INVESTIGATION OF HEAT TRANSFER DURING CHANGE IN THE STATE OF AGGREGATION OF A SYSTEM

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New differential equations are derived to describe the boundary conditions at a front defining a change of state. A method based on these equations is suggested for numerical calculation of the temperature field in a system undergoing a change of state.

Many processes in the metallurgical, chemical, building, and other industries involve a change in the state of aggregation of a system of solids. In these processes, a heat of transition, which is in general a function of position and time, is released (or absorbed) at the moving boundary G, where the change of state takes place.

The equations for the boundary conditions at the front G are known [1], and for the three-dimensional problem can be expressed in the form

$$\lambda_i \frac{\partial t_i(r, \tau)}{\partial n} - \lambda_k \frac{\partial t_k(r, \tau)}{\partial n} = s \frac{dn}{d\tau}. \tag{1}$$

When the transition from one state to another takes place at a boundary washed by a moving medium, the boundary conditions may be written:

$$\lambda \frac{\partial t(r, \tau)}{\partial n} - \alpha [t(r, \tau) - t_c] = s \frac{dn}{d\tau}. \tag{2}$$

Integration of the equation of thermal conductivity with boundary conditions (1) and (2) belongs to a class of problems with nonlinear boundary conditions, which have no exact solution.

For numerical solution of the problem, supplementary information is necessary regarding the behavior of the temperature function near the boundary G. This can be obtained as follows.

Assume that at time τ the temperature function t has finite derivatives to the second order in the interval from r to p = r - Δn; then

$$t[r(\tau), \tau] = t(p, \tau) + \Delta n \frac{\partial t(p, \tau)}{\partial n} + \frac{\Delta n^2}{2} \frac{\partial^2 t(p + \theta \Delta n, \tau)}{\partial n^2}, \quad 0 \leqslant \theta \leqslant 1. \tag{3}$$

The transition front passes through the point with radius vector p at time τ - $\Delta\tau$. Assuming that the temperature function at this point in the time interval from τ - $\Delta\tau$ to τ also has finite derivatives to the second order, we obtain

$$t[r(\tau - \Delta\tau), \tau - \Delta\tau] = t(p, \tau) - \Delta\tau \frac{\partial t(p, \tau)}{\partial \tau} + \frac{\Delta\tau^2}{2} \frac{\partial^2 t(p, \tau - \theta\Delta\tau)}{\partial \tau^2}. \tag{4}$$

Subtracting (4) from (3), and letting Δn tend to zero, we obtain an equation which, for convenience of later discussion, we shall write as follows:

$$\frac{dt(r, \tau)}{d\tau} = \frac{dn}{d\tau} \left[\frac{\partial t(p, \tau)}{\partial n}\right]_{p \to r} + \left[\frac{\partial t(p, \tau)}{\partial \tau}\right]_{p \to r}. \tag{5}$$

We replace the derivative dn/dτ by its value from equations (1), (2), to obtain the boundary conditions at the moving boundary G:

$$\frac{dt(r,\tau)}{d\tau}=\left[\frac{\lambda_i}{s}\frac{\partial t_i(r,\tau)}{\partial n}-\frac{\lambda_k}{s}\frac{\partial t_k(r,\tau)}{\partial n}\right]\times$$
$$\times\left[\frac{\partial t_i(p,\tau)}{\partial n}\right]_{p\to r}+\left[\frac{\partial t_i(p,\tau)}{\partial\tau}\right]_{p\to r}, \tag{6}$$

$$\frac{dt(r,\tau)}{d\tau}=\left\{\frac{\lambda}{s}\frac{\partial t(r,\tau)}{\partial n}-\frac{\alpha}{s}[t(r,\tau)-t_c]\right\}\times$$
$$\times\left[\frac{\partial t(p,\tau)}{\partial n}\right]_{p\to r}+\left[\frac{\partial t(p,\tau)}{\partial\tau}\right]_{p\to r}. \tag{7}$$

These equations give the rate of change of temperature of points situated near the surface G. From them the temperature at these points at time $\tau + \Delta\tau$ can be found, if the temperature distribution in the body at time τ is known. This offers a numerical method of calculating the temperature field during change of state in a system. On putting the thermal conduction equations [2, 3], and the boundary equations (1), (2), (6), and (7) in final form, a set of differences necessary for numerical calculation is obtained.

As an example of a calculation of this kind, consider the following problem. A layer of iron at its melting point is solidifying near a plane wall whose temperature is one degree less than the melting point of the metal.

The problem can be formulated mathematically as follows:

$$\frac{\partial t(x,\tau)}{\partial\tau}=a\frac{\partial^2 t(x,\tau)}{\partial x^2}; \tag{8}$$

$$t(0,\tau)=0;\ t(\xi,\tau)=t_3=1; \tag{9}$$

$$\lambda\frac{\partial t(\xi,\tau)}{\partial x}=\rho\gamma\frac{d\xi}{d\tau}; \tag{10}$$

$$\frac{\lambda}{\rho\gamma}\frac{\partial t(\xi,\tau)}{\partial x}\left[\frac{\partial t(x,\tau)}{\partial x}\right]_{x\to\xi}+\left[\frac{\partial t(x,\tau)}{\partial\tau}\right]_{x\to\xi}. \tag{11}$$

For the numerical solution of the set of equations (8) through (11), we introduce in the given region a family of planes perpendicular to the x axis, $x = i\Delta x$.

