ESTIMATING THE DIFFUSION RATE IN POROUS MEDIA BY MEANS OF A MATHEMATICAL EXPERIMENT

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Within the framework of the nonlinear model of diffusion, a method of determining the effective cementing of porous materials by means of a numerical computer experiment is proposed.

The technology of cementing metalloceramic parts is based on high-temperature diffusional processes. Parts of this kind are made from porous materials and it is notable that the diffusion rate in the latter exceeds the diffusion rate in continuous materials [1]. One explanation of this effect is that the presence of pores filled by gas with a significantly larger diffusion coefficient [2] facilitates the penetration of sorbent not only from the external but also from the "internal" surface of the medium forming the part.

To control the technological process of cementing, it is very useful to estimate the diffusion rate as a function of the degree of porosity of the material.

The mathematical experiment described below solves this problem within the framework of a characteristic mathematical model and leads to the plotting of nomograms which may be used to estimate the diffusion rate in cementing.

1. Since the porous medium is some microstructure, the problem may be considered within the framework of a plane model, representing the pores as rectilinear channels (Fig. 1) and assuming a periodic pore distribution. Since $D_{\text{pore}} \gg D_{\text{cont}}$, it is assumed that the sorbent instantaneously fills the pores, so that the process is described by a two-dimensional diffusion problem.

The rate of heat propagation in the cells considerably exceeds the diffusion rate. Therefore the temperature of the medium reaches a specified constant level in a short time. The law of temperature variation is insignificant here and is taken to be linear. Then, the next problem is to determine the concentration c(x, z, t) of the sorbent in the cell enclosed within the bold line in Fig. 1

$$\begin{gathered}
\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left[D(c)\frac{\partial c}{\partial x}\right] + \frac{\partial}{\partial z}\left[D(c)\frac{\partial c}{\partial z}\right] \equiv \Lambda_x c + \Lambda_z c, \\
0 < t \leqslant \bar{t}, \quad 0 < x < a, \quad 0 < z < l, \\
c(x, z, 0) = c^*, \quad c|_{z=0} = \hat{c}, \quad c|_{x=0} = \hat{c}, \\
\left.\frac{\partial c}{\partial z}\right|_{z=l} = 0, \quad \left.\frac{\partial c}{\partial x}\right|_{x=a} = 0,
\end{gathered} \tag{1}$$

where $\hat{c}$ is the carbon potential of the external medium; c^* is the carbon center before the onset of the cementing process; a and l are the cell boundaries; $\bar{t}$ is the total heating time.

Below, the diffusion coefficient D(c) in the continuous material is taken to be the diffusion coefficient of carbon in γ Fe: $D(c) = (0.04 + c\cdot 0.08)\exp\left(-\frac{31350}{1.987(T+273)}\right)$ cm^3/sec [3], thereby taking account of the significant concentration and temperature dependence of D for the cementing process.

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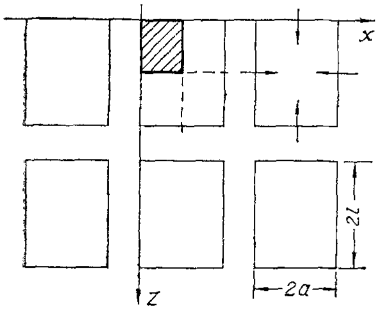

Fig. 1

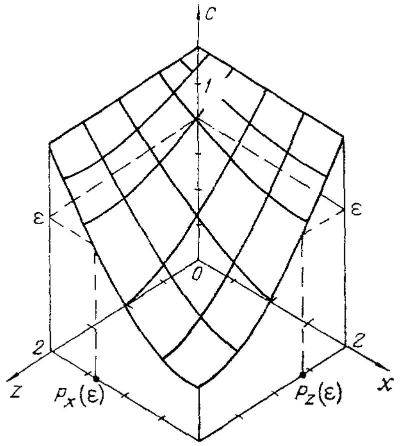

Fig. 2

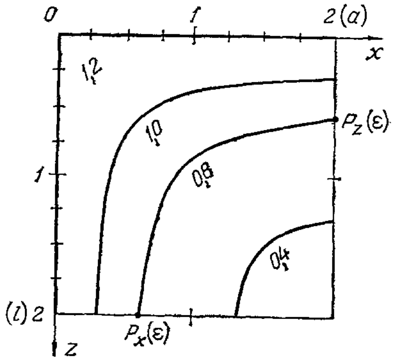

Fig. 3

Fig. 1. Two-dimensional periodic model of cell and pore distribution.

Fig. 2. Concentration field ($t = 7.4$ h; $a = l = 2$ mm); c, %.

Fig. 3. Lines of the concentration-field levels (the figures on the curves give values of the concentration $c = \varepsilon$; $t = 7.4$ h).

The problem in Eq. (1) is nonlinear, and it is solved in the grid $\{x_i, z_k\}$ using an iterative process within the framework of a longitudinal–transverse difference scheme [4] (implicit variable-direction method).

