

DISCUSSION OF A PARTICULAR MATHEMATICAL MODEL FOR CONTROLLING STEEL CARBURIZATION

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We formulate an inverse problem of controlling the carburization of steel parts in a gas furnace, when on termination of the process the partial pressures of gases in the atmosphere are determined by the prescribed characteristics of the distribution of carbon in the surface layer of the metal. Stable and economic algorithms are suggested for solving the problem.

The process of saturation of the surface layer of steel parts with carbon in gas furnaces is described by a nonlinear diffusion equation, which because of the smallness of the hardened layer thickness can be referred to a half-space: $0 < x < +\infty$ [1]. This process is preceded by the establishment of an equilibrium state of the gases forming the atmosphere, as a result of which a certain carbon potential of the atmosphere is produced, namely, the concentration of atomic carbon C in wt.% absorbed by the metal surface. In work [2], which was devoted to the problem of automating the process of carburization of carbon steels, the carbon potential was considered as a governing parameter that, along with the process duration t , provided *a priori* values of concentration at a given depth: $u = \{u_i(x_i, t)\}$, $i = 1, 2$. As means of such automation special nomograms were suggested that made it possible to assign in advance the optimum regime of carburization $q = \{C, t\}$ for specimens with different initial contents of carbon c_0 at different temperatures T of the furnace.

However, the value of C cannot be controlled directly. Therefore, in the present work as a governing parameter we take the set of partial pressures p of the gases forming the atmosphere. In this case the problem is divided into two problems: a) $u \rightarrow q$ and b) $q \rightarrow p$, so that the quantity C plays the part of an intermediate parameter. We propose a correct (in the sense of [3]) statement of these problems pertaining to the class of inverse problems [4].

Another feature that distinguishes the present work from previous ones is that instead of the nomograms, which inevitably limit the range of parameters, we suggest a universal economic algorithm based on asymptotic ($t \rightarrow \infty$) representations of the solution of a non-linear diffusion problem. Such an approach is justified by the long duration of carburization; it leads to determination of the desired pair of q from a closed system of nonlinear equations with two unknowns.

Finally, this algorithm is realized in a C computer program that accounts also for the alloying effect, with the corresponding parameter ϵ being determined automatically by the prescribed technological code.

1. The physical parameters of the carburization process are the diffusion coefficient D and the coefficient of mass exchange with the carbon-containing atmosphere β , expressed by the formulas: $\beta = \kappa_0 \exp(-b/T)$, $D = D(u) = D_0 k(u)$, where $k(u) = 1 + k_0 u$, and $D_0 = \kappa_1 \exp(-a/T + \epsilon)$. Here T, K , is the temperature; $k_0, \kappa_0, \kappa_1, a$, and b are numerical parameters that are independent of both the temperature and the type of the steel; ϵ is the alloying parameter, which is described by the formula $\epsilon = \ln 10 \cdot \sum_{i=1}^n (k_i'/T + k_i'') u_i$, where n is the number of impurities from the series $R \equiv \{Ni, Si, Cr, Mo, V, \text{etc.}\}$, u_i are the corresponding concentrations, k_i' and k_i'' are known constants for each impurity. The latter fact allows one to calculate in advance the value of ϵ by the prescribed technological code for the type of steel (for example, 15Kh, 18KhGT, etc.), while the C computer language makes