In its simplest form the difference system corresponding to equations (8)–(11) is as follows:

$$t_{i,k+1}=\left(1-\frac{2a\Delta\tau}{\Delta x^2}\right)t_{i,k}+\frac{a\Delta\tau}{\Delta x^2}(t_{i+1,k}+t_{i-1,k}), \tag{12}$$

$$t_{0,k}=0,\ t_{\xi,k}=t_3=1, \tag{13}$$

$$\frac{\lambda}{\rho\gamma}\frac{T_3-T_{m,k}}{\Delta x}=\frac{\xi_{k+1}-\xi_k}{\Delta\tau}, \tag{14}$$

$$\frac{\lambda}{\rho\gamma}\frac{T_3-T_{m,k}}{\Delta x}M+\frac{t_{m,k+1}-t_{m,k}}{\Delta\tau}=0, \tag{15}$$

where M is the derivative of the temperature function at point m, which can be obtained by drawing through the points $t_{m-1,k}$, $t_{m,k}$ and $t_{\xi,k}$ of the quadratic parabola $t = a_1x^2 + a_2x + a_3$:

$$M=\left[(t_{m,k}-t_{m-1,k})\frac{\xi-m\Delta x}{\Delta x}+\right.$$
$$\left.+(t_3-t_{k,m})\frac{\Delta x}{\xi-m\Delta x}\right]\frac{1}{\xi-(m-1)\Delta x}. \tag{16}$$

From (12)–(15) the temperature field at time $(k+1)\Delta\tau$ can be found, if the temperatures at points 0, 1, 2, ..., m and ξ_k at time $k\Delta\tau$ are known. The temperature at points 1, 2, ..., m-1 at time $(k+1)\Delta\tau$ is determined from

difference equation (12), the temperature $t_{m, k+1}$ from (15), the depth of solidification ξ_{k+1} from (14). The time for the solidification boundary G to advance to a depth $2\Delta x$ can be found from equation (14), if we make the approximation

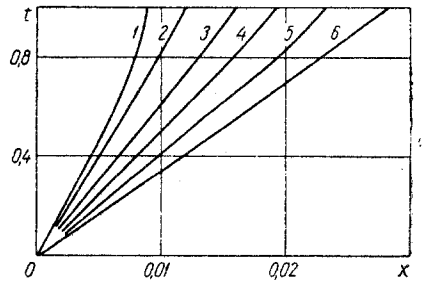

Fig. 1. Temperature field during change of state of the substance:
1 – at $\tau/3600 = 0.5$; 2 – 1; 3 – 2; 4 – 3; 5 – 5; 6 – 7.5

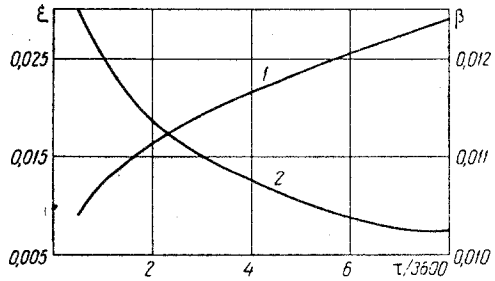

Fig. 2. Quantities ξ(1) and β(2) as functions of time of solidification.

that in this period the temperature field is linear with x. This time may be calculated more exactly after completing the calculations, from the quantity $\beta = \xi/\sqrt{\tau}$, which varies within narrow limits.

A computer program was devised for the difference set (12) to (15). Figs. 1 and 2 show the results of the calculations for values of the parameters: $a = 0.406 \cdot 10^{-5}/m^2$ sec, $\lambda = 23.3$ w/m · degree, $\gamma = 7200$ kg/m^3, $\rho = 272$ kj/kg, $\Delta x = 0.002$ m, $\Delta\tau = \Delta x^2/2a$ sec. It will be seen from Fig. 2 that at substantial ξ the value of β varies only very slightly, which agrees with experimental data, and also with the results of Stefan's investigation [1]. For $\xi = 0.028$ m, the calculated value of β is 4% above the value given by the approximate solution of Lamé and Clapeyron [1] for the conditions specified.

NOTATION

n – normal to moving front; r – radius vector of surface G; s – heat of transition released when unit area of moving front travels unit distance; t_c – temperature of medium washing surface; ξ – thickness of solidified layer of metal; ρ – heat of crystallization of metal; Δx – step value; i assumes successive values 0, 1, 2, ..., m; m – number of steps fully included in intercept at time τ; Δτ – step along time axis τ, chosen from condition (3) $\Delta\tau \leq \Delta x^2/2a$.

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