NUMERICAL METHOD OF DETERMINING THE BOUNDARY CONDITIONS AT THE SURFACES OF A CONTINUOUS CASTING FROM THE PROFILE OF THE SOLIDIFICATION FRONT

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A stable numerical method of solving the inverse Stefan type of heat-conduction problem is proposed. An applied thermophysical problem is then examined — that of calculating the boundary conditions on the cooled surface of a solidifying continuous circular casting under practically steady-state thermal conditions. The calculated results are compared with experimental data.

The quality of a continuous casting is largely determined by the profile of the cavity and its position in the mold. The cavity profile in turn depends on the boundary conditions at the surface of the casting, i.e., on the conditions of heat transfer in the mold and the zone of secondary cooling. The solution of the problem inverse to the problem of solidification (in which the cavity profile, optimized on the basis of some specific criterion, by reference to theoretical or practical data, is given in advance) enables us to find the corresponding boundary conditions, i.e., the optimum conditions for cooling the casting. In principle we may thus determine the constructional parameters of the mold giving the best results (from the point of view of any specific requirements imposed upon the castings) in advance. The solution of the inverse problem, furthermore, enables us to solve specific (Stefan-type) boundary problems by numerical methods, using the boundary conditions found in the manner indicated.

There have already been several attempts at formulating inverse heat-conduction problems (mainly transient) with due allowance for the phase transition: an approximate analytical solution for inverse one-dimensional problems was given in [1-4], and a two-dimensional steady-state problem was considered in [5], subject to certain specific assumptions. Considerable advances were made in [6, 7], in which effective numerical methods were proposed for solving inverse one-dimensional problems of the Stefan-type for the linear and quasilinear heat-conduction equations.

The inverse problem under consideration arises when solving the steady-state Stefan problem regarding the solidification of a cylindrical casting, and also when studying other technological processes: the welding of metals, melting processes (for example, in bath-type furnaces), and so on.

The steady-state presentation is most appropriate in our own case, since semicontinuous and continuous casting are mainly steady-state processes: even for semicontinuous casting (with a cycle of 25-30 min), under practical conditions more than 90% of the metal is cast at a constant velocity, i.e., in a practically steady-state manner.

In formulating the boundary problem we make the usual assumptions: heat transfer in both phases is effected by the conduction mechanism; there is no supercooling of the melt. The steady-state axisymmetrical temperature field in a continuous cylindrical casting $G = \{0 \le r \le R, 0 \le z \le H\}$ and the position of the solidification front are defined on the basis of the following conditions, using a system of stationary coordinates attached to the mold:

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$$c_i\gamma_i v \frac{\partial T}{\partial z} = r^{-1} \frac{\partial}{\partial r} \left(\lambda_i r \frac{\partial T}{\partial r} \right) + \lambda_i \frac{\partial^2 T}{\partial z^2}, \ (r, \ z) \in G_i, \ i = 1, \ 2,$$

$$G_1 = \{ 0 < r < \xi(z), \ 0 < z \le H \}, \ G_2 = \{ \xi(z) < r < R, \ 0 < z \le H \},$$
(1)

$$T|_{z=0} = T^{\circ}(r), \ T|_{z=H} = T^{1}(r), \ 0 \leqslant r \leqslant R,$$
(2)

$$\frac{\partial T}{\partial r}\Big|_{r=0} = 0, \ T|_{r=R} = T_{\text{sur}}(z) \ \left(\text{ on } \lambda_2 \frac{\partial T}{\partial r} \Big|_{r=R} = -q(z) \right), \ 0 < z \leq H,$$
(3)

$$T|_{r=\xi(z)} = T_{\text{sol}} \quad 0 < z \leqslant H,$$

$$\lambda_2 \left(\frac{\partial T}{\partial r} - \frac{\partial T}{\partial z} \cdot \frac{\partial \xi}{\partial z} \right) \Big|_{r=\xi(z)} - \lambda_1 \left(\frac{\partial T}{\partial r} - \frac{\partial T}{\partial z} \cdot \frac{\partial \xi}{\partial z} \right) \Big|_{r=\xi(z)}$$

$$= \rho \gamma_1 v \frac{\partial \xi}{\partial z}, \quad 0 < z \leqslant H.$$
(4)