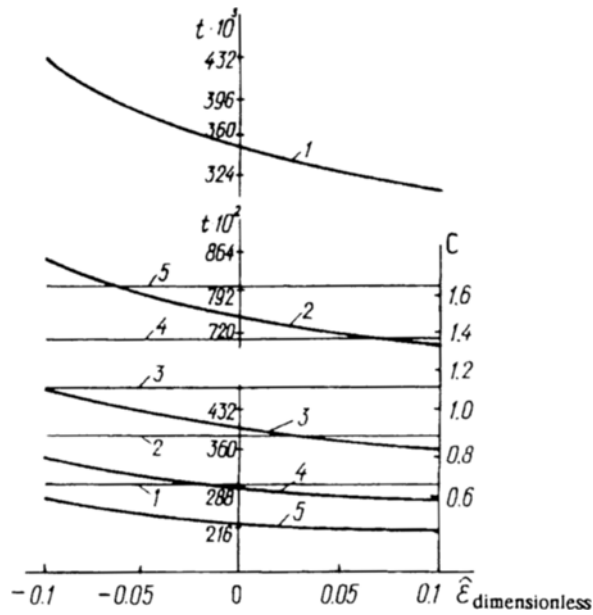


Fig. 1. Characteristic dependences of the optimum values of control parameters t (sec) and C (%) on the alloying parameter at different values of the surface concentration of carbon ($T = 1203$ K; $u_2 = 0.5\%$; $x = 0.001$ m): 1) $u_1 = 0.6\%$, 2) 0.8 , 3) 1 , 4) 1.2 , 5) 1.4 .

easy calculations for an arbitrary value of T by selection from a pair of tables. We realized this possibility in a special subroutine preceding the procedures described below.

In [5] it was shown that the concentration field for the geometrical model (adopted by us) of carbon diffusion into a metal is asymptotically equal to

$$u(x, t) = y_0(\xi) + (1/2\eta) k(C) y_0'(\xi) + O(1/\eta^2). \quad (1)$$

Here $\xi = x/(2\sqrt{D_0 t})$, $\eta = 2\beta\sqrt{t/D_0}$, C enters into Eq. (1) by virtue of the mass exchange condition $D(u)(\partial u/\partial x|_{x=0}) = \beta(C - u|_{x=0})$, and the function $y_0(\xi)$ is determined by the conditions

$$(k(y_0) y_0')' + 2\xi y_0' = 0, \quad y_0(0) = C, \quad y_0(+\infty) = c_0, \quad (2)$$

where c_0 is the initial content of carbon in the metal.

Now we use Eqs. (1) and (2) as a basis for formulating the first of the inverse problems for the control of carburization, the initial data for which, i.e., the objective of control, are the preassigned values of the concentration u_1 on the surface ($x_1 = 0$) and at a certain depth $u_2 = u(x_2, t)$ on termination of the process.

Then, after neglecting terms of the order of $1/\eta^2$, Eq. (1) leads to a system of two nonlinear equations for the pair of unknowns $q = \{C, t\}$, where t is the process duration.

Eliminating $\eta = \eta(q)$, we obtain an expression for $t = t(C)$, $t = D_0(k(C)y_0'(0)/2\beta(u_1 - C))^2$, that is defined, and in the only possible way, in the region of $C > u_1$. On the other hand, for C in the same region of definition we obtain a nonlinear equation with the left side prescribed algorithmically: $f(C) \equiv (y_0(\xi_2) - u_2)y_0'(0) + (u_1 - C)y_0'(\xi_2) = 0$, where $\xi_2 = \xi_2(C) \equiv \beta(x_2(u_1 - C)/D_0 k(C)y_0'(0))$.

An algorithm for solving the latter equation contains two essential elements: a) the quantity $y_0'(0)$ is determined at each C from condition (2) using a ballistic method by analogy with [6]; b) since $y_0'(0)$ is determined algorithmically, while $y_0(\xi_2)$ and $y_0'(\xi_2)$ can be found, for example, by the Runge-Kutta method from Eq. (2) at the prescribed values of $y_0(0)$ and $y_0'(0)$ on arrival at the point ξ_2 , then the function $f(C)$ is determined algorithmically and the root of the equation $f(C) = 0$ can be found by the fork method with preliminary (until a change of sign is detected) sounding of the semiaxis $C > u_1$.

Thus, parametrization of the problem, that is, replacement of the carburization profile by two reference points, leads to a mathematically correct [3] statement of this inverse problem.

Figure 1 gives some results of an automated calculation of the governing parameters q as functions of the alloying parameter in the range $|\epsilon| < 0.1$ typical for the considered set of types of steel. Also given in this figure are the values of the objective parameters u to which the above results refer.

2. The second problem of control involves the obtaining of information about the equilibrium partial pressures of the atmosphere components corresponding to the prescribed carbon potential C . Such an inverse problem has not been studied in the technological literature, but the initial premises used by us for calculating the quantity C from the prescribed state of the atmosphere are found, for example, in [1].

