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CONTROL OF HIGH-TEMPERATURE NITROCEMENTATION THROUGH A CONTINUOUS CHANGE IN THE CARBON POTENTIAL AND TEMPERATURE IN A GAS FURNACE

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The feasibility of automatic control of nitrocementation through a continuous change in the carbon potential and temperature of the environment has been studied by means of a mathematical experiment on the computer.

1. The idea of controlling the saturation process during cementation through a change in the parameters of the furnace atmosphere over time has been proposed in [1].

In [1, 2] the simpliest control method where the carbon potential of an external medium drops abruptly at a certain moment of time is considered and the question about choosing the latter so that the obtained carbon distribution over the diffusional layer approximate the prescribed profile as closely as possible was raised..

In [3] a mathematical simulation of a technological process (TP) controlled by a simultaneous change in time of the carbon potential and temperature of the saturating atmosphere of a furnace was carried out. The control functions were chosen from a prescribed class of functions permitting a simple realization (Fig. 1) and were parameterized accordingly.

In the case of the simpliest control through a carbon potential constant in time and of one or another level, informative nomograms have been developed in [4]. The nomographic method of describing functional relations is especially effective when they are given explicitly [5].

In the present work, mathematical simulation of the technological process of nitrocementation is carried out, similarly to the approach in [3] for cementation; here the technological process is controlled through a simultaneous change in time of the carbon potential and temperature of the furnace atmosphere and also of its nitrogen potential. The control functions, as in [3], are chosen from a given class of functions permitting a simple realization and are parameterized accordingly (Fig. 1). However, with a large number of control parameters (as in our case) and with an implicit character of their relationship with the results of technological process, a complete nomographic description of the process turns out to be impossible. Therefore, in the present work a basically new approach is employed: automated computer searching for the required regime parameters using assigned output characteristics of the process. This approach is similar to that used in [3]. Such an approach can be promising also for controlling nitrocementation in the dynamic regime, i.e., in real time, with operation specialized control computer on the production line.

This does not exclude employing nomograms in the programmed control of the technological process which can be used by an operator to assign the initial parameters for control programs. A variant of this kind of nomograms, allowing one to single out beforehand the duration of the carbon saturation process among a certain class of other parameters, is also suggested in the present study.

2. The physical basis of the technology of the saturation of a specimen is the process of nonlinear diffusion, which we consider in a two-dimentional case (when the specimen length is much larger than its thickness), so that

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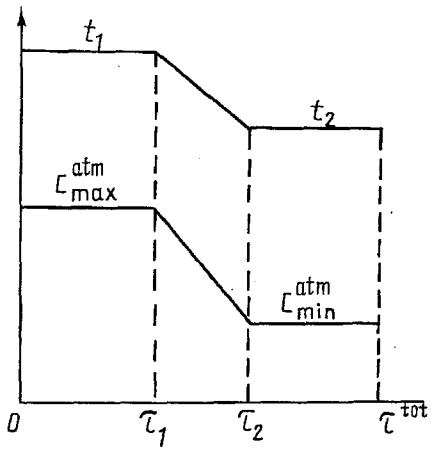

Fig. 1. Model of three-stage "smooth" control of furnace operation.

the concentrations of carbon C and nitrogen N depend on the spatial coordinate x and time τ: $C = C(x, \tau)$, $N = N(x, \tau)$, $0 \le x \le l$, $0 \le \tau \le \tau^{tot}$, where l is the specimen length.

In accordance with the technological conditions [6], it is assumed that the nitration process switches on later than the cementation, so that its duration not be so long.

Then C and N are determined by the following conditions:

$$\frac{\partial \tilde{C}}{\partial \tau} = \frac{\partial}{\partial x}\left(D_1(\tilde{C})\frac{\partial \tilde{C}}{\partial x}\right), \quad 0 < x < l, \quad 0 < \tau \leqslant \tau_2;$$

$$\tilde{C}(x, 0) = \hat{C}_0, \quad 0 \leqslant x \leqslant l; \quad D_1 \frac{\partial \tilde{C}}{\partial x}\Big|_{x=0} = \beta(\tilde{C} - C_{atm})|_{x=0}, \tag{1}$$

$$\frac{\partial \tilde{C}}{\partial x}\Big|_{x=l} = 0, \quad 0 \leqslant \tau \leqslant \tau_2,$$

