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

METHOD OF DESCRIPTIVE REGULARIZATION IN INVERSE PROBLEMS

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UDC 519.63

We propose algorithms for descriptive regularization that account for a priori concepts of the qualitative structure of the sought functions. The use of these concepts that possess stabilizing properties ensures rather high accuracy and quality of approximate solutions with an insignificant expenditure of computational resources.

The ideas of descriptive regularization developed in [1, 2] are very promising in creating effective algorithms for numerical solution of incorrect inverse problems of heat conduction. A specific feature of the descriptive regularization method is account for a priori concepts of the qualitative structure of the sought functions (knowledge of the regions of fixed sign, monotonicity, convexity, etc.). The use of these concepts that possess stabilizing properties [3, 4] ensures uniform convergence of approximate solutions.

1°. We consider the basic points of constructing algorithms for descriptive regularization using, as an example, a boundary-value inverse problem for the quasilinear Stefan problem that consists in determining the temperature distribution $u(x, t)$ in the region $Q = Q_1 \cup Q_2$, the front of phase transition $\xi(t)$ for $0 \le t \le T$, and the boundary conditions $v(t)$ for $0 \le t \le T$ from the conditions [5]

$$c(x, t, u)\, u_t - (a(x, t, u)\, u_x)_x + b(x, t, u)\, u_x = f(x, t, u),$$

$$(x, t) \in Q_1 = \{0 < x < \xi(t),\ 0 < t \le T\},$$

$$(x, t) \in Q_2 = \{\xi(t) < x < l,\ 0 < t \le T\}, \tag{1}$$

$$u|_{x=0} = v(t), \quad 0 < t \le T, \tag{2}$$

$$a(x, t, u)\, u_x|_{x=l} = p(t), \quad 0 < t \le T, \tag{3}$$

$$u|_{x=\xi(t)} = u^*(t), \quad 0 < t \le T, \tag{4}$$

$$\gamma(x, t, u)|_{x=\xi(t)}\, \xi_t = [a(x, t, u)\, u_x]_{x=\xi(t)} + \chi(x, t, u)|_{x=\xi(t)}, \quad 0 < t \le T, \tag{5}$$

$$u|_{t=0} = \varphi(x), \quad 0 \le x \le l, \quad \xi|_{t=0} = \eta_0 \tag{6}$$

and the additional condition at $x = l$

$$u|_{x=l} = g(t), \quad 0 \le t \le T. \tag{7}$$

Scientific-Research Computational Center of the M. V. Lomonosov Moscow State University. St. Petersburg State University. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 65, No. 6, pp. 695-702, December, 1993.

 1062-0125/93/6506-1200$12.50

We assume that the additional information contains data on monotonicity and convexity regions of the sought boundary function and has the form

$$v \in V_\mu, \quad V_\mu = \left\{ v \in V_R, \quad \mu(t)\, v_t(t) \geq 0, \quad 0 \leq t \leq T \right\}, \tag{8}$$

$$v \in V_\nu, \quad V_\nu = \left\{ v \in V_R, \quad \nu(t)\, v_{tt}(t) \geq 0, \quad 0 \leq t \leq T \right\}, \tag{9}$$

where $\mu(t)$ and $\nu(t)$ are parametric functions; $\mu(t) = \operatorname{sign} v_t(t)$; $\nu(t) = \operatorname{sign} v_{tt}(t)$; and V_R is a set of boundary functions $v(t)$:

$$\| v \|_{L_2[0,T]} \leq R, \quad R = \text{const} > 0.$$

The method of descriptive regularization of the inverse problem (1)-(7) based on account for the a priori constraints (8) and (9) reduces to the variational problem

$$\inf_{v \in V} J(v), \quad J(v) = \| u|_{x=l} - g \|^2_{L_2[0,T]},$$

in which V is a set of admissible boundary functions. Depending on the availability of one or another kind of a priori information, $V = V_\mu$, $V = V_\nu$, $V = V_\mu \cap V_\nu$, and $u|_{x=l}$ is the spur of the solution of the direct Stefan problem (1)-(6) corresponding to $v \in V$ at $x = l$.

