METHOD OF CALCULATING FROM EXPERIMENTAL DATA THE PARAMETERS IN BOUNDARY CONDITIONS OF THE THIRD KIND FOR THE DIFFUSIONAL SATURATION OF STEELS

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A method is proposed for the calculation, from experimental data, of parameters characterizing the mass transfer in the diffusional saturation of metals in conditions where the experimental time is limited.

The calculation of the kinetics of diffusional carburization of steel reduces to the solution of the diffusion equation for carbon

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D(c) \frac{\partial c}{\partial x} \right) \tag{1}$$

with the initial condition

$$c|_{t=0} = c^{i}(x), \tag{2}$$

where $c^i(x)$ is the initial distribution of carbon in the steel, the boundary condition

$$\left.\frac{\partial c}{\partial x}\right|_{x\to\infty} \to 0 \tag{3}$$

and the boundary condition at the surface being saturated, where x = 0. Here D(c) is the diffusion coefficient of carbon, which is a function of its concentration. In view of the complexity of the physicochemical processes occurring in the carburization of steel at the surface of the component (the formation of active atoms in the saturating medium, their transport to the surface being saturated and adsorption there, etc.), the carbon flux density through the surface of the component is usually specified by boundary conditions of the third kind [1]

$$-D\left.\frac{\partial c}{\partial x}\right|_{x=0} = V(c^0 - c|_{x=0}). \tag{4}$$

Here V is the mass-transfer coefficient; c^0 is the carbon concentration which would be established at the surface when $V \to \infty$. If diffusional saturation is not accompanied by phase transformations, the surface concentration of carbon $c|_{x=0}$ tends to c^0 with increase in the time of holding ($t \to \infty$). As a rule, equilibrium is established at the saturating medium—steel boundary when the concentration c^0 is reached. This suggests the possibility of calculating c^0 by equating the chemical potentials of carbon in the saturating medium and in steel or of finding it experimentally, for example, by saturating a thin film, etc. A number of methods have been developed for the experimental determination of the mass-transfer coefficients for a known value of c^0: from the saturation kinetics for a thin film, using the tangent method developed in heat engineering, from the time dependence of the surface concentration, etc. (see [2], for example).

In many cases the diffusional mass transfer of carbon in steel is accompanied by phase transitions. For example, the decarburization of steels may lead to the formation of alpha phase in the structure, and carburization to the formation and growth of carbide phase. In this case, the situation is different from that described above. For the first stage of the diffusion process, when the diffusion of carbon occurs in solid solution, the value of c^0 cannot be found independently of the mass-transfer coefficient. It is necessary to determine c^0 and V simultaneously in conditions of limited experimental time, so as to avoid the appearance of new phase in the diffusion region.

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In such cases, these parameters may be chosen by comparing the calculated and experimental distributions of the carbon concentration in the diffusional region for different c^0 and V.

The diffusion coefficient of carbon depends significantly on its concentration, and Eq. (1) is nonlinear. For example, in [3] it was established that neglecting the concentration dependence of the diffusion coefficient leads to considerable error in calculations of the carburization of ShKh15-steel rod in the time of heating. In [4] it was shown, by comparing a numerical calculation of the carbon distribution in ShKh15 steel after decarburization and restorative carburization at 1150°C with the corresponding analytic solution of the linear problem [5], that the linear approximation may only be used if a special value of the diffusion coefficient of carbon is chosen for each stage of the process. All this indicates that it is necessary to solve nonlinear diffusion problems in calculating real technological processes.

Before proceeding to an investigation of the present method of choosing the parameters c^0 and V for the nonlinear case, it will be analyzed for the case of constant diffusion coefficient, when it is possible to find an analytic solution of the diffusion problem.

