APPROXIMATE METHODS OF CALCULATING SOLIDIFICATION OF CASTINGS

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Two approximate methods are described for solving the problem of solidification of plane castings of a material crystalizing at constant temperature, under boundary conditions of the 3rd kind on a cooled surface.

1. We shall examine the process of solidification of a plane casting of thickness S undergoing heat transfer at its outer surface according to Newton's law of convection. The mathematical formulation of the problem includes the heat conduction equation

$$c\gamma \frac{\partial T}{\partial t} = \lambda \frac{\partial^2 T}{\partial x^2} \tag{1}$$

and the boundary conditions

$$\lambda \frac{\partial T}{\partial x}\bigg|_{x=0} = \alpha (T_s - T_c), \tag{2}$$

$$\rho\gamma \frac{d\varepsilon}{dt} = \lambda \frac{\partial T}{\partial x}\bigg|_{x=\varepsilon}, \tag{3}$$

$$T(\varepsilon, t) = T_{cr}, \tag{4}$$

$$T(x, 0) = \varphi(x), \tag{5}$$

$$\varepsilon(0) = \varepsilon_0, \tag{6}$$

the origin of coordinates (x = 0) being taken on the cooled surface of the casting. The thermophysical properties of the material are assumed constant; supercooling of the melt at the crystallization front is not taken into account; and the temperature of the liquid core of the casting is assumed to be unchanging and equal to the crystallization temperature.

In this form the problem has been examined by Veinik [1] using an integral method of heat balance with an assigned temperature profile at the solid crust ($0 \le x \le \varepsilon$) according to the formula

$$T(x, t) = T_{cr} - \frac{T_{cr} - T_c}{1 + n\lambda/\alpha\varepsilon}\left[1 - \frac{x}{\varepsilon(t)}\right]^n. \tag{7}$$

The value of the index m was determined by Veinik only for the case of a boundary condition of the first kind (Bi $\to \infty$) from comparison with the known exact solution for the problem.

Results are presented below of a determination of the index n on the basis of numerical solution of the problem, and then an approximate analytical method of computation is developed.

The numerical solution of the problem determined by the system (1)–(6) has been carried out by a finite difference method using the "extension network" proposed in reference [2]. In distinction from reference [2], however, the heat conduction equation was approximated by a network equation of implicit form

$$\frac{T_{i,k+1} - T_{i,k}}{\Delta t} = a\frac{T_{i+1,k+1} - 2T_{i,k+1} - T_{i-1,k+1}}{\Delta x^2},$$

from which it follows that

$$T_{i-1,k+1} - (2 + s_0)T_{i,k+1} + T_{i+1,k+1} = -s_0 T_{i,k}, \tag{8}$$

where $S_0 = \Delta x^2/a\Delta t$, $\Delta x = \varepsilon/M$, $a = \lambda/c\gamma$.

Equation (8) has been solved by the "screw" method [3], which leads to a computation relation of the type

$$T_{i,k+1} = A_{i,k+1}(B_{i,k+1} + T_{i+1,k+1}). \tag{9}$$

In the first stage of the screw, coefficients A_i and B_i are determined at the nodes of the network region according to the formulas

$$A_{i,k+1} = 1/(2 + s_0 - A_{i-1,k+1}),$$

$$B_{i,k+1} = A_{i-1,k+1}B_{i-1,k+1} + s_0 T_{i,k}. \tag{10}$$

The calculation there is carried out from the external surface of the casting, where the values A_0 and B_0 are known at the node of the network located at a distance $\Delta x/2$ from the surface outside the section (Fig. 1):

$$A_0 = \left(1 - \frac{\alpha\Delta x_k}{2\lambda}\right)\bigg/\left(1 + \frac{\alpha\Delta x_k}{2\lambda}\right),$$

$$B_0 = \frac{\alpha\Delta x_k}{\lambda} T_c \bigg/ \left(1 - \frac{\alpha\Delta x_k}{2\lambda}\right). \tag{11}$$

In the second stage of the screw the temperatures are determined at the nodes of the network region according to formula (9), beginning from a node coinciding with the solidification front.

Calculation of the increase of the crust in time Δt is performed according to the formula obtained from condition (3):

$$\Delta\varepsilon_k = \frac{\lambda\Delta t}{\rho\gamma\Delta x_k}(T_{cr} - T_{M-1}). \tag{12}$$

After determination of $\Delta\varepsilon_k$, the thickness of the crust is found at time k + 1, i.e., $\varepsilon_{k+1} = \varepsilon_k + \Delta\varepsilon_k$, as well as the new thickness of the elementary layers $\Delta x_{k+1} = \Delta x_k + \Delta\varepsilon_k/M$.