Numerical implementation of the descriptive regularization method entails the problem of nonlinear programming

$$\min_{\hat{v} \in \hat{V}} I(\hat{v}), \quad I(\hat{v}) = \sum_{j=0}^{N} \rho_j (u_{Mj} - g_j)^2, \tag{10}$$

where $\hat{v} = (v_0, \ldots, v_N)$ is a net boundary function on the net $\omega_\tau = \{t_j,\ 0 = t_0 < \ldots < t_N = T,\ t_j - t_{j-1} = \tau_j\}$; ρ_j are coefficients of the quadrature formula; $g_j = g(t_j)$, u_{ij} $(i = \overline{0, M},\ j = \overline{0, N})$ is a solution of the difference analog of the direct Stefan problem (1)-(6) on the nets $\omega_h \times \omega_\tau$ in the region Q, $\omega_h = \{x_i,\ 0 = x_0 < \ldots < x_M = l,\ x_i - x_{i-1} = h_i\}$; and $\hat{V}$ is a set of admissible functions $\hat{v}$ that comply with the constraints:

$$\sum_{j=0}^{N} \rho_j v_j^2 \leq R^2, \tag{11}$$

$$\mu_j (v_{j+1} - v_j) \geq 0, \quad j = \overline{0,\ N-1}, \quad \mu_j = \mu(t_j), \tag{12}$$

$$v_j \left(\frac{v_{j+1} - v_j}{\tau_{j+1}} - \frac{v_j - v_{j-1}}{\tau_j} \right) \geq 0, \quad j = \overline{1,\ N-1}, \quad v_j = \nu(t_j). \tag{13}$$

2°. The descriptive regularization algorithm devised in [5] relies on the method of projecting conjugate gradients for the numerical minimization (10)-(13), which has a sufficiently high rate of iteration convergence and permits structural features of the sought function to be revealed in a few steps. An iteration process of this method in the finite-dimensional analog $L_{2\tau}(\omega_\tau)$ of the space $L_2[0, T]$ is constructed proceeding from the initial approximation $\hat{v}^s$ $(s = 0)$ by the equations

$$\hat{v}^{s+1} = \mathcal{P}_{\hat{V}} (\hat{v}^s - \alpha_s \hat{r}^s), \quad s = 0, 1, \ldots,$$

$$\hat{r}^0 = \operatorname{grad}_{L_{2\tau}} I(\hat{v}^0), \quad \hat{r}^s = \operatorname{grad}_{L_{2\tau}} I(\hat{v}^s) - \beta_s \hat{r}^{s-1}, \quad s = 1, 2, \ldots,$$

$$\beta_s = \frac{(\operatorname{grad}_{L_{2\tau}} I(\hat{v}^s),\ \operatorname{grad}_{L_{2\tau}} I(\hat{v}^{s-1}) - \operatorname{grad}_{L_{2\tau}} I(\hat{v}^s))_{L_{2\tau}}}{\| \operatorname{grad}_{L_{2\tau}} I(\hat{v}^{s-1}) \|^2_{L_{2\tau}}}, \tag{14}$$

in which $\alpha_s > 0$ is a descent step chosen from the condition of monotonic decrease of the functional $I(\hat{v})$: $I(\hat{v}^{s+1}) \leq I(\hat{v}^s)$, $s = 0, 1, \ldots$, $\operatorname{grad}_{L_{2\tau}} I(\hat{v})$ is the gradient of the functional $I(\hat{v})$ in $L_{2\tau}(\omega_\tau)$, $\mathscr{P}_{\hat{V}}$ is the operator of projection onto the set $\hat{V}$:

$$\| \mathscr{P}_{\hat{V}}(\hat{v}) - \hat{v} \|_{L_{2\tau}} = \min_{\hat{w} \in \hat{V}} \| \hat{w} - \hat{v} \|_{L_{2\tau}}.$$

