A METHOD OF SIMULATING THE CRUST FORMATION IN THE ORE BATH OF SMELTING FURNACES

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The crust formation is analyzed as a problem of phase transformation with a random mode of heat transfer across the interphase boundary. A model of the process based on statistical testing is shown here.

The formation of a protective crust in an ore smelting furnace is associated with the optimum thermal conditions and with a stable lining. In the furnace crucible there forms a melt whose temperature is determined by the physicochemical properties of the charge. Under normal operating conditions there forms along the inner wall a protective layer of solidified material, which prevents a chemical decomposition of the furnace lining. The possibility of crust formation and its subsequent thickness at a given power level of furnace operation will determine the optimum crucible dimensions [1].

The performance of ore smelting furnaces is largely affected by processes which make it difficult to determine the thermophysical properties of a molten mass. Furthermore, results obtained by simulating the thermal processes in furnaces of various capacities cannot be scaled up from low-power to high-power apparatus.

In view of this, there arises the problem of devising a simulation method which would require the least time and equipment for testing and the mathematical description. A model for determining the crust thickness will be shown here which is based on statistical tests.

The model is shown schematically in Fig. 1. Electric power is supplied to the ore bath 1 in the furnace through electrode 2; a constant temperature is maintained at the outer wall consisting of a metal jacket 3 and a liner 4. The movement of the interphase boundary 5 is determined by the amount of heat flowing from the bath to the side walls. The problem is to determine the thickness of crust 6 at various power input levels. Crust formation is associated with a phase transformation in the liquid–solid system and, therefore, its analysis ties in with the Stefan problem [2].

The thermal circuits may be represented as follows. The solid phase consists of two layers: the liner and the crystallizing melt. The thickness of the latter comprises the width of the zone separating the wall from the interphase boundary. The thermophysical properties of the solid phase are functions of the coordinates and of the temperature, while those of the liquid phase are unknown functions of the temperature. The crust thickness is determined from the isotherm for a temperature below the temperature of the interphase boundary. One specifies boundary conditions of the third kind at the outside surface of the liner, and of the second kind along the solid surface in the upper part of the bath.

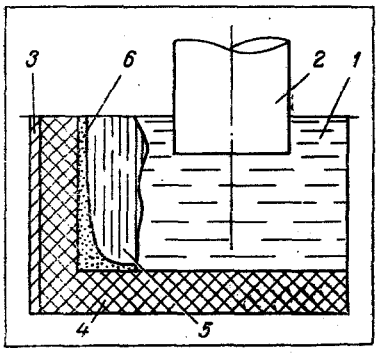

Fig. 1. Schematic diagram of ore bath in a smelting furnace.

The mathematical model of the crust formation process can, in this case, be described by the following system of equations:

$$c_1(x, y, T_1)\rho_1(x, y)\frac{\partial T_1}{\partial \tau} = \frac{\partial}{\partial x}\left(\lambda_1(x, y, T_1)\frac{\partial T_1}{\partial x}\right)$$

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$$+\frac{\partial}{\partial y}\left(\lambda_1(x, y, T_1)\frac{\partial T_1}{\partial y}\right), \quad (x, y)\in\Omega_1, \tag{1}$$

$$c_2(T_2)\rho_2(T_2)\frac{\partial T_2}{\partial \tau}=\frac{\partial}{\partial x}\left(\lambda_2(T_2)\frac{\partial T_2}{\partial x}\right)+\frac{\partial}{\partial y}\left(\lambda_2(T_2)\frac{\partial T_2}{\partial y}\right)$$

$$+c_2(T_2)\rho_2(T_2)\left(v_x\frac{\partial T_2}{\partial x}+v_y\frac{\partial T_2}{\partial y}\right)+f(x, y, \tau), \quad (x, y)\in\Omega_2, \tag{2}$$

$$\tau\in[0, t], \ \Omega=\Omega_1\cup\Omega_2.$$

At the interphase boundary Γ we have $T_1 = T_2$:

$$\lambda_1\frac{\partial T_1}{\partial n}\Big|_\Gamma-\lambda_2\frac{\partial T_2}{\partial n}\Big|_\Gamma=b\rho_2\frac{\partial l}{\partial \tau}. \tag{3}$$

We note that mass transfer and chemical conversions not accounted for in Eq. (2) are rather significant within region Ω_2. Furthermore, the conditions of heat transfer at the boundaries of the reaction zone and the physical phenomena occurring within the reaction zone are not in all ore smelting processes sufficiently understood yet. In view of this, one may regard the propagation of heat through region Ω_2 as a random process and assume that the heat flows in a chaotic pattern. One may then consider all the heat released in the volume underneath electrode 2 during a unit of time to become distributed over the nodes of the computation grid which covers region Ω_2.

