space $\tilde{W} \supseteq W$. This problem may be unstable since small variation in Aw in the set Φ may correspond to variation w(t) that is as large as is desired, generally speaking. Nevertheless, a regularized minimizing sequence $\{\tilde{w}_n\}$ may be constructed, on the basis of the assumptions that: a) the set W introduced a priori is a compact in $\tilde{W}$; and b) it is algorithmically ensured that $\{\tilde{w}_n\}$ belongs to this compact. The latter requirement is conveniently realized using a "stabilizer" [1] Ω(w), the construction of which depends on the choice of the compact W.

In [11, 12], a step control and a continuous control with one element were considered (Fig. 1) as an alternative to specifying a constant level of the carbon potential. This is equivalent to parameterizing the function w(t) and replacing it by a set of a small number of parameters $p = \{p_1, \ldots, p_n\}$. In this case $\tilde{W} \equiv R_n$, and the compactness of W is achieved by specifying a stabilizer of the form

$$\Omega(w) \equiv \|\overset{\circ}{w} - w\|^2_{R_n} = \sum_{i=1}^{n} q_i (\overset{\circ}{w}_i - w_i)^2, \tag{6}$$

where $\overset{\circ}{w}$ is a specified vector; q_i are specified constants ($q_i > 0$).

Continuous control $w = w(t)$ of sufficiently arbitrary profile gives broader possibilities. In this case, $\tilde{W} \equiv C[0, \hat{t}]$, and the compactness of W is achieved by introducing a stabilizer

$$\Omega(w) \equiv \|w\|^2_{C[0,\hat{t}]} = \int_0^{\hat{t}} [q_1 w'(t)^2 + q_2 w(t)^2]\, dt, \tag{7}$$

where q_1 and q_2 are specified constants.

In both cases, the minimizing sequence may be constructed from extremals of the "smoothing" functional

$$F(z) = \rho^2_\Phi(Aw, \hat{\varphi}) + \alpha\Omega(w), \tag{8}$$

considered in a sequence $\{\alpha_n\}$ which converges to zero.

In the case where an estimate δ of the tolerance for deviation of the approximation of the metric Φ is known in advance — $\rho_\Phi(A\tilde{w}, \hat{\phi}) \leq \delta$ — and where the problem of choosing w from a set defined by this mixed inequality is correct, this inequality may be used to interrupt the sequence of extremals $w_n \equiv w^{\alpha_n}$ according to the condition

$$\min_n |\rho^2_\Phi(Aw^{\alpha_n}, \hat{\varphi}) - \delta^2|. \tag{9}$$

This condition, corresponding to the discrepancy principle in interpretation problems [1], allows the approximation to the extremal to be chosen in the given case.

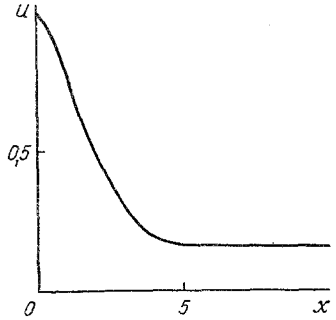

Fig. 4

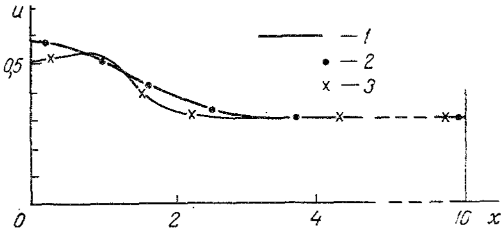

Fig. 5

Fig. 4. Concentration profile with model step control, corresponding to curve 4 in Fig. 3a; T = 930°C, u_0 = 0.5% C, $\hat{t}$ = 30 h. x, mm.

Fig. 5. Concentration profiles: 1) specified a priori; 2) corresponding to continuous control; 3) "exponential"; T = 930°C, u_0 = 0.30% C, $\hat{t}_1$ = 5 h, $\hat{t}_2$ = 7.5 h, $\hat{f}$ = 10 h.