One of the main problems in realizing process (14) is an effective method of calculating the gradient. To solve this problem, we resort to results [6] regarding differentiability of the functionals determined in the solutions of the quasilinear Stefan problem. From discrete analogs of the relations for the increment $\Delta J(v)$ relative to the increment $\Delta v \in V$:

$$\Delta J(v) = (\operatorname{grad}_{L_2} J(v),\ \Delta v)_{L_2[0,T]} + o(\| \Delta v \|_{L_2[0,T]}),$$

$$\Delta J(v) = (\operatorname{grad}_{W_2^2} J(v),\ \Delta v)_{W_2^2[0,T]} + o(\| \Delta v \|_{W_2^2[0,T]})$$

and the representation established in [6]:

$$\Delta J(v) = \int_0^T a(x, t, u)\, \psi_x|_{x=0}\, \Delta v(t)\, dt + o(\| \Delta v \|_{W_2^2[0,T]}),$$

we may obtain, by virtue of the equivalence of the norms in finite-dimensional spaces, an equation for calculating the gradient

$$\operatorname{grad}_{L_{2\tau}} I(\hat{v}) = (I'_0, \ldots, I'_N), \quad I'_j = a_{0j} \frac{\psi_{1j} - \psi_{0j}}{h_1}, \quad j = \overline{0, N}, \tag{15}$$

in which ψ_{ij} is a solution of the difference analog of the conjugate problem [6] on the nets $\omega_h \times \omega_\tau$; and a_{0j} is the value of the coefficient $a(x, t, u)$ at $x = 0$, $t = t_j$, and $u = u_{0j} = v_j$. The form of the conjugate problem for the inverse Stefan problem considered is presented in the article "Inverse Stefan problems" by N. L. Gol'dman in this same issue of the journal.

Determination of the gradient of the functional $I(\hat{v})$ on each iteration of the process (14) incorporates three steps:

1) numerical solution of the difference analog of the direct Stefan problem (1)-(6) with the boundary function $\hat{v}^s = (v_0^s, \ldots, v_N^s)$ for determining u_{ij}, ξ_j, $i = \overline{0, M}$, and $j = \overline{0, N}$;

2) subsequent solution of the difference analog of the conjugate problem using the obtained u_{ij} and ξ_j for determining ψ_{ij}, $i = \overline{0, M}$, $j = \overline{0, N}$; and

3) calculation of the components of the vector $\operatorname{grad}_{L_{2\tau}} I(\hat{v})$ from Eq. (15) using the obtained ψ_{ij}.

The suggested method for calculating the gradient provides a noticeable savings in computer time. The volume of computational operations (of the order of $M \times N$) is determined only by the effectiveness of the numerical algorithms for solving the direct Stefan problem and the corresponding conjugate problem. At the same time, the approximate method of calculating I'_j ($j = \overline{0, N}$) via a difference approximation of the partial derivatives $\partial I / \partial v_j$ results in an $(N+1)$-fold numerical solution of the direct Stefan problem, i.e., requires a computational expenditure at least N times as great and, furthermore, has a poor accuracy.

Another problem of numerical minimization, viz., construction of an effective procedure of projection onto the set of constraints (11)-(13), is solved with allowance for the specific properties of these constraints.

If the the structure of $\hat{V}$ is determined by conditions (12), use is made of an explicit form of the projector onto a set of piecewise monotonic functions [7] that provides a mean-square approximation in this class of functions in N^2 operations. For monotonically increasing admissible functions (i.e., $\mu_j \equiv 1$, $j = \overline{0, N-1}$, the algorithm for mean-square approximation proposed in [8] permits the projection onto such a set in $\simeq 2N$ operations and includes three steps:

1) for the projected function $v(t)$, the integral

$$w_0(t) = \int_0^t v(y)\, dy;$$

is calculated;

2) for the function $w_0(t)$, the upper envelope $w^0(t)$ of convex functions located on the section $[0, T]$ below $w_0(t)$ is constructed;

3) the derivative $d/dt = w^0(t)$ is calculated, which is exactly the solution for the projection problem.