$$\frac{\partial C}{\partial \tau} = \frac{\partial}{\partial x}\left(D_1(C, N)\frac{\partial C}{\partial x}\right),$$

$$0 < x < l, \quad \tau_2 < \tau \leqslant \tau^{tot},$$

$$\frac{\partial N}{\partial \tau} = \frac{\partial}{\partial x}\left(D_2(C, N)\frac{\partial N}{\partial x}\right),$$

$$C(x, \tau_2) = \tilde{C}(x, \tau_2), \quad N(x, \tau_2) = \hat{N}_0, \quad 0 \leqslant x \leqslant l;$$

$$D_1 \frac{\partial C}{\partial x}\Big|_{x=0} = \beta(C - C_{atm})|_{x=0}, \quad N(0, \tau) = N_{atm}, \tag{2}$$

$$\frac{\partial C}{\partial x}\Big|_{x=l} = 0, \quad \frac{\partial N}{\partial x}\Big|_{x=l} = 0, \quad \tau_2 \leqslant \tau \leqslant \tau^{tot}.$$

Here, the diffusion coefficients depend not only on the concentration, what makes the problem nonlinear, but also on the temperature of the furnace t, which, in its turn, is the function of time: $t = t(\tau)$.

Since diffusional processes are considerably slower than thermal ones, we can neglect the time it takes to reach the prescribed temperature, so that the process depends on t as on a functional parameter.

The carbon potential of the furnace atmosphere, which depends on time: $C_{atm} = C_{atm}(\tau)$ and the nitrogen potential N_{atm} are also control parameters.

For the characteristics D_1, D_2, β of the material the following expressions are taken [7]:

$$D_1(C, N, t) \equiv D_1 = (0{,}04 + 0{,}08(C + N))\exp(-31350/(1{,}987t_k)), \ \text{cm}^2/\text{sec},$$

$$D_2(C, N, t) \equiv D_2 = (1{,}0 + 0{,}5(C + N))\exp(-27883/(1{,}987t_k)) \cdot 0{,}0144, \ \text{cm}^2/\text{sec},$$

$$\beta = 1{,}36 \cdot 10^{-3}\exp(-11100/(1{,}987t_k)), \ \text{cm/sec}, \quad t_k = t + 273{,}15 \ \text{K}.$$

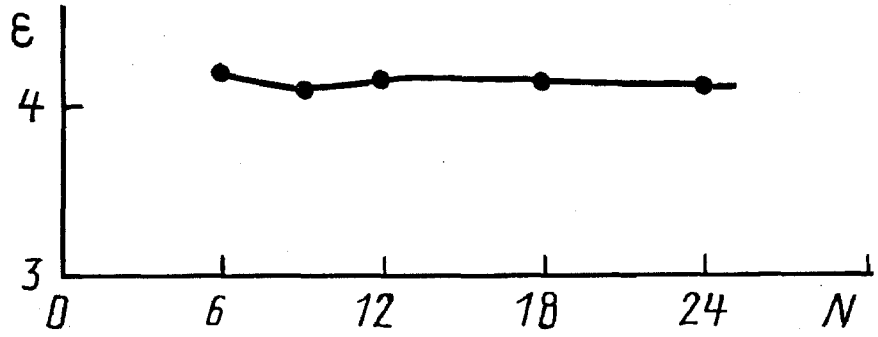

Fig. 2. Dependence of the norm of the relative deviation $\varepsilon \equiv \max_i |\hat{p}_i - \hat{p}_{*i}| / |\hat{p}_i|$ (%), where $\hat{p}_i$, $\hat{p}_{*i}$ are the i-th components of the vectors $\hat{p}$, $\hat{p}_*$, respectively, on the number of reference points $s + 1 \equiv N$.

Problem (1), (2) makes it possible to predict the concentration field for each prescribed set of control parameters. For this purpose, we use an implicit finite-difference scheme of second-order accuracy in x and first-order accuracy in τ [8], solved by the trial run method within the framework of a double iteration process attributed to the nonlinearity of problem (1), (2). We turn to the problem of controlling the nitrocementation process.

3. For the control model under consideration (Fig. 1) and for the given grade of steel, one can single out a discrete set of control parameters $\hat{p}$ characterizing the potential and temperature of the furnace atmosphere.