The realization of the given algorithm in computer programs includes the following elements: a) minimization of the functional in Eq. (8) for each α_n by the method of "formal search," analogous to the method of coordinate descent [13]; b) repeated solution of the boundary problem in Eq. (1) within the framework of the given minimization algorithm, using an iteration–difference procedure similar to that in [14], with an accuracy $O(\Delta x^2 + \Delta t)$ [15].

4. Mathematical experiments have been conducted for the cementation problem with the following physical parameters

$$D(u) = (0{,}04 + 0{,}08u)\exp(-31350/1{,}987T_h)\ (\text{cm}^2/\text{sec}),$$

$$\beta(u) = 1{,}36\cdot 10^{-3}\exp(-11100/1{,}987\cdot T_h)\ (\text{cm/sec})\ [12],$$

$$T_h = T + 273{,}15,\quad l = 10\ \text{mm},\ \Delta x = \frac{1}{25}l,\ \Delta t = \frac{1}{40}\hat{t}.$$

A. The question of the effectiveness of controlling the cementation by choosing a constant (over time) level w of the atmospheric carbon potential is resolved by the following experiment.

The range w∈[0.9; 1.21% C] is considered, and the controlling parameters also include the temperature $\hat{T}$∈[910; 930°C] and the cementation time $\hat{t}$∈[30; 100 h]. The numerical characteristics $\hat{\phi}(x)$ are chosen as follows: $\hat{\phi}(x) = \{\hat{u}_{sur}, \hat{h}_{bo}, \hat{h}_{tot}\}$, where $\hat{u}_{sur} = u(0, \hat{t})$, $\hat{h}_{bo}$ and $\hat{h}_{tot}$ correspond to the depth of the layer (from the surface) with concentration u_{bo} = 0.8% C and $u_{bo} = u_0$ + 0.05% C (at t = $\hat{t}$), respectively.

Finally, an analog of the functional of the problem in Eq. (4) is introduced

$$\tilde{\rho}_{R_3} = \sum_{i=1}^{3}(f_i(\mathbf{p})/\hat{\varphi}_i)^2,\ f_1(\mathbf{p}) = u_{sur}(\mathbf{p}) - \hat{u}_{sur},\ f_2(\mathbf{p}) = h(u_{bo}, \mathbf{p}) - \hat{h}_{bo},$$

$$f_3(\mathbf{p}) = h(u_{tot}, \mathbf{p}) - \hat{h}_{tot}$$

Since in this case the problem reduces to minimizing a function of three variables, the problem is stable. Direct approximate estimation of its solution by the "formal-search" method leads to the following values of the characteristics of the cementation profile and the corresponding controls

$$w \simeq 1{,}21\%\ \text{C},\ T \simeq 910\ ^\circ\text{C},\ \hat{t} \simeq 30\ \text{h};$$

$$u_{sur} \simeq 1{,}02\%\ \text{C},\ h_{bo} \simeq 0{,}14\ \text{mm},\ h_{tot} \simeq 2{,}05\ \text{mm}.$$

Experiment shows that, within the framework of the given algorithm, optimal values may be obtained within limits specified in advance. Note that, if a less sharp drop in concen-

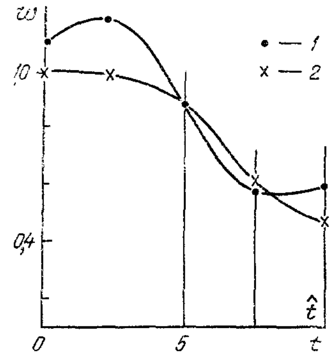

Fig. 6 Control corresponding to concentration profile in curve 2 (1) and 3 (2) in Fig. 5.

tration with depth ($h_{bo} \gg 0.1$ mm) is of interest, the character of the control w(t) must be changed.