First, consider the preliminary problem of establishing how much the accuracy with which the initial concentration distribution $c^i(x)$ and the surface concentration $c^s(t)$ are determined affects the results of calculating the concentration distribution for a diffusion equation with a boundary condition of the first kind

$$c\,|_{x=0} = c^s(t). \tag{5}$$

The solution of this well-known problem is written as follows

$$c(x,\ t) = \int\limits_0^\infty c^i(\xi)\,G(x,\ \xi,\ t)\,d\xi + \int\limits_0^t c^s(t-\xi)\,\frac{x\exp\left(-\dfrac{x^2}{4D\xi}\right)}{\sqrt{4\pi D\xi^3}}\,d\xi, \tag{6}$$

where

$$G(x,\ \xi,\ t) = (4\pi Dt)^{-\frac{1}{2}}\left[\exp\left(-\frac{(x-\xi)^2}{4Dt}\right) - \exp\left(-\frac{(x+\xi)^2}{4Dt}\right)\right].$$

The difference between the two solutions $c(x, t)$ and $\hat{c}(x, t)$ may be determined from the difference between their initial $c^i(x)$ and $\hat{c}^i(x)$ and boundary $c^s(t)$ and $\hat{c}^s(t)$ conditions. Writing $c(x, t)$ and $\hat{c}(x, t)$ in the form in Eq. (6) yields

$$|c(x,\ t) - \hat{c}(x,\ t)| \leqslant \sup|c^i(x) - \hat{c}^i(x)| + \sup|c^s(t) - \hat{c}^s(t)|\ \operatorname{erfc}\left(\frac{x}{2\sqrt{Dt}}\right). \tag{7}$$

In many cases of practical importance, the chemicothermal treatment proceeds in stages (e.g., the decarburizing and restorative carburizing of mechanical-engineering steels): At a temperature T_1 for a time t_1, and then at a temperature T_2 for a time t_2. Using Eqs. (6) and (7) for the concentration distribution of carbon after the first stage of diffusion ($t \leq t_1$), the following inequality is obtained for the second stage

$$\begin{aligned} |c(x,\ t) - \hat{c}(x,\ t)| \leqslant \sup|c^i(x) - \hat{c}^i(x)| + \sup|c_2^s(t) -{} \\ - \hat{c}_2^s(t)|\ \operatorname{erfc}\left(\frac{x}{2\sqrt{D^{(2)}t}}\right) + \sup|c_1^s(t) - \hat{c}_1^s(t)|\,\psi\left(\frac{x}{2\sqrt{D^{(1)}t_1}},\ \sqrt{\frac{D^{(1)}t_1}{D^{(2)}t_2}}\right). \end{aligned} \tag{8}$$

Here the superscript α ($\alpha = 1, 2$) denotes that the diffusion coefficient is taken at the temperature T_α; $c_1^S(t)$ and $c_2^S(t)$ are the surface concentrations for the first and second stages. The function

$$\psi(z,\ \gamma) = \frac{2}{\pi}\int\limits_0^\infty d\xi \int\limits_{\gamma(z-\xi)}^{\gamma(z+\xi)} \exp(-\xi^2 - \eta^2)\,d\eta$$

decreases monotonically with increase in z for fixed γ and

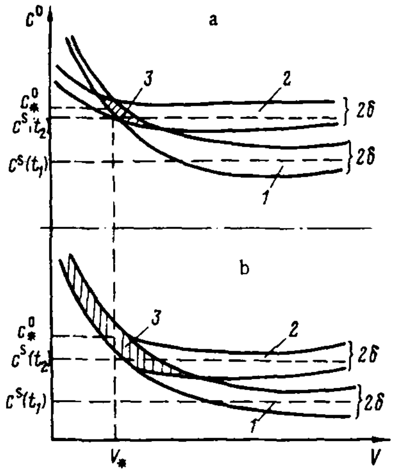

Fig. 1. Region of values of c^0 and V found from Eq. (9) for the first (1) and second (2) measurements of the surface concentration, and for both (3), with an error $\pm\delta$: a) $[c^s(t_2) - c^\infty + \delta]/\sqrt{t_2} < [c^s(t_1) - c^\infty - \delta]/\sqrt{t_1}$; b) $[c^s(t_2) - c^\infty]/\sqrt{t_2} \approx [c^s(t_1) - c^\infty]/\sqrt{t_1}$.