The atmosphere will be considered as a closed constant-volume medium filled with the gases H_2 , H_2O , CH_4 , CO , CO_2 , and O_2 , to which the partial pressures p_i ($i = 1, \dots, 6$) correspond. According to [1], in the equilibrium state these quantities are connected by three independent relations:

$$p_4 = K_1 p_2 p_3 / p_1^3, \quad p_5 = (K_1^2 / K_2) p_2^2 p_3 / p_1^4, \quad p_6 = (K_1^2 / K_3) p_2^2 / p_1^2, \quad (3)$$

where $K_j = K_j(T)$, $j = 1, 2, 3$ are the equilibrium constants. In turn, the quantity $\eta = 4.65 \cdot 10^{-2} C$, i.e., the equilibrium concentration of carbon in atomic fractions, at small concentrations ($\eta < 0.2$) is determined from the equation

$$\psi(\eta) = \ln(\eta / (a_C (1 - 5\eta))) + b_0 + b_1/T + (b_2 \eta / (1 - \eta)) / T + \epsilon = 0, \quad (4)$$

where b_0 , b_1 , and b_2 are known constants [1], a_C is the activity of atomic carbon in its interaction with a metal. This activity can be determined, for example, on the basis of the reaction $2CO \rightleftharpoons C + CO_2$, and if $K^* = K^*(T)$ is the corresponding equilibrium constant [1], then

$$a_C = K^* p_4^2 / p_5 \equiv K^* K_2 p_3 / p_1^2. \quad (5)$$

Thus, in order to calculate the carbon potential for the indicated composition of the atmosphere, it is sufficient to know two independent partial pressures: p_1 and p_3 . We note that if, in addition to these pressures, the vapor pressure p_2 is also given, we can determine the full set of partial pressures in the equilibrium state.

Now we turn our attention to the inverse problem of interest for us. It is evident that at a prescribed C , i.e., η , the equation $\psi(\eta) = 0$ determines a_C unambiguously. But then Eq. (5) determines a set of equilibrium states for which

$$p_3 = q p_1^2, \quad (6)$$

where $q = a_C / K^* K_2$. In this case, as we can see according to Eqs. (3) and (5),

$$p_4 = K_1 q (p_2 / p_1), \quad p_5 = (K_1^2 q / K_2) (p_2 / p_1)^2, \quad p_6 = (K_1^2 / K_3) (p_2 / p_1)^2, \quad (7)$$

so that the set of equilibrium states corresponding to the given C turns out to be dependent on two parameters: the hydrogen pressure p_1 and the relative humidity of the atmosphere $\lambda = p_2 / p_1$. Consequently, the inverse problem considered in its natural ("primary") formulation is no longer correct, because of the absence of uniqueness.

To select a unique solution of their possible number, it is necessary to use additional information about it and to prescribe the pair; for example, according to the technological conditions, $\{p_1, \lambda\}$ is sufficient for the purpose. On the other hand, as seen from Eq. (4), large variations of a_C and, consequently, of pressures p_4 and p_5 at fixed values of p_1 and λ can correspond to small variations of C near the right boundary of the region of admissible values of $C \in (0; 4.3)$. However, by eliminating a rather wide half-neighborhood of the point $C_{cr} = 4.3$, it is possible to guarantee stability.

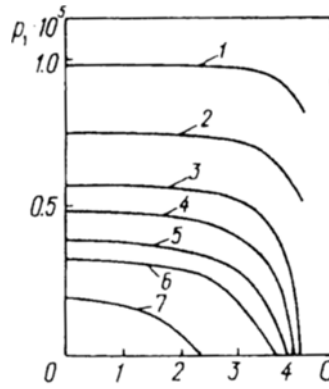


Fig. 2. Characteristic (for $\hat{p} \cong 10^5$ Pa) dependences of the hydrogen pressure in the furnace atmosphere on C (%) at different levels of relative humidity λ ($T = 1203$ K, $\hat{p} = 10^5$ Pa): 1) $\lambda = 0.1$, 2) 0.3, 3) 0.7, 4) 1.0, 5) 1.5, 6) 2.0, 7) 5.0. p_1 , Pa; C, %.