Condition (4) at the solidification front is obtained from the well-known Stefan thermal-balance relationship, on the assumption of a unique representation of the front in the form

$$r = \xi(z), \ 0 \leqslant z \leqslant H, \ \max |\xi_z| < \infty.$$

Estimates of the thermal fluxes in the direction of the z and r axes show that in a number of cases (for example, that of a continuous steel casting [8-10], and also a copper casting up to a specific thickness of the crust [5]) the axial flux is negligibly small by comparison with the radial component, and need not be taken into account. The term $\lambda_i (\partial^2 T/\partial z^2)$ in Eq. (1) may then be neglected, as a result of which we obtain an equation of the parabolic type (v = const > 0, c_i, $\gamma_i > 0$)

$$c_i \gamma_i v \frac{\partial T}{\partial z} = r^{-1} \frac{\partial}{\partial r} \left(\lambda_i r \frac{\partial T}{\partial r} \right), \tag{5}$$

in which z plays the part of the time t. The condition based on Eq. (2_1)

$$T|_{z=0} = T^{\circ}(r), \ 0 \leqslant r \leqslant R \tag{6}$$

becomes the initial condition (the condition at z = H is not needed).

In the region of the liquid phase $G_1 = \{0 \le r \le \xi(z), 0 \le z \le H\}$, neglecting overheating of the melt, we may consider that $T(r, z) \equiv T_{SOI}$, i.e., Eq. (5) is only applicable to the solid phase (one-phase problem), $G_2 = \{\xi(z) \le r \le R, 0 \le z \le H\}$.

As one of the boundary conditions we use Eq. (3). The other boundary condition is also formulated at $r = \xi(z)$, and represents a direct consequence of (4) if we know the profile of the cavity $r = \xi(z)$:

$$\lambda_2 \frac{\partial T}{\partial r} \bigg|_{r=\xi(z)} = \rho \gamma_1 v \frac{\partial \xi}{\partial z}.$$
(7)

The inverse Stefan problem lies in finding the boundary condition $T|_{r=R}$ (or $\lambda_2 (\partial T/\partial r)|_{r=R}$ and T(r, z) in \overline{G}_2 from the conditions (5)-(7) and (3). We note that at the boundary $r = \xi(z)$ of the region \overline{G}_2 two conditions (3) and (7) (Cauchy conditions) are specified, while at the other boundary -(r=R) the values of T_{sur} are unknowns. For an equation of the parabolic type, problems incorporating Cauchy data belong to the category of "incorrect" (A. N. Tikhonov) problems; in particular, instability of the solution with respect to perturbations of the conditions (3) and (7) may occur. The problem may be regularized, for example, by separating out the permissible set of solutions [11, 12]. This approach was employed in [5] to obtain an approximate analytical solution.

Another approach to the approximate solution of inverse problems of the Stefan-type for parabolic equations was established in [6, 7]. This lay in reducing the original problem to an equivalent extremal problem. The method enables us to find a smooth solution to the inverse Stefan-type of problem (when this exists), and to construct smooth quasi-solutions in the general case.

The inverse problem (5)-(7), (3) is replaced by the problem of minimizing the functional

$$J(V) = \int_{0}^{H} \int_{\xi(z)}^{R} (\overline{T} - \overline{\overline{T}})^2 \, dr dz, \tag{8}$$



Fig. 1. Profile of the cavity in a continuous copper casting 180 mm in diameter, subject to the calculated (designed) technological casting conditions: $0', 1, 2, \ldots, 9$ are the computing intervals over the height of the cavity.