Then the concentration fields determined by problem (1), (2) at the end of the process $\tau = \tau^{tot}$ turn out to be functionals of $\hat{p}$:

$$C = C[x, \hat{p}], \quad N = N[x, \hat{p}].$$

The desired result of nitrocementation can be characterized by a set of s + 1 "reference" points x_k, at which the required values of the concentrations C_k and N_k are assigned at the moment of time τ^{tot} (k = 0, 1, ... , s).

Let δ be the allowable standard deviation of the calculated concentrations from the required values at the reference points, and let the set P from which the control parameters are chosen be assigned. Then the quality of the result of nitrocementation at any assigned moment of time can be characterized by the requirement:

$$F(\hat{p}) \equiv \sum_{k=0}^{s} \left(\frac{C[x_k, \hat{p}] - C^{(k)}}{C^{(k)}} \right)^2 + \sum_{k=1}^{s} \left(\frac{N[x_k, \hat{p}] - N^{(k)}}{N^{(k)}} \right)^2 \leqslant \delta^2, \quad \hat{p} \in P. \tag{3}$$

The latter condition includes explicit quantitative restrictions on the components $\hat{p}$ corresponding to the values admissible in practice. This ensures [9] the correctness of the formulation of quasiminimization problem (3) in the case of its applicability for the given τ^{tot} and δ, i.e., if

$$\inf_{\hat{p}} F(\tau^{tot}, \hat{p}) < \delta^2. \tag{4}$$

On the other hand, the condition $\hat{p} \in P$ can include an implicit requirement on the qualitative behavior of the carbon profile at the end of a process: monotonicity of the curve C(x), etc. (see Sec. 4).

As numerical experiments on minimization of $F(\hat{p})$ for various s and for profiles of carbon and nitrogen distribution prescribed beforehand, corresponding to some $\hat{p}_*$, have shown, it is sufficient to take two reference points, assuming: $x_0 = 0$, $C^{(0)} = C_{surf}$, $x_1 = h_b$, $C^{(1)} = C_b$, $N^{(1)} = N_b$.

An increase in the number s does not lead to a noticeable improvement of the choice of $\hat{p}$. This is not surprising, since we are not free to choose the shapes of the nitrocementation profiles: this is the solution of boundary problem (1), (2) at $\tau = \tau^{tot}$. In particular, a generally accepted characteristic of the result such as the total depth of cementation ($h_{tot.C}$, for which $C^{(2)} = C_0 + 0.05\%$ [2]), is not controlled when a value of the effective thickness $h_{b.C}$ different from it is assigned, but it acquires the value which is "prescribed" by the diffusion law for the chosen parameters. Thus, the result of the technological process is characterized by the set $\hat{q} = \{C_{suf}, h_b, C_b,$

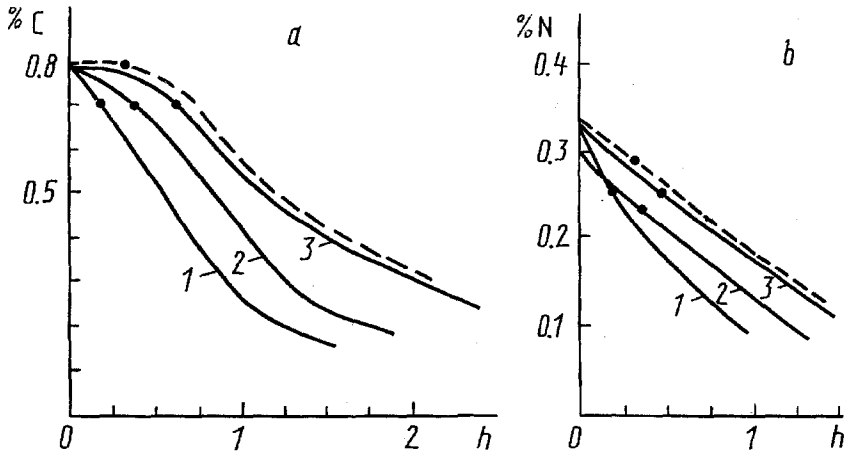

Fig. 3. Carbon and nitrogen profiles in the case of continuous control of the temperature regime for the first (1), second (2), and third (3) sets of parameters in Table 1. h, mm.

$N_b\}$ prescribed beforehand. This conclusion is illustrated in Fig. 2, where the dependence of the norm of the relative deviation of $\hat{p}$ from $\hat{p}_*$ is presented.