Should the set $\hat{V}$ include constraints (13) of the piecewise convexity of admissible functions, an algorithm [9] is employed to realize the projection. This algorithm accounts also for constraints prescribed as

$$\underline{\mu}_j \le (v_{j+1} - v_j)/\tau_{j+1} \le \bar{\mu}_j, \quad j = \overline{0, N-1},$$

where $\underline{\mu}_j$ and $\bar{\mu}_j$ are known quantities. The algorithm for projection onto a set of downward convex functions (i.e., for $v_j \equiv 1$, $j = \overline{1, N-1}$) suggested in [8] is very efficient.

Concluding the presentation of the basic points of constructing the descriptive regularization algorithm, we note its universality in a wide class of inverse Stefan problems. This should be attributed to the quantity of the algorithm: specifying the form of the purpose functional and the equation for calculating its gradient for the inverse problem under consideration, it is possible to effectively use one and the same software for the numerical minimization of the functional, the procedure of projecting onto a set of constraints, and the numerical solution of the direct Stefan problem and the conjugate problem.

3°. We present the results of numerical experiments on using the descriptive regularization algorithm in solving various inverse Stefan problems.

In model calculations for the boundary-value inverse Stefan problem (1)-(7) we sought the boundary conditions at $x = 0$ [5]:

$$v_{ex}(t) = 0.75 + 0.25\,(t+1)^2, \quad 0 \le t \le 1,$$

and the corresponding exact solution of the direct Stefan problem (1)-(6):

$$u_{ex}(x, t) = 0.75 + 0.25\,(t+1)^2 - x, \quad \xi_{ex}(t) = 0.25\,(t+1)^2$$

with the following input data:

$$0 \le x \le 1, \quad 0 \le t \le 1, \quad a = 10 + u, \quad b = -(1+x), \quad c = 1, \quad d = 0,$$

$$f = x + 0.5\,(t+1), \quad p = -9.75 - 0.25\,(t+1)^2, \quad u^* = 0.75,$$

$$\gamma = 0.5, \quad \chi = 0.25\,(t+1), \quad \varphi = 1 - x, \quad \eta_0 = 0.25.$$

The additional information (7) is prescribed at $x = 1$:

$$g(t) = 0.25\,(t+1)^2 - 0.25.$$

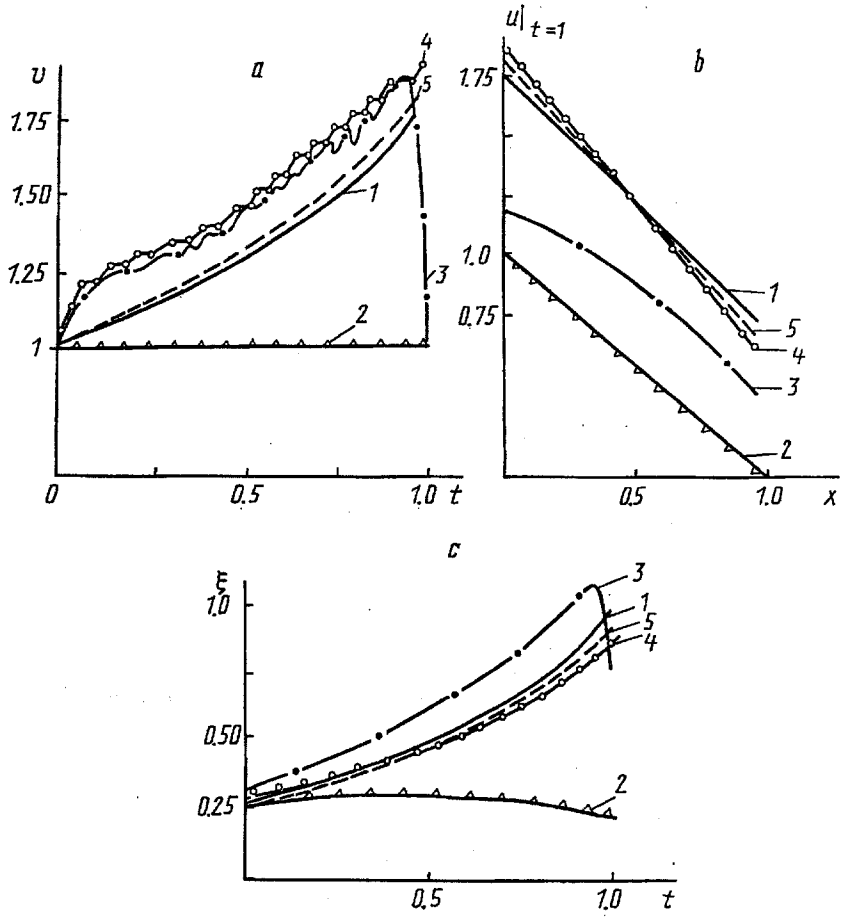

Fig. 1. Model problem: 1) exact solution, 2) initial approximation, 3-5) approximate solutions: 3) without conditions (8) and (9); 4) with condition (8); 5) with conditions (8) and (9).

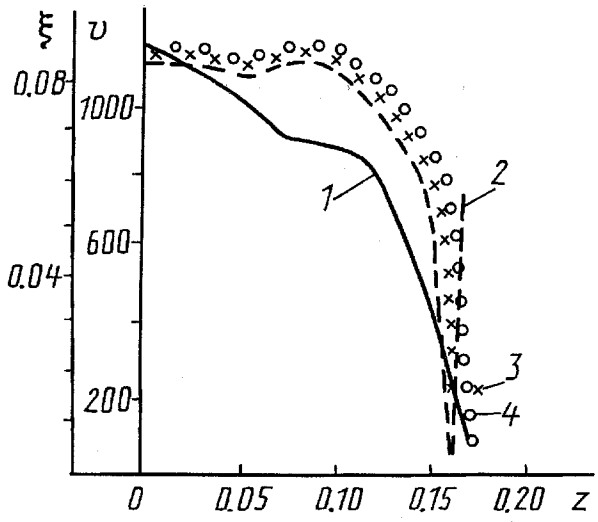

Fig. 2. Problem of a continuous ingot: 1) hole profile, 2-4) temperature at the ingot surface: 2) without conditions (8) and (9); 3) with condition (8); 4) with conditions (8) and (9). ξ, z, m; ν, $^{\circ}$C.

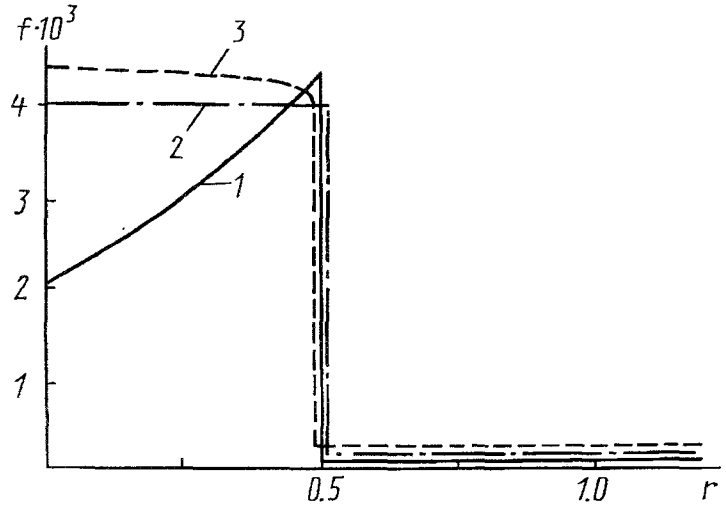

Fig. 3. Problem of plate melting: 1-3) heat pulse of: 1) parabolic; 2) uniform; 3) Gaussian type. f, cal/(cm^2·sec); r, cm.