Fig. 2. Results of a numerical calculation of the boundary conditions on the surface of a casting: 1) q; 2) T_{sur} ; 3) q distribution according to experimental data [14].

defined in terms of the solutions $\overline{T} = \overline{T}(\mathbf{r}, \mathbf{z})$, $\overline{\overline{T}} = \overline{\overline{T}}(\mathbf{r}, \mathbf{z})$ of the auxiliary boundary problems of Eq. (5) in a region G_2 with a movable boundary $\xi(\mathbf{z})$. As boundary condition at $\mathbf{r} = \xi(\mathbf{z})$ we respectively use (3) and (7) for \overline{T} and $\overline{\overline{T}}$; at $\mathbf{r} = \mathbf{R}$ the boundary conditions are $\overline{T}_{|\mathbf{r}|=\mathbf{R}} = \overline{T}_{|\mathbf{r}|=\mathbf{R}} = V(\mathbf{z})$ where $V(\mathbf{z})$ is a certain sufficiently smooth function:

$$(I_{T}) \begin{cases} c_{2}\gamma_{2}v \frac{\partial \overline{T}}{\partial r} = r^{-1} \frac{\partial}{\partial r} \left(\lambda_{2}r \frac{\partial \overline{T}}{\partial r}\right), (r, z) \in G_{2}, \\ \overline{T}|_{r=\xi(z)} = T_{sol} \quad 0 < z \leq H, \\ \overline{T}|_{r=R} = V(z), \quad 0 < z \leq H, \\ \overline{T}|_{z=0} = T^{\circ}(r), \quad \xi(0) \leq r \leq R, \end{cases}$$

$$(II_{T}) \begin{cases} c_{2}\gamma_{2}v \frac{\partial \overline{T}}{\partial r} = r^{-1} \frac{\partial}{\partial r} \left(\lambda_{2}r \frac{\partial \overline{T}}{\partial r}\right), (r, z) \in G_{2}, \\ \lambda_{2} \frac{\partial \overline{T}}{\partial r} \Big|_{r=\xi(z)} = \rho\gamma_{1}v \frac{\partial \xi}{\partial z}, \quad 0 < z \leq H, \\ \overline{T}|_{r=R} = V(z), \quad 0 < z \leq H, \\ \overline{T}|_{r=0} = T^{\circ}(r), \quad \xi(0) \leq r \leq R. \end{cases}$$

In order to minimize the functional J (V) in the set

$$Q_{C} = \{V(z) \in W_{2}^{1}[O, H], \|V\|_{W_{2}} \leq C, V(0) = T^{\circ}(R)\}, C = \text{const} > 0,$$

we may use the iterative gradient method. Specifying the initial approximation $V^{(0)} \in Q_C$, we find the next approximations by using the equation:

$$V^{s+1} = P_{Q_c} \{ V^s - \alpha^s \operatorname{grad} J(V^s) \}, \ s = 0, \ 1, \ \dots,$$
(9)

where P_{Q_C} is the operator for projection on the set Q_C ; $\alpha^S > 0$ is the step of the gradient method; grad J (V^S) is the gradient of the functional J (V) in the s-th iteration.

The following relationship is then valid [6, 7]:

$$\operatorname{grad} J(V) = a \left(\frac{\partial \overline{\Psi}}{\partial r} + \frac{\partial \overline{\Psi}}{\partial r} \right) \Big|_{r=R}, \ a = \lambda_2 \left(\upsilon c_2 \gamma_2 \right)^{-1}, \tag{10}$$

where $\overline{\Psi} = \overline{\Psi}(\mathbf{r}, \mathbf{z}), \ \overline{\Psi} = \overline{\Psi}(\mathbf{r}, \mathbf{z})$ are the solutions of the boundary problems conjugate to the problems I_T , II_T :

$$\begin{split} & I_{\Psi} \begin{cases} -\frac{\partial \overline{\Psi}}{\partial z} = a \frac{\partial^2 \overline{\Psi}}{\partial r^2} - a \frac{\partial}{\partial r} (r^{-1} \overline{\Psi}) - 2 (\overline{T} - \overline{T}), \ (r, \ z) \in G_2, \\ \overline{\Psi}|_{r=\xi(z)} = 0, \ 0 < z \leqslant H, \\ \overline{\Psi}|_{r=R} = 0, \ 0 < z \leqslant H, \\ \overline{\Psi}|_{z=H} = 0, \ \xi(H) \leqslant r \leqslant R, \end{cases} \\ & II_{\Psi} \begin{cases} -\frac{\partial \overline{\Psi}}{\partial z} = a \frac{\partial^2 \overline{\Psi}}{\partial r^2} - a \frac{\partial}{\partial r} (r^{-1} \overline{\Psi}) + 2 (\overline{T} - \overline{T}), \ (r, \ z) \in C_2, \\ a \frac{\partial \overline{\Psi}}{\partial r} - \left(ar^{-1} + \frac{\partial \xi}{\partial z} \right) \overline{\Psi}|_{r=\xi(z)} = 0, \ 0 < z \leqslant H, \\ \overline{\Psi}|_{r=R} = 0, \ 0 < z \leqslant H, \\ \overline{\Psi}|_{r=R} = 0, \ \xi(H) \leqslant r \leqslant R. \end{split}$$