The search for $\hat{p} = \hat{p}(\tau^{tot})$ ensuring the required quality is realized in automatic regime on a computer by Rosenbrock method [10] using the given initial approximation $\hat{p}_0$. The minimization process is interrupted under condition (3), or the nonvalidity of the statement of the problem for the given τ^{tot} and δ (condition (4)) is ascertained.

The solution of problem (3) determines the values of the control parameters $\hat{p}$ for which the carbon concentration profile of the required quality is obtained in the least time.

The object functional $\tau^{tot}(\hat{p})$ corresponding to this requirement can be defined by the condition $F(\tau^{tot}, \hat{p}) = \delta^2$, and the optimum saturation time τ^{tot}_{min} in the indicated sense is obtained by solving the following variational problem:

$$\tau^{tot}_{min} = \inf \tau^{tot}\ (\hat{p}), \quad \hat{p} \in P^{min}_{\delta}, \tag{5}$$

where $P^{min}_{\delta} = \{\hat{p} \in P\colon F(\tau^{tot}, \hat{p}) = \delta^2\}$. It is natural to seek the solution of this problem in the set of values $\{\tau^{tot}_l\}$. This means that for each τ^{tot}_l the quasiminimization problem (3) is solved with respect to the rest of the control parameters. An algorithm for its solution is, therefore, a component of the complex of methods for solving the problem of optimum control in the indicated sense. This main part is supplemented by a condition for choosing the value of τ^{tot}_l: choose the least value of $\tau^{tot}_{l,min} \in \{\tau^{tot}_l\}$ for which the condition $\hat{p} \in P^{min}_{\delta}$ is still valid.

Below, the results of a mathematical experiment on the automated search for the parameters of optimum control in the sense of (3) or (5) are presented.

4. We consider a variant of three-stage (see Fig. 1) control of the nitrocementation process. A decrease in furnace temperature from t_1 to t_2 in the time interval $\tau_2 - \tau_1$ and the corresponding decrease in the temperature of the metal at this stage of the process should reduce diffusion flows in the surface layes and, thus, should promote the outflow of carbon into the depth of the metal due to the significant gradient of it established previously at the boundary of the "effective layer." A decrease in temperature thus acts in the same direction as a decrease in the carbon potential of the furnace atmosphere.

With a prescribed value of τ^{tot} and a fixed value of t_1 ($t_1 = 870$, 930, or 1050°C), the control is characterized by the set

$$\hat{p} = \{C^{atm}_{max},\ C^{atm}_{min},\ \tau_1,\ \tau_2,\ N_{atm}\}.$$

The corresponding compact set P of values of $\hat{p}$ is determined by the technological conditions: $1.21 \geq C^{atm}_{max} \geq C^{atm}_{min} \geq 0.8\%$; $840\ ^{\circ}C \leq t_2 < t_1$; $\tau_1 + 0.25\ h \leq \tau_2 < \tau^{tot}$; $l = 10$ mm, $0.2\% \leq N_{atm} \leq 0.4\%$; $\hat{C}_0 = 0.15\%$, $N_0 = 0.0\%$.

TABLE 1

Set number	t_1, °C	τ^{tot}, h	$\hat{q}$, $\frac{C_{surf}}{h_b/C_b/N_b}$	C^{atm}_{max}, %	C^{atm}_{min}, %	N_{atm}, %	t_2, °C	τ_1, h	τ_2, h
1	1050	2.5	$\frac{0.8}{0.2/0.7/0.25}$	1.04	0.84	0.32	840	1.5	2.0
2		5	$\frac{0.8}{9.3/0.7/0.23}$	1.01	0.82	0.30	850	3.1	4.0
3		10	$\frac{0.8}{0.5/0.7/0.25}$	1.05	0.85	0.33	1000	6	8

TABLE 2

Set number	t_1, °C	τ^{tot}, h	$\hat{q}$, $\frac{C_{surf}}{h_b/C_b/N_b}$	C^{atm}_{max}, %	C^{atm}_{min}, %	N_{atm}, %	τ_1, h	τ_2, h	t_2, °C
1	870	10	$\frac{0.8}{0.2/0.7/0.25}$	1.05	0.83	0.32	6.5	8.5	850
2	930	5	$\frac{0.8}{0.2/0.7/0.25}$	1.04	0.86	0.33	2.0	4.0	850

In Fig. 3 the profiles of carbon and nitrogen distributions are presented for sets 1, 2, 3 in Table 1. The optimum profiles obtained in the course of optimization for $\hat{q} = \{C_{surf} = 0.8\%, h_b = 0.3$ mm, $C_b = 0.8\%, N_b = 0.28\%\}$ are depicted by dashed lines.