Before repeating the calculation of displacement is carried out of the values of temperature to a node of the new (extended) network by means of the interpolation formula

$$T_i' = T_i - \frac{i - 0.5}{M}\frac{\Delta\varepsilon_k}{\Delta x_k}(T_{i+1} - T_i),$$

where i = 1, 2, 3, ..., M − 1 (beginning from the node adjacent to the surface of the casting).

The use of the implicit scheme of the network equation, which is stable during the computations for any values of the intervals Δx and Δt, allowed the volume of computation to be cut down by a factor of ten in comparison with the explicit scheme, which is limited by the condition that the interval Δt must be selected

$\leq \Delta x^2/2a$. In carrying out the calculations, accomplished on a "Minsk-1" computer, the solid cross section was divided into 9.5 intervals Δx; evaluation of the accuracy of calculations showed that the error in determining the temperature field did not exceed one or two tenths of one per cent.

The result of the calculations allowed construction of a graph of the total duration of solidification t_f, of the casting, expressed by means of the parameter $(Fo)_f = at_f/S^2$, as a function of the parameters Bi and K_1 (Fig. 2). The top corner of the figure shows values of the parameter $(Fo)_{in}$, corresponding to time of growth of the initial thickness of the crust $\varepsilon_0 = 0.1s$, from which calculation by the network method commences. Values of $(Fo)_{in}$ have been calculated from Veinik's formula (1, page 63) with $\delta_0 = \varepsilon_0/S = 0.1$.

The data of the calculations by the network method were used further to determine the index n in formula (7). As analysis shows, the value of n rapidly becomes stablized with time; the values of n thus determined are shown in Fig. 3 as a function of parameters Bi and K_1.

2. An approximate analytical solution of the problem (1)–(6) was obtained in [1] by the integral heat balance method. An interesting idea is to use for this purpose variational methods of solution with the objective of increased accuracy of calculation.

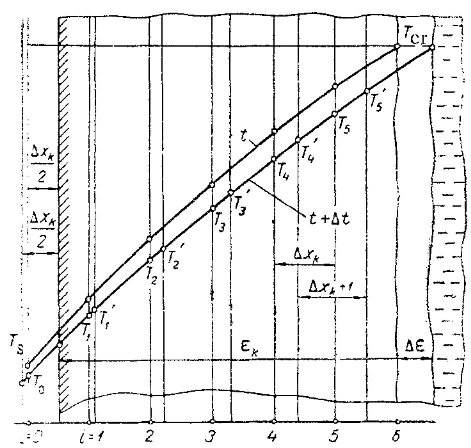

Fig. 1. Schematic temperature distribution in the solid cross section.

We therefore made use of the variational method of Biot [4–6] to solve the problem (1)–(6). According to the procedure of this method, for one-dimensional unsteady heat conduction problems there is a differential equation of the Lagrange type

$$\frac{\partial W}{\partial q} + \frac{\partial D}{\partial q} = \Theta_{inc} \frac{\partial H}{\partial q}\Big|_{inc}, \qquad (13)$$

where

$$W = \frac{1}{2} c\gamma \int_0^s \Theta^2 dx; \quad D = \frac{1}{2\lambda} \int_0^s \dot{H}^2 dx;$$

$$H = -c\gamma \int_s^x \Theta\, dx + \text{const}; \quad \Theta = T_{cr} - T;$$

q is a generalized coordinate for which we have used the thickness of the solidified layer, ε, below.

Setting

$$\frac{\partial H}{\partial \varepsilon} = \rho\gamma - c\gamma \frac{\partial}{\partial \varepsilon} \int_\varepsilon^x \Theta\, dx,$$

we shall satisfy boundary condition (3), since the heat flux vector H is determined by the equation

$$c\gamma\Theta = -\operatorname{div} H$$

and, in addition,

$$\dot{H} = \frac{\partial H}{\partial \varepsilon}\dot{\varepsilon} = -\lambda \frac{\partial \Theta}{\partial x}.$$

We shall assign the temperature profiles at the solid cross section with the aid of formula (7), which we shall rewrite in the form

$$\Theta = \frac{\Theta_c}{1 + n\lambda/\alpha\varepsilon}\left(1 - \frac{x}{\varepsilon}\right)^n. \qquad (7a)$$

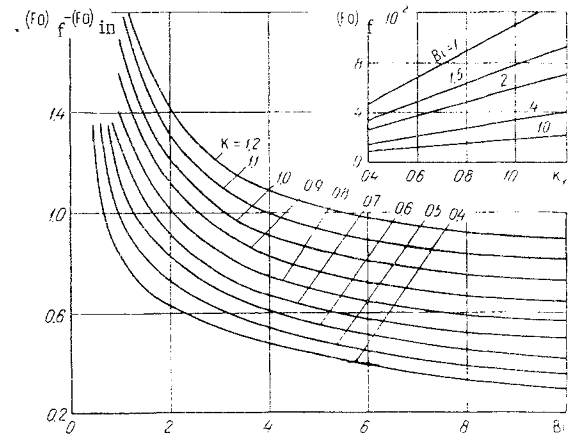

Fig. 2. $(Fo)_f = at_f/S^2$ versus parameters Bi and K_1.