In accordance with (9) and (10), the determination of $V^{S+1}(z)$ (s = 0, 1, ...) involves the solution of the boundary problems I_T , II_T for $V(z) = V^S(z)$, with subsequent solution of the conjugate problems I_{Ψ} , II_{Ψ} in which \overline{T} and $\overline{\overline{T}}$ are the solutions of problems I_T , II_T for $V(z) = V^S(z)$. The gradient-descent iteration process is regarded as completed when $V^S(z)$ and $V^{S+1}(z)$ coincide to a specified accuracy. As the element yielding the minimum J (V) in Q_C , we then take V^{S+1} .

We call the following pair of functions the quasi-solution to the inverse Cauchy problem (5)-(7), (3) in the set $Q_{\rm C}$

 $\{T_{C}^{\mu}, V_{C}\},\$

where $V_C \in Q_C$ gives a minimum J (V) in Q_C ; T_C^{μ} is a linear combination of the solutions \overline{T} , $\overline{\overline{T}}$ of the problems I_T, II_T corresponding to the function $V_C(z)$:

$$T_C^{\mu} = \mu \overline{T} + (1 - \mu) \overline{T}, \ 0 < \mu < 1.$$

The value of the numerical parameter μ is chosen from the condition

$$\mu = \frac{\|\overline{T}\|_{r=\xi(z)} - T_{\mathrm{SOI}}\|_{L_{2}[0, H]}^{2}}{\|\overline{T}\|_{r=\xi(z)} - T_{\mathrm{SOI}}\|_{L_{2}[0, H]}^{2} + \left\|\left(\frac{\partial\overline{T}}{\partial r} - \frac{\partial\overline{T}}{\partial r}\right)\right\|_{r=\xi(z)}\left\|_{L_{2}[0, H]}^{2}\right\|_{L_{2}[0, H]}^{2}}$$

The quasi-solution may be defined in any set Q_C , C > 0. If the input data of the inverse problem are sufficiently smooth and its solution $\{T(r, z), T_{sur}(z)\}$ exists, it follows that a quasi-solution $\{T_C^{\mu}, V_C\}$ exists in the set Q_C , within the range $0 < C < C^*$ ($C^* = \inf_{\substack{(T_{sur})}} \|T_{sur}\|_{W_2^1} = \|T_{sur} \min\|$), and that it is more-over the only one. As $C \rightarrow C^*$ we find that $\{T_C^{\mu}, V_C\}$ converges to the solution of the inverse problem $\{T, T_{sur}\}$ [7]. The stability of the quasi-solutions relative to smooth perturbations of all the input data was also established in [7]. In order to construct smooth quasi-solutions for the case of input data perturbed in L_2 , preliminary smoothing of the perturbations must be carried out [7].

For a numerical solution of the problem under consideration it is convenient to make a substitution to "straighten" the front [13]:

$$y=\frac{r-\xi(z)}{R-\xi(z)}, \ z'=z,$$

so converting the region $\overline{G}_2 = \{\xi (z) \le r \le R, \ 0 \le z \le H\}$ into a rectangle of fixed width $\overline{\Pi} = \{0 \le y \le 1, 0 \le z \le H\}$. Into $\overline{\Pi}$ we then introduce the network $\Omega = \omega h \times \omega_{\tau}$, where $\omega h = \{y_0 = 0, y_1, \dots, y_i = y_{i-1}\}$

+ h, ..., $y_N = 1$, h = 1/N is the y network and $\omega_\tau = \{z_0 = 0, z_1, \ldots, z_j = z_{j-1} + \tau_j, z_n = H\}$ is a non-uniform z network.