$$\psi(z,\ \gamma) < \psi(0,\ \gamma) = \frac{2}{\pi}\ \mathrm{arctg}\,\gamma.$$

In fact, Eqs. (7) and (8) illustrate the well-known general fundamental result that parabolic equations (both linear equations with variable coefficients and nonlinear equations) are stable with respect to perturbations of the initial and boundary conditions (see [6, 7], for example). Unfortunately, there is a lack of estimates of the minimum values of $\sup|c^s(t) - \hat{c}^i(x)|$ and $\sup|c^s(t) - \hat{c}^s(t)|$ permissible in Eqs. (7) and (8) for the given class of functions appearing in the equations, not only for nonlinear equations but also for linear parabolic equations with variable coefficients. It follows from Eqs. (7) and (8) that, if the calculated concentration distribution of an element in the diffusion region is to be close to the experimental distribution, it is necessary to choose a surface concentration $c^s(t)$ and an initial distribution $c^i(x)$ that are close to the corresponding experimental results. This is also true of nonisothermal diffusional saturation.

Thus, the present method of determining the unknown parameters in the boundary condition in Eq. (4) at the surface being saturated involves, first of all, choosing these coefficients from a comparison of the numerically calculated time dependence of the surface concentration with the experimental function $c^s(t)$. This allows the bulk of experiments required to be considerably reduced. It is important to stress that this method may also be used to find the parameters in a nonlinear boundary condition at the surface being saturated. Because of the difficulty of determining the minimum value of the coefficients permissible in Eqs. (7) and (8), it is impossible to rule out the possibility that additional comparison of the calculated concentration distribution in the diffusion region with that found experimentally would improve the estimate of these parameters made solely on the basis of the measured surface concentrations. Therefore, after choosing the parameters in the boundary condition from the experimental surface concentration, it is necessary, if such a possibility exists, to compare the calculated concentration distribution over the whole of the diffusion region with the corresponding experimental data. In the case of a constant diffusion coefficient, this comparison cannot be made; see Eqs. (7) and (8). This result is a consequence of a special form of the maximum principle, which is valid for a broad class of parabolic equations [6, 7].

The next step is to determine the uniqueness of the values of the unknowns c^0 and V determined from the experimental surface concentrations in conditions where the experimental time is limited.

The solution of the diffusion problem in Eqs. (1)-(4) for a constant diffusion coefficient leads to the following expression for the surface concentration

$$c^s(t) \equiv c|_{x=0} = \varphi\left(V\sqrt{\frac{t}{D}}\right)c^0 + \int\limits_0^\infty R(\xi,\ t)\,c^i(\xi)\,d\xi, \tag{9'}$$

where

$$\varphi(z) = 1 - \exp(z^2)\,\mathrm{erfc}(z);\quad R = \frac{\exp\left(\frac{-\xi^2}{4Dt}\right)}{\sqrt{\pi D t}}$$

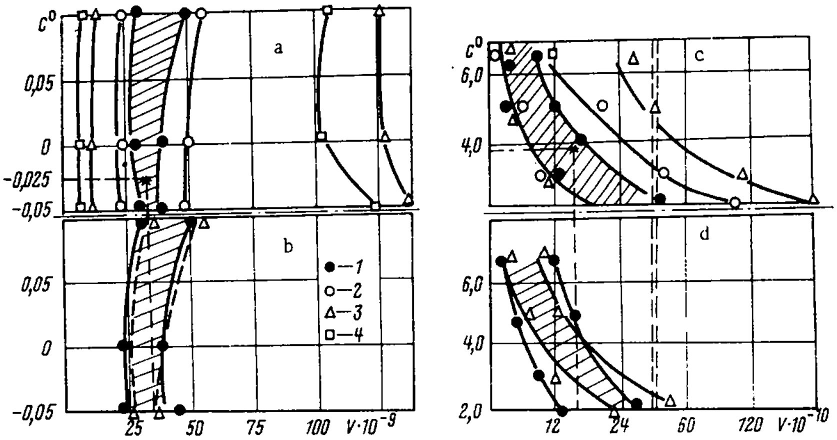

Fig. 2. Region of permissible values of c^0 (mass %) and V (m/sec) for the decarburization (a, b) and restorative carburization (c, d) of ShKh15 steel at 900°C for 1 (a) and 5 (c) h at different distances from the external surface of the sample: 1) at the surface; 2) 100 μ; 3) 200 μ; 4) 300 μ; and for the surface of the sample at different times: 1) 1 h (b, d); 3) 2 h (b), 5 h (d). The shading denotes the common region for several measurements.