Using expression (7a) to determine the components of relation (13), we arrive at the equation

$$dy\left[K_1^2(y+N)^4 + \frac{2K_1 y}{(n+1)(n+2)}(y+N)^2(2y+3N) + \frac{(5n+3)y^4 + (16n+9)y^3N + (13n+7)y^2N^2}{(n+1)^2(2n+1)(2n+3)}\right] \times$$

$$\times\left[K_1(y+N)^3 + y(y+N)\frac{y+2N}{n+1} - \frac{(y+N)(y+3N)y}{2(2n+1)}\right]^{-1} = d\text{Fo}, \qquad (14)$$

for

$$N = n\,\text{Bi}, \quad y = \varepsilon/s.$$

Integrating the latter equation with the initial condition $y(0) = 0$, we obtain the calculation relation

$$M_1\text{Fo} = 2(a_1 - \beta_1)y + y^2 + 2\gamma_1 A_2 \ln\frac{|y_* - y|}{y_*} +$$

$$+ \gamma_1 B_2 \ln\left(\frac{1}{b_2}|y^2 + a_2 y + b_2|\right) + \gamma_1(2C_2 - B_2 a_2) J(y), \qquad (15)$$

where

$$J(y) = \frac{2}{\sqrt{4b_2 - a_2^2}}\left(\operatorname{arctg}\frac{2y + a_2}{\sqrt{4b_2 - a_2^2}} - \operatorname{arctg}\frac{a_2}{\sqrt{4b_2 - a_2^2}}\right).$$

if $4b_2 - a_2^2 > 0$;

$$J(y) = \frac{1}{\sqrt{a_2^2-4b_2}} \times$$

$$\times \ln \frac{\left|(2y+a_2-\sqrt{a_2^2-4b_2})/(2y+a_2+\sqrt{a_2^2-4b_2})\right|}{\left|(a_2-\sqrt{a_2^2-4b_2})/(a_2+\sqrt{a_2^2-4b_2})\right|},$$

if $4b_2 - a_2^2 < 0$;

$$J(y) = -2\,[1/(2y+a_2) - 1/a_2],$$

if $4b_2 - a_2^2 = 0$; y_* a root of the equation $y^3 + \beta_1 y^2 + \beta_2 y + \beta_3 = 0$;

$$A_2 = (y_*^2 + a_1 y_* + b_1)/(y_*^2 + a_2 y_* + b_2),$$

$$B_2 = 1 - A_2; \quad C_2 = (A_2 b_2 - b_1)/y_*,$$

$$a_1 = \gamma_2/\gamma_1; \quad b_1 = \gamma_3/\gamma_1; \quad a_2 = \beta_1 + y_*; \quad b_2 = -\beta_3/y_*.$$

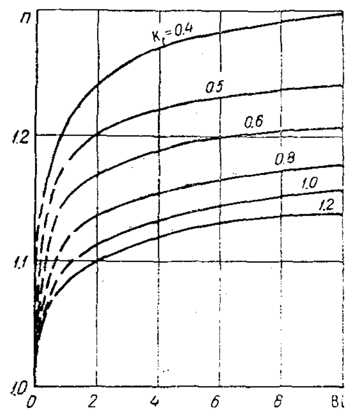

Fig. 3. Index n versus parameters Bi and K_1.

Here

$$b_2 - a_2 y_* = \beta_2; \quad \gamma_1 = (\alpha_2 - \beta_2) - \beta_1(\alpha_1 - \beta_1),$$

$$\gamma_2 = (\alpha_3 - \beta_3) - \beta_2(\alpha_1 - \beta_1),$$

$$\gamma_3 = \alpha_4 - \beta_3(\alpha_1 - \beta_1); \quad \alpha_1 = B_1/A_1, \quad \alpha_2 = C_1/A_1,$$

$$\alpha_3 = D_1/A_1; \quad \alpha_4 = E_1/A_1; \quad \beta_1 = G_1/F_1, \quad \beta_2 = H_1/F_1,$$