Two characteristic kinds of carbon distribution over the diffusional layer can be observed: one, corresponding to small values of τ^{tot}, has a sufficiently abrupt linear drop in concentration with depth; the other, formed at large values of τ^{tot}, is distinguished by the surface layer with a more slowly decreasing concentration. Thus, by regulating the time of nitrocementation and choosing the appropriate parameters it is possible to provide the quality of carbon distribution over the surface layer that conforms to the goal set during design work: a part is to be designed for short-term intense impact loads or for long-duration uniform loads, which solves the problem of increased fatigue strength.

Similar distributions are characteristic also for other values of $\hat{q}$ at $C_{surf} = 0.8\%$ in the ranges $0.1 \le h_b \le 1.0$, $0.5\% \le C_b \le 0.8\%$, $0.15\% \le N_b \le 0.28\%$.

Table 1 presents the optimum values of $\hat{p}$, found in automatic regime, at $t_1 = 1050$°C for different τ^{tot} and "medium" h_b from the indicated range. One can note that among the control parameters N_{atm} turns out to be the least "active": for close values of it profiles of differing quality can be obtained (corresponding to various τ^{tot}). On the other hand, it turns out that close results of nitrocementation C(x), N(x) can be obtained for different sets of control parameters, including the total time τ^{tot}. The appropriate comparison is presented in Table 2. Precisely this fact allows one to formulate the problem on the search for the minimum time of nitrocementation without loss of quality.

At the same time, the characteristic specific features of the profiles noted above enable one to formulate additional conditions on the set P for solving the problem of time optimization in automatic regime.

We use such conditions for a variant of control with continuous change in the furnace atmosphere temperature. (In this variant the temperature t_2 is fixed ($t_2 = 840$°C), and the control is characterized by the set $\hat{p} = \{C^{atm}_{max}, C^{atm}_{min}, \tau_1, \tau_2, t_1, N_{atm}\}$.)

For profiles ensuring the heightened resistance to impact effects (profile A), the following requirement can serve as an optimality criterion in automated selection:

a) the negative derivative of the carbon concentration at the surface should differ slightly or as little as possible from the angular coefficient of the chord passing through the points (C_{surf}, $h_b = 0$) and (C_b, h_b).

With account for the allowance δ_1, in calculating the derivative at the surface $\tilde{C}'_{surf}$ using a certain approximation formula, this means the satisfaction of the following inequality:

TABLE 3

Set number	t_2, °C	τ^{tot}, h	$\hat{q}$, $\frac{C_{surf}}{h_b/C_b/N_b}$	C^{atm}_{max}, %	C^{atm}_{min}, %	N_{atm}, %	τ_1, h	τ_2, h	t_1, °C
1	840	2.5	$\frac{0.8}{0.5/0.5/0.15}$	1.05	0.83	0.32	1.5	1.9	1047.5
2		2.5	$\frac{0.8}{1.3/0.7/0.24}$	1.07	0.84	0.31	1.5	2.0	970
3		5	$\frac{0.8}{0.3/0.7/0.21}$	1.09	0.84	0.28	3.1	4.0	1023
4		10	$\frac{0.8}{0.3/0.8/0.28}$	1.14	0.82	0.33	6.0	8.0	1050

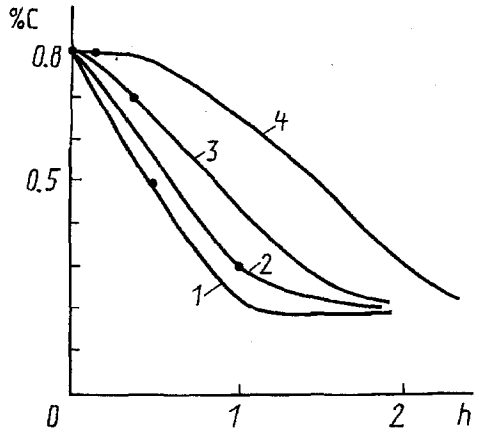

Fig. 4. Optimum carbon profiles of two kinds in time in "smooth" control: 1) type A for set 1 of control parameters (Table 3); 2) type A for set 2; 3) type B for set 3; 4) type B for set 4.

$$\|\tilde{C}'_{surf}| - |\tilde{C}'\| \leqslant \delta_1,$$

where $C' = (C_b - C_{surf})/h_b$.