Under the effect of the boundary conditions $\nu_{ex}(t)$, the phase transition front $\xi_{ex}(t)$ moves to the right, reaching the right boundary of the region $x = 1$ at $t = 1$. A set of admissible boundary conditions is composed of monotonically increasing downward-convex functions, i.e., in a priori information (8) and (9), $\mu(t) \equiv 1$ and $\nu(t) \equiv 1$ for $0 \le t \le 1$. The value of R is taken to be 10.

The difference algorithms of the direct Stefan problem and the conjugate problem were constructed using variational-difference schemes on the uniform net ω_h with a mesh width of $h = 0.04$ (the number of mesh points was $M = 25$) and the nonuniform net ω_τ with mesh widths of $\tau_{max} = 0.1$ and $\tau_{min} = 0.025$ (the number of mesh points was $N = 37$).

Figure 1 gives for comparison the predictions (the boundary conditions and the corresponding solution of the difference Stefan problem) obtained with allowance for constraints (12) and (13) and without them. The predictions are conducted in the presence of errors in all input data of the inverse problem introduced by random disturbances with dispersions of $\sigma = 0.05$ distributed uniformly on [-1, 1]. The descriptive regularization permits obtaining approximations (curves 4 and 5) that are quite satisfactory from the viewpoint of accuracy and quality, though the initial approximation in the process (14) is rather "crude" in comparison with the exact solution (curves 1 and 2, Fig. 1a). A lack of a priori information as to the qualitative behavior of the sought conditions leads to worse results (curve 3). In particular, the difficulties of determining the boundary functions near the final instant of time $t_N = 1$ fail to be overcome. These difficulties stem from the fact that the component I'_N of the vector $\mathrm{grad}_{L_{2\tau}} I(\hat{\nu})$ is equal to zero. Therefore the minimization process (14) depends strongly on the choice of the initial approximation at $t = t_N$: $\nu_N^s = \nu_N^0$ when $s > 0$.

It took five iterations of the method (14) and insignificant expenditures of computer time (from 60 to 110 sec on a BESM-6 computer) to attain the results presented in Fig. 1. Here the values of the minimized functional manage to decrease to the level of the total errors of the input data and the approximation error introduced in conversion from the initial problem to its difference analog. Subsequently, as the number of iterations increases, the process of refining the approximation in the vicinity of the exact solution slows down sharply. This property of the projection method for conjugate gradients is appropriate for use as a halt criterion.

Figure 2 gives the results of applying the descriptive regularization algorithm to calculations of the boundary conditions on a cooled surface of a crystallized continuous cylindrical copper ingot [10]. The corresponding boundary-value inverse Stefan problem on determining the temperature $\nu(z)$ at the ingot surface $r = r_{cr}$ that ensures the desired shape of the hole (of the crystallization front $\xi(z)$) reduces to the variational problem

$$\inf_{\nu \in V} J(\nu), \quad J(\nu) = \| u|_{r=\xi(z)} - u^* \|_{L_2[0,H]},$$