A thermal flux element contained in point (x, y) at the time $\tau + \Delta\tau$ is determined by the thermal fluxes in the surrounding points at time τ:

$$u(x, y, \tau+\Delta\tau)=p^{+1}u(x+\Delta x, y, \tau)+p^{-1}u(x-\Delta x, y, \tau)$$

$$+p^{+2}u(x, y+\Delta y, \tau)+p^{-2}u(x, y-\Delta y, \tau), \quad p^{\pm1}+p^{\pm2}=1, \tag{4}$$

where $p^{\pm1}$ and $p^{\pm2}$ are the transient probabilities.

Equation (4) is the difference analog of the Einstein–Kolmogorov differential equation [3]

$$\frac{\partial u}{\partial \tau}=\frac{1}{4}D_x\frac{\partial^2 u}{\partial x^2}+\frac{1}{4}D_y\frac{\partial^2 u}{\partial y^2}-c_x\frac{\partial u}{\partial x}-c_y\frac{\partial u}{\partial y}. \tag{5}$$

The form of Eq. (5) is the same as the equation of heat conduction in a moving stream. Its coefficients D_x and D_y have the dimension of thermal diffusivity (m^2/sec), while c_x and c_y have the dimension of velocity (m/sec).

The physical meaning of Eq. (5) is that it describes the law of heat distribution in region Ω_2, with u being a function of the source density. Since it is necessary to determine the thermal flux transmitted through the side walls, hence the boundary conditions will be written as

$$u(x_l, y_l, t)=1, \quad u(x, y, t)=0. \tag{6}$$

In other words, the model described by Eqs. (1) and (5) replaces now the model described by Eqs. (1) and (2).

Thus, the solution of the problem consists of two stages: in the first stage we consider the heat distribution in the ore bath (region Ω_2) and determine the thermal flux Q_T transmitted across the interphase boundary; in the second stage we solve Eq. (1) and determine the isotherm of the crust.

In order to determine the thermal flux $Q_T=\sum^{N_t} u(x, y, t)$, we replace Eq. (5) by its difference analog. The bath volume underneath the electrode will be subdivided into a uniform grid of dimensions (k + 1)(m + 1). The entire thermal flux Q_0 entering the bath is assumed to distribute over the grid nodes. With the phase-transition boundary regarded as an absorbing shield, we apply the method of a random walk [4] to determine the number of points u(x, y, τ) which reach this shield after t steps and obtain

$$Q_T=Q_0\frac{N_T}{N}=\sum^{N_T}u(x, y, \tau)=(p^{+1}+p^{-1})Q_0. \tag{7}$$

The probability that the thermal flux concentrated at some node (i, j) will reach the phase-transition boundary after t steps is given in Eq. (4), and this equation may be rewritten in a more convenient form

$$u^{s+1}(i, j)=p^{+1}u^s(i+1, j)+p^{-1}u^s(i-1, j)+p^{+2}u^s(i, j+1)+p^{-2}u^s(i, j-1) \tag{8}$$

(s denoting a discrete time interval) with the boundary conditions

$$u(0,\ j) = 1, \quad u(k+1,\ j) = 1,$$
$$u(i,\ 0) = 0, \quad u(i,\ m+1) = 0, \tag{9}$$

where

$$\frac{(\Delta x)^2}{\Delta\tau} = 4D_x, \quad \frac{(\Delta y)^2}{\Delta\tau} = 4D_y, \tag{10}$$

$$p^{\pm 1} = \frac{1}{4} \pm \frac{c_x}{4D_x}\Delta x, \quad p^{\pm 2} = \frac{1}{4} \pm \frac{c_y}{4D_y}\Delta y. \tag{11}$$

Analytic solutions to Eq. (8) with conditions (9) are known only for certain special cases. For this reason, it would be appropriate to solve Eq. (8) by the Monte Carlo method [6].

Having determined the thermal flux passing through the side walls at different power levels M' and M", one can rephrase condition (3) as follows:

$$Q_T' - Q_T'' = b\rho\frac{\partial l}{\partial\tau}, \tag{12}$$

$$\lambda_1 \frac{\partial T_1}{\partial n}\bigg|_\Gamma = 2Q_T' - Q_T''. \tag{13}$$

The transient probabilities in this statistical model are playing the role of similarity criteria. In the physical sense they correspond to the Peclet number. Unlike in physical models, where the similarity criteria are constant, here the transient probabilities will fluctuate from 0 to 1. Their values can be determined when thermal equilibrium in the test furnace ceases to prevail, whereupon c_x and c_y are calculated according to formulas (11). The initial location of the interphase boundary in the test apparatus is also determined then.

The process is now scaled up according to simple rules: when the scale factor is appropriately multiplied, then the grid step changes and the number of steps (process time) necessary for a point to reach the state of heat absorption also changes, but quadratically according to (10).