For profiles solving the problem of heightened fatigue strength (profile B), with account for the allowance δ_2 for the nonuniformity of carbon distribution in the surface layer, we shall consider the distribution and, thereby, the corresponding τ^{tot} to be optimum when one of the following criteria (or both) is fulfilled:

b) $|C_{max} - C_{surf}| \leq \delta_2$;

c) $|\tilde{C}'_{surf}| \leq \delta_2$ or passage of $\tilde{C}'_{surf}(0, \tau^{tot})$ (the derivative at the surface) through zero as τ^{tot} changes by a step of the mesh introduced here.

In subsequent experiments, for δ_1 and δ_2 we took the value 0.02% C, matching the accuracy of the measurement of the carbon concentration in practice.

Figure 4 shows the optimum concentration profiles of type A and B in time for different sets of reference points $\hat{q}$, respectively, marked by dots in the figures. The values of control parameters corresponding to approximate values of τ^{tot}_{min}, obtained on the grid 1 h $\leq \tau^{tot} \leq$ 10 h, $\Delta\tau$ = 0.5 h are presented in Table 3. We note that the nitrocementation process should not last more than 10 h, since nitrogen can exist in a free state only for a relatively brief period (then it combines with other chemical elements), and the results obtained satisfy this requirement.

The comparison of the results of various kinds of control presented here shows that a smooth change in both control parameters (both the temperature of the furnace atmosphere and the carbon concentration in it) enables one to achieve better, as compared to the traditional, quality in a shorter period of time. The temperature variation here plays a significant role if one solves the problem in a sufficiently wide range of the values of $\hat{q}$. The simplest control variant, proposed earlier in [1], yields satisfactory results only for small values of h_b, C_b: $h_b \leq$

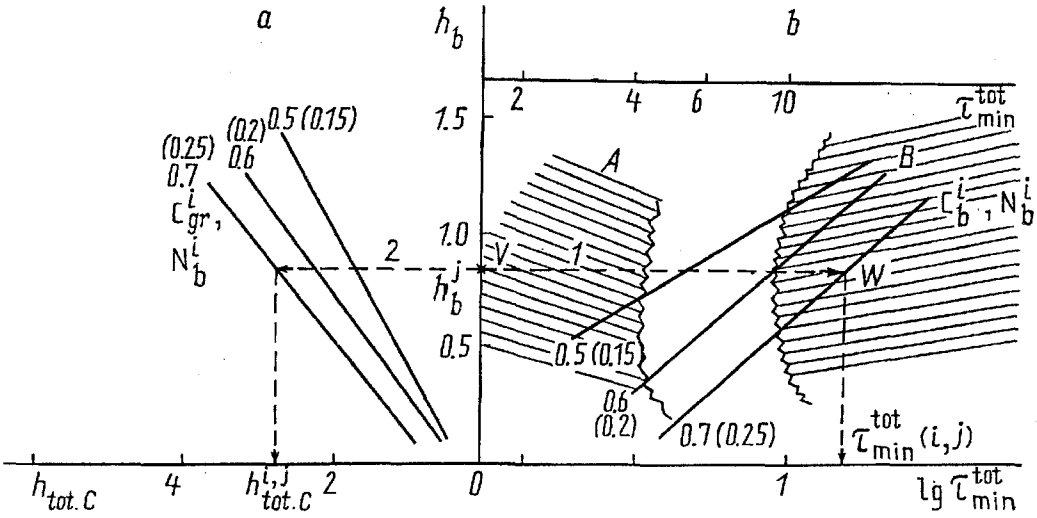

Fig. 5. Nomograms of the relation h_b - τ^{tot}_{min} - $h_{tot.C}$ for several pairs of concentration values $\{C_b, N_b\}$ (the values on the curves; the values of N_b are in the brackets) and the scheme for using them. $h_{tot.C}$, h_b, mm; τ^{tot}_{min}, h.

0.2 mm, $C_b \leq 0.6\%$. In other cases, the duration of the process that is optimum in time for smooth control turns out to be clearly insufficient for obtaining an effect that is at least close to the required one.

The optimum values of model parameters corresponding to this duration [1] lead to carbon profiles characterized by a clearly expressed maximum near the specimen surface, the value of which reaches 20% of the prescribed value of the carbon concentration at the surface. A reduction (for other τ^{tot}_{min}) of the level of this maximum by two-fold results in a deviation of the concentration profile from the depth reference point by up to 30%.