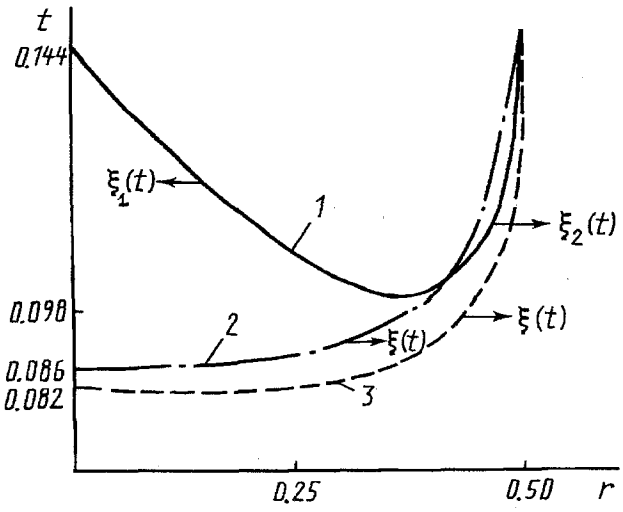

Fig. 4. Advance of melting fronts in a plate, corresponding to a heat pulse of: 1) parabolic; 2) uniform; 3) Gaussian type. ξ, cm; $t \cdot 10^{-1}$, sec.

where $u(r, z)$ is a solution of the boundary-value problem for equations of the type (1) (the role of x and t is fulfilled by the variables r and z) in the region $\xi(z) \leq r \leq r_{cr}$, $0 \leq z \leq H$ with the specificed boundary $r = \xi(z)$; H is the length of the calculated section of the ingot; and u^* is the crystallization temperature. The calculations are carried out with consideration of a priori concepts of a monotonic decrease in the boundary temperature and flux at the crystallizer exit based on experimental data. This a priori information can be utilized in specifying the set of admissible boundary conditions.

The case of a copper ingot is less favorable compared to metals and alloys with a lower thermal conductivity because the ranges of applicability of one-dimensional casting models for copper do not exceed distances equal to 3/4 of the hole depth. A descriptive regularization method based not only on quantitative but also on qualitative information on the temperature and flux behavior at the ingot surface permits obviation of this difficulty. For the hole profile $\xi(z)$ (curve 1, Fig. 2), we obtained approximate solutions that are quite satisfactory in terms of accuracy and quality throughout the hole depth, as opposed to the approximation found without account for such information (compare curves 2-4 in Fig. 2).

We now present the results of applying the descriptive regularization algorithm to numerical study of the effect exerted by the shape of the heat pulse of a laser source of energy on the formation of a molten opening of prearranged size in a thermally thin plate. Studies [11, 12] present statements of the corresponding coefficient inverse Stefan problems in accordance with the character (uniform, Gaussian, or parabolic) of the spatial distribution of the intensity of the thermal effect. The descriptive regularization algorithm allows finding the shape of the heat pulse that possesses the required qualitative characteristics and provides the desired course of the plate melting process. Curves 1-3 in Figs. 3 and 4 reflect the results of numerical calculations for melting of a Duralumin specimen in producing an opening of the same radius $r_0 = 0.5$ cm over a time $t = 0.0144$ sec by the action of heat sources with different intensity distributions across the radius of the irradiation spot. With a parabolic heat pulse (curves 1, Figs. 3 and 4), at the instant of time $t_{melt} = 0.0098$ sec two melting fronts are formed, one of which $\xi_1(t)$ moves toward the center of the irradiation spot and the other $\xi_2(t)$, toward the spot boundary $r_0 = 0.5$ cm. By the instant of time $t = 0.0144$ sec, the whole of the required opening is molten. Under the effect of uniform and Gaussian heat fluxes (curves 2 and 3, Figs. 3 and 4), at the center of the irradiation spot a single melting front is formed at the instants of time $t_{melt} = 0.0086$ sec and, correspondingly, $t_{melt} = 0.0082$ sec that moves toward the spot boundary $r_0 = 0.5$ cm and reaches it at the instant of time $t = 0.0144$ sec. The calculations took 90 sec of computer time on a BESM-6 computer.

Analysis of the numerical results permits the conclusion that the suggested descriptive regularization algorithm appreciably improves the quality of approximate solutions of inverse problems with an insignificant increase in the volume of computational operations.

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