$$-\frac{V}{D}\exp\left(\frac{\xi V}{D}+\frac{V^2 t}{D}\right)\operatorname{erfc}\left(\frac{\xi}{\sqrt{4Dt}}+V\sqrt{\frac{t}{D}}\right).$$

If the concentration distribution is initially uniform, this expression is simplified

$$c^s(t)=c^\infty+(c^0-c^\infty)\varphi\left(V\sqrt{\frac{t}{D}}\right). \tag{9''}$$

This result involves the use of the relation

$$\int_0^\infty R(\xi,\ t)\,d\xi=1-\varphi\left(V\sqrt{\frac{t}{D}}\right).$$

Using Eq. (9), it is not possible to determine the mass-transfer coefficient V and the concentration c^0 simultaneously from a single measurement of the surface concentration; it is only possible to find the region of possible values of c^0 and V satisfying Eq. (9) within the limits of experimental accuracy in measuring $c^s(t)$. If diffusional saturation is not accompanied by phase transitions, c^0 may be determined independently of the mass-transfer coefficient, and Eq. (9) can then be used to find V.

Consider the case when the surface concentration of the elements is measured at several different times. Using the asymptotic formula for erfc(z), the following result is obtained

$$c^s\approx 2V\sqrt{\frac{t}{\pi D}}\left[c^0-\sqrt{\pi}\int_0^\infty c^i(\sqrt{4Dtu})\operatorname{erfc}(u)\,du\right]$$

$$+\frac{2}{\sqrt{\pi}}\int_0^\infty c^i(\sqrt{4Dtu})\exp(-u^2)\,du \quad \text{when} \quad V\sqrt{\frac{t}{D}}\ll 1,$$

$$c^s\approx c^0-\frac{1}{V}\sqrt{\frac{D}{\pi t}}\left[c^0-\int_0^\infty c^i(\sqrt{4Dtu})\exp(-u)\,du\right] \text{when } V\sqrt{\frac{t}{D}}\gg 1.$$

If the concentration dependence is initially uniform, then

$$c^s \approx c^\infty + 2V\sqrt{\frac{t}{\pi D}}\,(c^0 - c^\infty) \quad \text{when} \quad V\sqrt{\frac{t}{D}} \ll 1,$$

$$c^s \approx c^\infty - \frac{1}{V}\sqrt{\frac{D}{\pi t}}\,(c^0 - c^\infty) \quad \text{when} \quad V\sqrt{\frac{t}{D}} \gg 1.$$

Since the asymptotic expansions for $V \le \sqrt{D/t}$ and $V \ge \sqrt{D/t}$ are different, the region of possible values of c^0 and V satisfying Eq. (9) is reduced as the number of surface-concentration measurements increases. This may be illustrated in more detail for the case when the initial concentration distribution is uniform. The surface concentration varies over time in accordance with Eq. (9) with some parameters c_*^0 and V_* in the boundary conditions; these values are found from two measurements of the surface concentration at times t_1 and t_2 ($t_2 > t_1$). The concentrations are found with an error of ±δ. From Eq. (9"), the region of possible values of c^0 and V for the first and second measurements is found

$$\frac{c^s(t_1) - c^\infty - \delta}{\varphi\left(V\sqrt{\frac{t_1}{D}}\right)} \leqslant c^0 - c^\infty \leqslant \frac{c^s(t_1) - c^\infty + \delta}{\varphi\left(V\sqrt{\frac{t_1}{D}}\right)}, \qquad (10')$$

$$\frac{c^s(t_2) - c^\infty - \delta}{\varphi\left(V\sqrt{\frac{t_2}{D}}\right)} \leqslant c^0 - c^\infty \leqslant \frac{c^s(t_2) - c^\infty + \delta}{\varphi\left(V\sqrt{\frac{t_2}{D}}\right)}. \qquad (10")$$