As has been said earlier, the second stage is solving Eq. (1) with condition (13) stipulated at the interphase boundary Γ. According to the procedure adopted for calculating the crust, Eq. (1) can be solved by the Monte Carlo method, the gist of which is to represent the difference scheme for the differential equation as a Markov chain with a finite number of states. Problems associated with the application of the Monte Carlo method to heat conduction have already been discussed in [7, 8].

Another good reason for using the method of statistical tests is that the values given for the thermophysical properties of materials are, as a rule, widely spread and no simple analytic relation between these properties and the temperature is known. With the use of statistical methods it is convenient to simultaneously simulate the thermophysical properties of the materials involved. We will briefly describe here the method of solving Eq. (1), which has already been described more thoroughly in [9]. Since the heat conducting medium is heterogeneous and the thermal conductivities are functions of the temperature, hence each zone is subdivided into a uniform grid. The values of thermal conductivity between node points are generated according to the rule of random sampling. It is necessary here to specify the range of possible values for each zone.

Having calculated the temperatures at the grid nodes n times, each time anew generating the values of thermal conductivity between nodes, one now determines the mean temperature at node (i, j) according to the formula

$$\overline{T}_{i,j} = \frac{\sum_{r=1}^{n} T_{i,j}^r}{n}, \tag{14}$$

where $T_{i,j}^r$ denotes the temperature at node (i, j) based on the r-th sampling of thermal conductivity values.

The temperature at node (i, j) is calculated according to the formula

$$T_{i,j}^{s+1} = \frac{T_{i+1,j}^s \lambda_{i,j}^{+1} + T_{i-1,j}^s \lambda_{i,j}^{-1} + T_{i,j+1}^s \lambda_{i,j}^{+2} + T_{i,j-1}^s \lambda_{i,j}^{-2}}{\lambda_{i,j}^{+1} + \lambda_{i,j}^{-1} + \lambda_{i,j}^{+2} + \lambda_{i,j}^{-2}}, \tag{15}$$

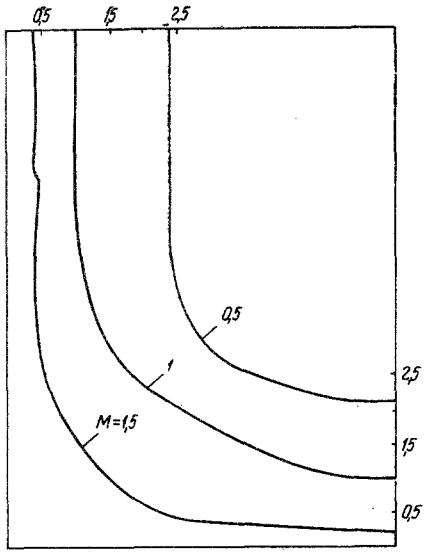

Fig. 2. Crust profile at various power levels.

where $\lambda_{i,j}^{\pm 1}$ denotes the thermal conductivity between nodes (i, j) and (i ± 1, j) while $\lambda_{i,j}^{\pm 2}$ denotes the thermal conductivity between nodes (i, j) and (i, j ± 1).

Formula (15) may be interpreted as representing a random walk among grid nodes, with the peripheral nodes in the state of absorption [9]. The transient probabilities in this case are determined according to the formula

$$p_{i,j}^{\pm m} = \frac{\lambda^{\pm m}}{\sum_{r=1}^{2} (\lambda_{i,j}^{+r} + \lambda_{i,j}^{-r})}. \quad (16)$$

The fact that this is a Markov process ensures its stability [10] and the convergence of the approximate solution to the exact one.

For simulating the crust formation process by the method of statistical tests, one must know the initial location of the interphase boundary in the model and the range of possible values of thermal conductivities. The accuracy of the model depends on the dispersion of temperature values at the grid nodes. For estimating purposes, the maximum dispersion is

$$\sigma_{\max}^2 = \frac{\sum_{q=1}^{n} (T_{i,j}^q - \bar{T}_{i,j})^2}{n-1}. \quad (17)$$

With more samplings n, of course, the accuracy improves proportionally to $\sqrt{n}$.

It serves no useful purpose to sample more than 30 times for engineering problems when an accuracy of 15-20% is required, especially since doing so would lengthen the computer time considerably.

A crust profile within the crystallization zone is shown in Fig. 2, based on this simulation procedure. It has been assumed here that the interphase boundary is also the surface of maximum electric current density, also that as much heat is transmitted by conduction as by convection. All results are given here in relative units.

NOTATION

T_1	is the temperature in the crystallization zone of a melt;
T_2	is the temperature in the reaction zone;
λ	is the thermal conductivity;
ρ	is the density of the melt;
b	is the heat of phase transformation;
l	is the distance from the center of the electrode to the interphase boundary;
Q_T' and Q_T''	are the thermal fluxes transmitted, per unit time, from the bath across the interphase boundary at a power level M' and M'';
N_T	is the number of points reaching the absorption state;
N	is the number of grid nodes.

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