$$\beta_3 = L_1/F_1; \quad M_1 = 2F_1/A_1.$$

Also

$$M_1 = \left\{2K_1 + \frac{3n+1}{(n+1)(2n+1)}\right\} \Big/ \left[K_1^2 + \frac{4K_1}{(n+1)(n+2)} + \frac{5n+3}{(n+1)^2(2n+1)(2n+3)}\right],$$

$$A_1 = K_1^2 + \frac{4K_1}{(n+1)(n+2)} + \frac{5n+3}{(n+1)^2(2n+1)(2n+3)},$$

$$B_1 = N\left[4K_1^2 + \frac{14K_1}{(n+1)(n+2)} + \frac{16n+9}{(n+1)^2(2n+1)(2n+3)}\right],$$

$$C_1 = N^2\left[6K_1^2 + \frac{16K_1}{(n+1)(n+2)} + \frac{13n+7}{(n+1)^2(2n+1)(2n+3)}\right],$$

$$D_1 = N^3\left[4K_1^2 + \frac{6K_1}{(n+1)(n+2)}\right], \qquad E_1 = N^4 K_1^2,$$

$$F_1 = K_1 + \frac{3n+1}{2(n+1)(2n+1)},$$

$$G_1 = N\left[3K_1 + \frac{4n+1}{(n+1)(2n+1)}\right],$$

$$H_1 = N^2\left[3K_1 + \frac{5n+1}{2(n+1)(2n+1)}\right], \quad L_1 = N^3 K_1. \tag{15a}$$

In particular, when Bi $\to \infty$ ($N \to 0$), the solution takes the form

$$y = \sqrt{M_1 \mathrm{Fo}}, \tag{16}$$

where M_1 is determined by formula (15a).

The values of the coefficient M_1, as calculated from formula (15a) as a function of n are shown by the solid inclined lines on Fig. 4.

The horizontal straight lines on the same figure correspond to values found from the exact solution of Stefan [7], from the transcendental equation

$$\frac{\sqrt{\pi}}{2}\sqrt{M_1' K_1}\exp\left(\frac{M_1'}{4}\right)\operatorname{erf}\left(\frac{1}{2}\sqrt{M_1'}\right) = 1. \tag{17}$$

The points of intersection of the curves M_1 and M_1' determine the values of the index n, corresponding to the exact solution of the problem.

Values of the coefficient $M''_1 = [2n(n+1)] / [1 + K_1(n+1)]$ which appears in the well known solution of Veinik [1], are shown on the same figure by dotted lines.

It may be seen from the figure that the values of the coefficients M_1 and M''_1 are close together at points of intersection with the lines corresponding to the exact values of M'_1.

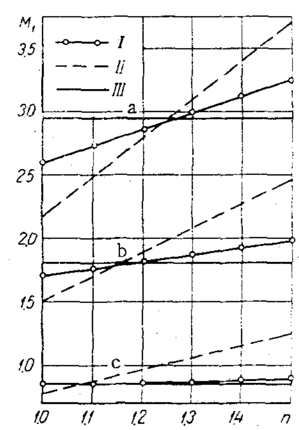

Fig. 4. Comparison of the coefficients M_1, calculated by a variational method (I) and according to Veinik's formula (II), with the exact solution of Stefan (III): a is for $K_1 = 0.413$; b is for $K_1 = 0.823$; c is for $K_1 = 2.03$, where $K_1 = \rho/c\,(T_{cr} - T_c)$.

With increasing deviation from the above point, the discrepancies between M_1, M''_1 and M'_1 increase while, for the Veinik solution, the difference in the coefficients M''_1 and M'_1 increases much more rapidly than for the solution obtained by the variational method. The advantage of the variational method is clearly seen in the stability of the index M_1 as regards oscillations of the index n.

Similarly, for finite values of the Biot number, the results of calculations according to relations (15), (15a) depend to a lesser degree on oscillations of the index n, than in the calculations according to the Veinik formulas. In addition, for a boundary condition of the third kind on the surface of the casting, the variational method leads to excessively awkward relations in comparison with the formulas of reference [1]. When using the exact values of the index n (in particular for a plane casting according to the graphs of Fig. 3) calculations according to the Veinik formulas lead to results which are practically concident with the data of the network method and of the variational method (the initial data of the calculation being identical).

NOTATION

T is the temperature; t is the time; x is the coordinate; ε is the thickness of the solidified layer; λ, c, γ are the thermal conductivity, specific heat, material density; ρ is the specific heat of crystallization; α is the heat transfer coefficient; $Bi = \alpha S/\lambda$ is the Biot number; $Fo = at/S^2$ is the Fourier number; $K_1 = \rho/c(T_{cr} - T_c)$ is the heat emission intensity criterion; M is the number of layers of the network region.

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