Another possibility for correct formulation of the inverse problem is the assignment of a certain combination of p_i as additional information. The sum of the equilibrium pressures $\sum_{i=1}^6 p_i = \hat{p}$, with $p_i > 0$, is the simplest of these. From here, with allowance for Eqs. (6) and (7) as well as the equation $p_2 = \lambda p_1$ it follows that $p_1 = (((1 + \lambda)^2 + 4q(\hat{p} - \varphi(\lambda)))^{1/2} - (1 + \lambda))/2q$, where $\varphi(\lambda) = \lambda K_1(q + K_1 \lambda((q/K_2) + (1/K_3)))$. The condition of positivity of p_1 imposes a restriction on λ from above: we can see that $\lambda \in (0, \hat{\lambda})$ if $\hat{\lambda}$ is the only positive root of the quadratic trinomial $\varphi(\lambda) - \hat{p}$, which is explicitly expressed in terms of q and three equilibrium constants.

Figure 2 presents the functions $p_1(C)$ at different values of λ for a typical temperature of carburization. We can see that at small values of λ there are regions of the values of C in which control is virtually unstable: variations of C, being substantial for control purposes, correspond to small variations of p_1 . On the other hand, for each quantity C it is possible to indicate a value of λ in whose neighborhood C is stable with respect to small variations of p_1 , and the inverse problem under consideration also has the property of stability.

In this connection, as a second condition for a selecting a solution it is natural to require that the value of $\partial p_1 / \partial C$ differ from -1 at the minimum. We note that the indicated derivative is determined explicitly by the expressions for p_1 and a_C , and, due to the monotonicity of $p_1(C)$, at each $\lambda \in (0, \hat{\lambda})$ this requirement uniquely determines the relative level of atmosphere humidity: $\lambda^* = \lambda(C)$. When $\lambda = \lambda^*$, the value of $p_1^*(C)$ is also uniquely determined.

Both inverse problems are combined in a single C program that can serve as a tool for solving problems of carburization control within the framework of the physicomathematical model considered here. The latter can also be extended on the basis of the statements used above.

3. Of interest for "manual" selection of the necessary parameters of the atmosphere is the problem of prediction of the carbon potential from given initial conditions p_{i0} ($i = 1, \dots, 6$) obtained experimentally. Such data allow one to supplement undefined system (3) with three equations following from the mass conservation law. Since the number of atoms of each element in the composition of gas molecules (H, C, O) in a closed atmosphere is invariable, and, according to the Clapeyron–Clausius law, this number for each gram-molecule of a compound containing one or another gas is proportional to the pressure of the corresponding gas, then the following linear combinations of pressures remain unchanged:

$$p_2 + p_4 + 2p_5 + 2p_6 = \alpha_0, \quad 2p_1 + 2p_2 + 4p_3 = \beta_0, \quad p_3 + p_4 + p_5 = \gamma_0, \quad (8)$$

where α_0 , β_0 , and γ_0 are just determined by the initial pressures.

System of Eqs. (3) and (8), which determines the equilibrium state, is closed. Its possible inconsistency, established by a mathematical experiment, implies that for the prescribed initial state equilibrium is impossible.

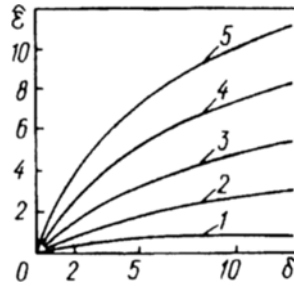


Fig. 3. Error in the determination of C versus the inaccuracy of pressure assignment at different values of the carbon potential (ϵ , %; δ , %; $T = 1203$ K; $\hat{p} = 10^5$ Pa): 1) $C = 4\%$, 2) 3, 3) 2, 4) 1, 5) 0.5.

For experimental calculations, an algorithm based on the following considerations appears to be effective.