Correspondingly, at each moment of time, from the specified sequence $\{t_j\}$, the grid function c_{ik}^{j+1} approximating solution of the problem in Eq. (1) is determined by the equations

$$\frac{c^{j+1/2} - c^j}{0.5\tau} = \Lambda_x c^{j+1/2} + \Lambda_z c^j,$$
$$\frac{c^{j+1} - c^{j+1/2}}{0.5\tau} = \Lambda_z c^{j+1} + \Lambda_x c^{j+1/2}, \tag{2}$$

where transition form time layer t_j to t_{j+1} ($j = 0, 1, 2, \ldots, M$, $t_0 = 0$, $t_M = \bar{t}$) is accomplished in two stages with a step of 0.5τ (for the sake of brevity, the subscripts i, k on c_{ik} are omitted).

The fitting method is used to solve them for each iteration s [5].

Computer calculations allow an idea of the dynamics of the process to be obtained as a function of the cell dimensions of the structure. In particular, the carbon concentration field at time $t = 7.4$ h is shown in Fig. 2 in an isometric projection for the parameters: $a = l = 2$ mm; $c^* = 0.2\%$; $\hat{c} = 1.2\%$; $\bar{t} = 10$ h; T varies linearly from 20 to 920°C at $t \leqslant 24$ min and $T = 920$°C at $t > 24$ min. The parameters c^*, $\hat{c}$, $\bar{t}$, and T are common to all the illustrations below. Note that the diffusion coefficient may also be considered as a functional parameter of the problem, since an autonomous procedure is calculated in its solution.

2. A nomographic description of the result similar to that in [6, 7] is very useful in estimating the cementing effect with the aim of controlling this process. For the periodic structure assumed, the pore density is evidently characterized by the linear cell dimension along the x axis (Fig. 1).

The characteristic adopted for the effect is the layer thickness (measuring from the surface $z = 0$) h^* saturated by sorbent of concentration no less than a specified value ε, %.

Using a computer, the analysis of the results accumulated in calculating the function $c(x, z, t)$ may be organized according to the following scheme.

A. The intersection of the plane of specified carbon concentration $c = \varepsilon$ with the concentration surface $c(x, z, t_{fix})$ on the plane (x, z) is estimated: for example, in Fig. 2, these are the points $P_x(\varepsilon)$ and $P_z(\varepsilon)$. The set of such points $\{P_x(\varepsilon)\}$ and $\{P_z(\varepsilon)\}$ for each value of ε is shown by a nomogram in Fig. 3. This reduces to

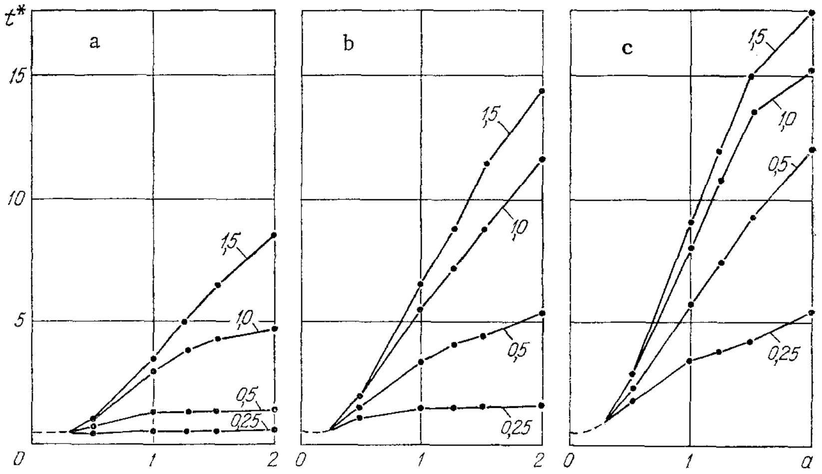

Fig. 4. Nomograms of the heating time t*, h, to the specified carbon concentration ε at a fixed depth when *l* = 2 mm (the figures on the curves are values of h*); ε = 0.4% (a), 0.8 (b), 1.0 (c).

numerical solution of the equation c(x, z, t) = ε on a computer, with specified t_{fix}. As a result of subsequent interpolation, the curves of z = $f_{tfix}(x)$ in Fig. 3 are obtained.

B. From the curve of the concentration c(*a*, h*, t) as a function of the time at several fixed depths h* when x = *a*, the time t* corresponding to a specified concentration ε is sought. To this end, the equation c(*a*, z, t) is solved numerically on a computer at fixed z = h*, and subsequent interpolation leads to curves of $t=\varphi_{h^*}(a)$, the nomograms of the cementing process in Fig. 4.

On the figures corresponding to different ε, curves of the cementing time as a function of the cell dimensions are shown; each curve corresponds to a definite depth h* of interest for technology. The common point on the nomogram curves corresponds to the onset of the constant temperature 920°C after a time t = 24 min.

Note that the cementing rate actually increases with increase in pore density which confirms the initial hypothesis regarding the influence of porosity. It is evident in particular (Fig. 4b) that the concentration of 0.8% carbon at a depth of 0.25 mm with a cell "dimensions" *l* = 2 mm, *a* = 1 mm (Fig. 1) may be reached after 1.6 h.

The results obtained may facilitate the solution of the problem of energy economy in the corresponding technological process.

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