5. The problem on the optimum saturation time without loss of quality can be stated similarly to (3) with introduction of the process duration τ^{tot} into the quantity of control parameters: $\hat{p}_{min} = (\hat{p}, \tau^{tot})$. However, as our calculation experiments show, automated choice of $\hat{p}_{min}$ results in a significant increase in the processing time of computer. A similar effect is caused by a reduction in the size of the grid $\{\tau^{tot}_l\}$ in the algorithm of solution of problem (5) proposed above.

Therefore, the design of nomograms which compare the minimum optimum time τ^{tot}_{min} with each set of reference points $\hat{q}$ turns out to be useful. Then the search for the optimum regime in time for each $\hat{q}$ is reduced to the solution of problem (1), (2) in the case of a fixed, certainly optimal process duration.

Since the equation whose solution is the desired relation is prescribed implicitly, for the construction of such nomograms the set of carbon profiles of the required quality obtained by solving problem (1), (2) on the grid $\{\tau^{tot}_l\}$, is subjected for each $\hat{q}$ to processing according to criteria a), b), and c). This makes it possible to visualize the relation $\tau^{tot}_{min} = \tau^{tot}_{min}(\hat{q})$.

The base of the nomogram developed by us is the series of curves $h_b = h_b(\tau^{tot}_{min})$, each of which corresponds to one of the pairs of values $\{C_b, N_b\}$.

In the semilogarithmic scale $\tau^{tot}_{min} \rightarrow \lg \tau^{tot}_{min}$, the indicated curves are represented by straight-line segments (see Fig. 5b), and the relations $h_{tot.C} = h_{tot.C}(h_b)$ are presented in Fig. 5a.

As stated above, the point ($h_{tot.C}$, $C_b = \hat{C}_0 + 0.05\%$) is not included in the quantity of reference points and the values of $h_{tot.C}$ are obtained as a result of solving problem (1), (2). Thus, Fig. 5a gives additional information on the total saturation depth that is expected in the optimum regime. Finally, the criteria indicated above allow one to mark on the nomogram sheet (Fig. 5) the regions (τ^{tot}_{min}, $\hat{q}$) in which one should expect the profiles of A and B, respectively. (Each such sheet corresponds to one of the values of C_{surf}; in the calculation performed C_{surf} = 0.8%.)

A scheme of possible use of a nomogram for one of the required values of parameters is also presented in Fig. 5. Suppose it is necessary to know the optimum nitrocementation time for obtaining the concentrations C^i_b, N^i_b at a boundary layer of thickness h^i_b. The search path is represented in this scheme by dashed line 1, whose

beginning is at point V on the h_b axis. Movement along the horizontal up to the straight line corresponding to the given C_b^i, N_b^i with subsequent "descent" to the τ_{min}^{tot} axis enables one to find the sought value of $\tau_{min}^{tot}(i, j)$. Here, one can also point out $h_{tot.C}^{i,j}$ moving to the left from the point V along dashed line 2 up to the given numerical specification for C_b^i, N_b^i; moreover, simultaneously we establish the type of carbon concentration profile. In the example considered, point W belongs to a region of type B in the scheme and we obtain the "flat" surface region of thickness $\leq h_b^j$. The value of $\tau_{min}^{tot}(i, j)$ found can be employed by an operator in computer calculations of the optimum value of $\hat{p}_{min}$ in quality, corresponding to the required $\hat{q} = \{C_{surf}, h_b^j, C_b^i, N_b^i\}$, using the algorithm solving problem (1), (2).

NOTATION

D_1, coefficient of carbon diffusion, cm^2/sec; D_2, coefficient of nitrogen diffusion, cm^2/sec; β, coefficient of carbon mass transfer, cm/sec; C_{atm}, carbon potential of the atmosphere, %; t, process temperature, ^0C; t_k, process temperature, K, $t_k = t + 273.15$ K; $C(x, \tau)$, carbon concentration as a function of the spatial coordinate x and time τ; $N(x, \tau)$, nitrogen concentration as a function of the spatial coordinate x and time τ; $\hat{p}$, the set of control parameters; $F(\hat{p})$, quality functional; $\hat{q}$, the set of parameters characterizing the result of a process; τ^{tot}, total time of specimen saturation by carbon and nitrogen; $\hat{C}_0$, $\hat{N}_0$, initial contents of carbon and nitrogen.

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