The problem of finding the quasi-solution $\{T_C^{\mu}, V_C\}$ is replaced by that of finding a function defined in Ω , ω_{τ} , namely, the network function $\{(T_C^{\mu})_{ij}, (V_C)_j\}$. For the numerical solution of the boundary problems I_T , II_T , I_{Ψ} , II_{Ψ} (written in variables y, z) we here use the monotonic difference schemes of [15].

Making use of the algorithm just described, we carried out some calculations in the BESM-6 computer for several tens of M1 copper castings produced in a copper mold 176-185 mm in diameter by the semicontinuous method. We judged the accuracy of the solution from the values of the functional J, and also from the mean square deviations σ of the calculated temperatures at the solidification from the specified T_{sol}.

In setting out the input data for the majority of experimental cavities, the profile (and hence the derivative $d\xi/dz$) was specified in the following way: in the upper region we used piecewise-linear interpolation; in the lower region we approximated the cavity by a parabola (using the method of least squares). Here we considered only the monotonic approximations of the cavity profile ($d\xi/dz \le 0$). Calculations showed that this method of representing the cavity profile ensured reliable results.

The foregoing algorithm enables us to restore boundary conditions of both the first and second kinds. The results of the calculations show that boundary conditions of the first kind may be restored (reconstituted) far more accurately and stably (relative to the original approximation and method of specifying the cavity profile) than those in which the thermal flux q is defined (i.e., conditions of the second kind). The flux is in this case determined from the solution for the temperature field [as the derivative $\lambda (\partial T/\partial r)|_{r=R_1}$.

By way of example, Fig. 1 shows the profile of the cavity in a copper casting of radius R = 90 mm for v = 10 m/h, obtained by flooding the casting with lead; Fig. 2 shows the results of a numerical calculation for q and T_{sur} . Figure 2 also shows the experimental data relating to the q distribution over the height of the mold under the casting conditions specified (these data were taken from [14]). In this calculation the following initial data were taken: $T_{sol} = 1083 \text{ °C}$; $c_2 = 418.68 \text{ J/kg} \cdot \text{deg}$, $\gamma_2 = 8700$, $\gamma_1 = 8300 \text{ kg/m}^3$; $\gamma_2 = 350 \text{ W/m} \cdot \text{deg}$; $\rho = 205 \text{ kJ/kg}$. The temperature of the liquid phase was taken as constant and equal to T_{sol} .

An analysis of the results shows that, within that part of the casting preceding the cross-section in which the ratio of the thickness of the solidified crust ξ to the radius of the casting exceeds 0.4, the experimental data agree reasonably well with calculation (the difference is no greater than 15%), i.e., the axial flux may validly be neglected. In the present example this condition is valid along the whole length of the casting, up to the sixth interval inclusively ($\xi = 0.036$ m), i.e., a distance of almost 2/3 the depth of the cavity. In this region the problem may be regarded as one-dimensional. As the crust grows further, the influence of the axial flow of heat becomes rapidly greater, in accordance with the situation already encountered in [8, 14], and the one-dimensional model is no longer applicable. Clearly, as the thermal conductivity of the metal diminishes, the axial flow of heat does likewise, and the range of applicability of the one-dimensional model expands. In this respect the case of a copper casting under consideration is the least favorable.

The peak of the q curve (Fig. 2) in the second interval indicates that a gas gap has developed at this point between the casting and the mold wall, causing a sharp fall in q. The subsequent course of the curve reflects the influence of the changing gap and contact between the casting and the mold.

The proposed numerical solution of the inverse problem may be used directly in practical calculations, and also in specifying the necessary boundary conditions and obtaining initial approximations for the solution of direct problems of the Stefan type by numerical methods.

NOTATION

 γ , density; ρ , heat of solidification; c, specific heat; λ , thermal conductivity; v, rate of pulling the solidifying material (ingot, casting); H, length of the working (computed) part of the casting; $T_{sur}(^{\circ}C)$, q (mW/m²), temperature and thermal flux on the surface of the casting respectively.

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