1) After substitution of Eq. (3) into Eq. (8) the extreme equations in Eqs. (8) turn out to be cubic with respect to p_2 , so that one of these can be replaced by the resultant of the both. Denoting for brevity $p_1 \equiv x$, $p_2 \equiv y$, and $p_3 \equiv z = 0.5(\beta_0/2 - x - y)$, we arrive at to the following system:

$$y_s = p(x) + (-1)^{s+1} (D(x))^{1/2} \quad (s = 1, 2), \quad (9)$$

$$\varphi_s(x) \equiv 0.5z_s(x) (x^4 + K_1 y_s(x) x + A y_s^2(x)) - \gamma_0 x^4 = 0.$$

Here $p(x) \equiv 0.5(K_1(\beta_0/2 - x) - 2x^3)/(K_1 + 4Bx)$; $D(x) = p^2(x) - q(x)$; $q(x) \equiv 2(\lambda_0 + x)x^3/(K_1 + 4Bx)$; $\lambda_0 \equiv 2\gamma_0 - \alpha_0 - \beta_0/2$; $A \equiv K_1^2/K_2$; $B \equiv K_1^2/K_3$.

2) Since it is known in advance that $x > 0$, $y > 0$, and $z > 0$, we are interested only in solutions that satisfy the condition $0 < (x + y) < \beta_0/2$ and, in particular, $x < \beta_0/2$. We denote the root of the equation $D(x) = 0$ nearest to zero by x^* if it is smaller than $\beta_0/2$; otherwise, we assume that $x^* = \beta_0/2$. Since it is evident that $D(0) > 0$, then the solution of the equation $\varphi_s(x) = 0$ in algorithmic determination of $y_s(x)$ and $z_s(x)$ can be sought on $(0, x^*)$.

3) For this purpose it is reasonable to use the fork method with preliminary sounding of $(0, x^*)$.

A mathematical experiment based on such an algorithm leads us to the conclusion that only one of the functions $\varphi_s(x)$ (either at $s = 1$ or $s = 2$) can have a root on $(0, x^*)$.

Thus, at prescribed initial pressures the equilibrium state of the atmosphere is either nonexistent or unique. In turn if such a state is found and consequently the value of a_C is determined unambiguously, then the equation $\psi(\eta) = 0$ determines the carbon potential unambiguously. Actually, $\psi'(\eta) > 0$ with $\psi(\eta) \rightarrow -\infty$ when $\eta \rightarrow 0$ and $\psi(\eta) \rightarrow +\infty$ when $\eta \rightarrow 0.2$.

Moreover, taking into account the fact that all the elements of the algorithm are stable, the problem of predicting the carbon potential by the prescribed initial state of the atmosphere should be regarded as a conventionally correct problem [3]; employing another algorithm, for example, the Newton method, for the initial system of Eqs. (3) and (8), the solution can appear unstable, because of the proximity of the Jacobian of the system to zero, as evidenced by a corresponding mathematical experiment.

The proposed algorithm for calculating C makes it possible to obtain an estimate of the stability of the result; this estimate involves the experimentally incorrect assignment of the atmosphere state found in the inverse problem. In this case the values of p_i obtained in the problem should be taken as the initial values, introducing into them a controlled error that imitates an experimental one. As a measure of the latter, we can adopt the value of $\delta = \max_{1 \leq i \leq 6} (|\Delta p_i / p_i|)$, where $\Delta p_i = p_i \delta \xi_i$, ξ_i is a random variable uniformly distributed on $[-1, 1]$. As an estimate of the error in the result we take $\hat{\epsilon} = |\Delta C / C|$, where $\Delta C = C - \bar{C}$ if \bar{C} corresponds to the disturbed state of the atmosphere. The dependence $\hat{\epsilon} = \hat{\epsilon}(\delta)$ (Fig. 3) provides indication of the control stability in the case of random malfunctionings in the assignment of equilibrium state.

Thus, a mathematically correct statement of the problem of controlling carburization by varying the equilibrium state of the furnace atmosphere as well as of the problem of predicting the carbon potential by the initial state of the atmosphere turns out to be possible. Corresponding economic algorithms realized in a C-program can form a basis for the development of on-line control systems for production installations.

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NOTATION

C , carbon potential of the furnace atmosphere; t , process duration; x , coordinate of point of carburized layer; u , carbon concentration in layer; T , furnace temperature; D , diffusion coefficient; β , mass exchange coefficient; ϵ , alloying parameter; c_0 , initial concentration of carbon in metal; p_i , partial pressure of the i -th component of the atmosphere; K_j , K^* , equilibrium constants of chemical reactions; η , equilibrium concentration of carbon in atomic fractions; a_C , carbon activity; \hat{p} , total pressure of gases; cr , critical value.

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