If $c^S(t_2) - \delta > c^S(t_1) + \delta$, then as $V \to \infty$ the region in Eq. (10) lies below that in Eq. (10"). Consider the positions of these regions as $V \to 0$. Replacing the functions $\varphi(V\sqrt{t_1/D})$ and $\varphi(V\sqrt{t_2/D})$ by the first terms of their asymptotic expansions as $V \to 0$, it is found that the relative positions of the regions in Eqs. (10') and (10") depend on the relation between the quantities

$$\frac{c^s(t_1) - c^\infty}{\sqrt{t_1/D}} = (c_*^0 - c^\infty)\,V_*\,\frac{\varphi(V_*\sqrt{t_1/D})}{V_*\sqrt{t_1/D}},$$

$$\frac{c^s(t_2) - c^\infty}{\sqrt{t_2/D}} = (c_*^0 - c^\infty)\,V_*\,\frac{\varphi(V_*\sqrt{t_2/D})}{V_*\sqrt{t_2/D}}.$$

From the integral expression

$$\frac{\varphi(z)}{z} = \frac{2}{\sqrt{\pi}}\left(1 - \int_0^\infty \frac{\exp(-u)}{\sqrt{\frac{u}{z^2}} + \sqrt{(1+u)/z^2}}\,du\right)$$

it is evident that the function $\varphi(z)/z$ is monotonically decreasing, and therefore

$$\frac{c^s(t_2) - c^\infty}{\sqrt{t_2/D}} < \frac{c^s(t_1) - c^\infty}{\sqrt{t_1/D}}.$$

Thus for,

$$\frac{c^s(t_2) - c^\infty + \delta}{\sqrt{t_2/D}} < \frac{c^s(t_1) - c^\infty - \delta}{\sqrt{t_1/D}}$$

the region in Eq. (10') lies above that in Eq. (10") as $V \to 0$. This case is shown in Fig. 1a. If both the measurements of the surface concentration are made for t_1, $t_2 \ll D/V^2$, then

$$\frac{c^s(t_2) - c^\infty}{\sqrt{t_2/D}} \approx \frac{1}{\sqrt{\pi}}\,(c_*^0 - c^\infty)\,V_* \approx \frac{c^s(t_1) - c^\infty}{\sqrt{t_1/D}}$$

and the regions in Eqs. (10') and (10") practically overlap as $V \to 0$ (Fig. 1b).

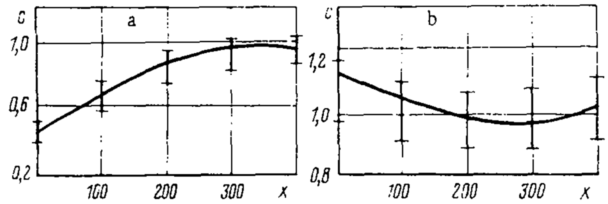

Fig. 3. Comparison of the distribution of the carbon concentration (in mass %) over the layer thickness after decarburization (a) and restorative carburization (b) of ShKh15 steel at 900°C with the parameters c^0 and V marked by an asterisk (*) in Fig. 2a for decarburization and in Fig. 2c for carburization: the vertical lines show the error of the experimental determination of the carbon concentration; the continuous lines show the results of computer calculation.

For a nonlinear diffusion equation, the region of possible values of V and c^0 is constructed by comparing computer-calculated surface concentrations with experimental values of $c^S(t_i)$; $i = 1$—N, where N is the number of measurements.

The present method has been used to determine the parameters V and c^0 characterizing the mass transfer at the external surface of ShKh15 steel for decarburization and restorative carburization at 900°C. Prolonged decarburization of this steel leads to the appearance of alpha phase at the surface, and prolonged carburization to the growth of carbide phase. Therefore, the diffusion of carbon in a single-phase system (at sufficiently high temperatures only a gamma region exists) occurs in a limited time.