B. The next experiment concerns verification of the effectiveness of the algorithm here developed on well-known models. In this case, from the specified controlling function w(t), the "final" cementation profile $\hat{\phi}(x) = u(x, \hat{t})$ is determined by solving Eq. (1), and then the inverse problem is solved using Eqs. (8) and (9).

Since $\hat{\phi}(x) \in AW$ in this experiment, δ is determined solely by the errors of the computational scheme (relative error $\sim 10^{-3}$), so that the algorithm operates essentially as for the problem of interpreting initial data that are close to the accurate data. To simulate specification of $\hat{\phi}(x)$ outside the limits AW, perturbations at different levels are introduced, according to the formula

$$\tilde{\varphi}(x_i) \equiv \tilde{\varphi}_i = \hat{\varphi}_i + \delta\xi_i \Big/ \sum_{i=1}^{N} \xi_i^2,$$

where $\xi_i \in [-1, 1]$, $\delta = 10^{-3}, 10^{-2}, 10^{-1}$.

The following control models are considered: w constant over time; w(t) piecewise constant; and w(t) continuous and piecewise smooth. The parameters of these functions are shown in Figs. 2-6.

The results of solving the inverse problem are shown in Figs. 2 and 3 in comparison with those specified by the models, and the concentration profile corresponding to Fig. 3a is shown in Fig. 4.

On the basis of these results, the error in specifying the carbon potential required in order for the tolerance in the concentration distribution with depth to fall within specified limits may be determined. For example, the error 1-2% in Fig. 3a corresponds to a tolerance of 10^{-2} ($\delta < 10^{-2}$).

C. Finally, consider the result of searching for a control ensuring the profile specified in advance in Fig. 5 (curve 1). Searching for the solution w(t) in a set of continuous functions, even for a small number of points (n = 5), leads to the result in Fig. 6 (curve 1), corresponding to curve 2 in Fig. 5.

Also in Figs. 5 and 6, the experimentally achievable concentration profile (curve 3) and control (curve 2) found using the algorithm in Eqs. (8) and (9) are shown.

Thus, the analysis allows the type of control ensuring the required cementation structure of the samples to be effectively predicted.

5. Without significant change, the given algorithm may be extended to the problem of controlling the temperature field in dynamic conditions. However, the final result of the thermal process – the creation of a near-uniform temperature field – is more interesting. The corresponding problem is solved using the given algorithm.

In this case, the whole formulation is changed. With specified tolerance on the nonuniformity δ, it is required to choose the controlling potential w(t) so that the given result is obtained in minimal time. The mathematical formulation of the problem in variational form is

$$\hat{t} = \inf t(w), \tag{10}$$

where t(w) is implicitly specified by the condition $\rho_{\Phi}^{(t)}(Aw, \hat{\phi}) = \delta$ at specified δ and constant temperature level $\hat{\phi}$, under the condition that $w \in W$, a compact specified in advance.

For the limiting case $\beta(u) = \infty$, a similar problem which will not be discussed in detail here was solved in [6].

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APPLICATION OF ITERATIVE REGULARIZATION FOR THE SOLUTION OF INCORRECT INVERSE PROBLEMS

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UDC 536.24

The solution of inverse heat-conduction problems using regularizing gradient algorithms is considered.

Many structures in various engineering fields operate in conditions of intensive and often extremal thermal treatment. The general trend is associated with increase in the number of thermally loaded engineering objects and with increasingly rigorous conditions of thermal loading, with simultaneous increase in reliability and working life and decrease in volume of the material. Questions regarding the maintenance of thermal conditions also occupy an important position in the design and development of technological processes associated with the heating and cooling of materials, for example, in the continuous casting of steel, various methods of heat treatment of metals, glass production, foundry processes, growing high-temperature single crystals from melt, etc.

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Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 53, No. 5, pp. 843-851, November, 1987. Original article submitted March 17, 1987.

0022-0841/87/5305-1335 $12.50