The region of possible values of c^0 and V was calculated from the measured carbon distribution over the layer thickness after decarburization. Computer calculations were carried out for eight values of c^0 and for ten values of V for each fixed c^0. The computer program was described in [8]. The region of possible values of c^0 and V chosen for 1 h and different distances from the surface is shown in Fig. 2a. In fact, as is evident from Fig. 2a, to describe the carbon distribution over the layer thickness it is sufficient to find the parameters c^0 and V at which the calculated and experimental values of the carbon concentration at the surface are the same. Increase in the decarburization time from 1 to 2 h does not lead to any significant improvement in the values of c^C and V (see, for comparison, Fig. 1b).

Analogous investigations were made for a two-stage process: decarburization for 1 h and subsequent restorative carburization (Fig. 2c, d). The values of c^0 and V marked by an asterisk (*) in Fig. 2a were chosen for the calculations of the carbon distribution after decarburization. It is evident from Fig. 2c that for the description of restorative decarburization it is again sufficient to measure only the surface concentration of carbon. Increase in the time of carburization from 1 to 5 h also leads to no significant improvement in the values of the mass-transfer parameters (Fig. 2d).

A comparison (Fig. 3a, b) of the calculated carbon distributions after decarburization and carburization with the parameters c^0 and V marked by an asterisk in Fig. 2a, c in the region of permissible values with the corresponding experimental data shows the possibility of using the present method for practical purposes.

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FILTRATION OF A COMPRESSIBLE GAS IN AN APPARATUS WITH A DIAPHRAGM

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Results of an experimental investigation of the filtration of a compressible gas in an axisymmetric apparatus with a diaphragm mounted in the layer of charge or at the exit from the apparatus are presented. A dependence is given to compute the resistance of the apparatus—charge system.

Technological processes realized in an apparatus with fluid or gas filtration through a charge of finely dispersed or bulk materials are extensively used in different industrial branches. The correct organization of these processes depends greatly on knowledge of the aerodynamic fluid motion conditions in such an apparatus.

The authors of [1, 3, 4, 7, 11] investigated the condition of the influence of the side walls on the hydraulic drag of the charge in a uniform flow field of the filtering fluid when examining the charge and the apparatus in combination. In addition to the conditions described above, different nonuniformities at the entrance to and exit from the charge are produced most often in real technological apparatus. A number of papers [2, 5, 6, 9, 10] are devoted to a study of such technological apparatus.

Mathematical models of a low-speed filtration flow in an apparatus are considered in [2, 9]. The resistance of an apparatus with precompression, i.e., when the gas is supplied to or removed from the charge through a hole smaller than the cross section of the apparatus, is experimentally studied on rectangular models in [5, 6, 10].

A number of physical statements of the picture of filtration with precompression directly in a cylindrical apparatus are refined in the present study, and a dependence between the hydraulic drag coefficient and the parameters of the gas stream, the charge, and the apparatus is set up. In comparison to [5], the variation range of the precompression parameter and of the working pressure in the apparatus is hence extended to quantities used in an industrial apparatus of the feeder type in pneumatic transport systems.

The gas flow picture in an apparatus with a charge can be estimated by means of the pressure distribution. The most characteristic pattern permitting an assessment of the filtration flow in an axisymmetric apparatus is the pressure diagram along the apparatus axis. Such diagrams were recorded on a unit (Fig. 1) consisting of interchangeable steel sections with the following diameters: D = 300, 100, 46 mm. Diaphragms with a center hole were used to assure different precompression values. They were mounted both within the charge layer and at the exit from the apparatus. The charge was formed from spherical polystyrene particles. The mean suspended particle diameter d was determined for each fraction obtained between two sieves. The porosity was determined by means of the true and the bulk density of the material [1]. The geometric characteristics of the fractions used in the research are presented in Table 1. The charge was held in the apparatus by a metal mesh with a porosity greater than the layer being studied. Air was used as the filtering agent. The gas pressure at the apparatus axis was measured by means of thin tubes passing through the side wall. U-shaped and pointer manometers were used as recording devices.

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