AN INVERSE PROBLEM OF CARBONITRIDING

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The problem of determining diffusion coefficients of carbon and nitrogen during carbonitriding has been stated and solved.

1. The technological process of steel carbonitriding [1] is described, under certain additional conditions, by a nonlinear system of parabolic equations, coupled through diffusion coefficients dependent on the system solution, i.e., on concentrations of carbon (u_1) and nitrogen (u_2): $D_i = D_i(u_1, u_2)$; i = 1, 2. Either linear representations [2] or experimental equations are used for the functions D_i. However, even such approximations are known not for all technological processes. A problem arises determining D_i from indirect measurements above the diffusion fields, which falls into the class of inverse problems [3].

The present study states and solves this problem for a standard linear model of coefficients, which depends on few parameters. The uniqueness of the solution is established in the relevant class of models, a stable algorithm is formulated to search the problem parameters, and a modulus of solution continuity relative to an error of indirect data regarding the parameters sought is studied by conducting the mathematical experiment on a computer.

2. The linear model of diffusion coefficients is defined by the equations

$$D_i = \bar{a}_{0,i} + \bar{a}_{1,i}u_1 + \bar{a}_{2,i}u_2, \tag{1}$$

where $\bar{a}_{0,i}$, $\bar{a}_{1,i}$, $\bar{a}_{2,i}$, i = 1, 2 are certain temperature functions of the process.

With temperatures not too high, the interaction of processes is neglected ($D_i = \bar{a}_{0,i}$), and the concentration field problem splits into two independent ones. At a high temperature T, regarded as a parameter, two modifications will be discerned. For the model (α): $\bar{a}_{1,i} = \bar{a}_{2,i} \equiv \bar{a}_{1,i}$, when the interaction is determined by the sum of concentrations. Here, we will consider the sought quantity to be $\mathbf{p}_\alpha = \{\bar{a}_{0,i}, \bar{a}_{1,i}\}$, i = 1, 2, with components constant at a fixed T. For the model (β): $\bar{a}_{1,i} \neq \bar{a}_{2,i}$, but the values of $\bar{a}_{0,i}$ are assumed known from indirect observations of uncoupled diffusion fields. In this case, the sought quantity is $\mathbf{p}_\beta = \{\bar{a}_{1,i}, \bar{a}_{2,i}\}$, where the components are invariable as well.

We would like to note that the values of $\bar{a}_{0,i}$ in the case (β) can be determined unambiguously also if $\bar{a}_{0,i} = \bar{a}_{0,i}(u_i)$, with constraints which are not too stringent imposed on the class of such functions [4] and even when the available information on diffusion fields is incomplete, i.e., it is sufficient that the concentrations should be specified as functions of time: $u_i(0,t) = \varphi_i(t)$, along with ordinary boundary conditions of the second or third order [5].

In the framework of the adopted models with assigned initial concentrations and linear boundary conditions of any type [6], the diffusion process is described by a system of equations

$$L_i(u_1, u_2) \equiv \frac{\partial u_i}{\partial t} - \frac{\partial}{\partial x}\left[D_i(u_1, u_2)\frac{\partial u_i}{\partial x}\right] = 0, \quad i = 1, 2,$$
$$(x, t) \in Q \equiv [0, l] \times [0, \hat{t}]. \tag{2}$$

Let M_p denote a set of the values of $\mathbf{p}_\alpha$(or $\mathbf{p}_\beta$), and M_u represent a set of solutions $\mathbf{u} = (u_1, u_2)$ for the system (2) with specified initial and boundary conditions, and $\mathbf{p}_\alpha \in M_p$ (or $p_\beta \in M_p$). The following condition is evident: $\mathbf{u} \in M_u$ assures a solution to the inverse problem.

The diffusion fields will be referred to as degenerate in a certain subregion Q, if $(\partial^2 u_i/\partial x^2) \equiv 0$ or $(\partial/\partial x)[(u_1 + u_2)/(\partial u_1/\partial x)] \equiv \alpha\,(\partial^2 u_i/\partial x^2)^{1/2}$ at some $\alpha \neq 0$, i = 1, 2.

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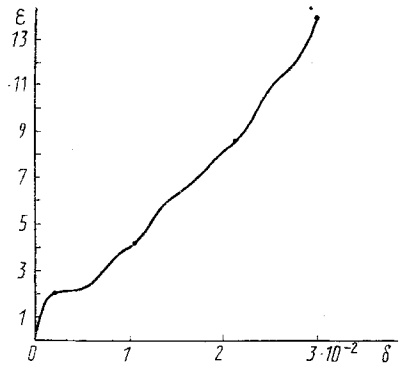

Fig. 1. Relation $\epsilon(\delta)$, %.

Theorem. Let $\mathbf{u} \in M_u$ be known in a certain vicinity ω_{M_0} of any point $M_0(x_0, t_0) \in Q$, and the diffusion fields be nondegenerated in ω_{M_0}. Then, the solution for the inverse problems $\mathbf{u}_\omega \to \mathbf{p}_\alpha$ and $\mathbf{u}_\omega \to \mathbf{p}_\beta$ is unique.

To prove this theorem, for example, in the case (α) we consider the function $F(\mathbf{p}_\alpha) \equiv \int_\omega \int_{M_0} [L_1^2(\mathbf{u}) + L_2^2(\mathbf{u})] d\sigma$.

Obviously, $\inf F(\mathbf{p}_\alpha) = 0$, and any solution of the inverse problem is the solution for this variational one.

Critical points of the system are $(\partial F/\partial \bar{a}_{k,i}) = 0$, $k = 0, 1$, $i = 1, 2$. It is not difficult to make certain that the point of global extremum be nonunique only in the case of degenerated fields, whence it follows that the theorem is valid.

We should note that the degeneracy conditions lead either to breaking down of the diffusion fields for u_1 and u_2 into independent ones, or (as in [6]) to a specific structure inconsistent with the problem conditions (2). On the other hand, the formulated uniqueness conditions are of local character and can apply to a vicinity as small as desired, and also to a half-vicinity of any point. At the same time, these conditions are sufficient and relate, as usual [7], to a precise assignment of the input information. This does not hinder the employment of less detailed information on the fields in the mathematical experiment, and, if the data are inaccurate, requires construction of a regularizing algorithm [4]. We used the model (α).

3. Proceeding to the formulation of such an algorithm, let us write an inverse coefficient [8] problem for any modification ((α) and (β)) in the operator form

$$Az = v, \tag{3}$$

where $z \in D$ pertains to a metric space of the linear functions of the form (1), and $v \in V$ to a metric space of the concentration fields observed on a specified set of values of the argument (in particular, ωM_0). The operator A is defined by the system (2) at any given coefficients z.

Evidently, only with a precise definition of the fields v the problem (3) can be assumed (by virtue of the proven theorem) conditionally proper [4] on the compactum $\hat{D}$, a priori determined by explicit restrictions imposed on the coefficients of linear functions.

However, when the information on the fields is specified approximately, problem (3), generally, has no solution, and, if only for this reason, has been stated incorrectly. In this case, a proper statement of the problem can be obtained by referring to the quasisolution:

$$z_0 = \arg\inf \rho_V^2 (Az, v), \tag{4}$$

where ρ_v is the metric of an appropriate space, expressed in the considered case as an integral of the squared deviation of v from Az. It should be remarked that the statement (4) can also prove to be improper (inconsistent), since the error of input data δ in the metric space V and the quantitative limitations defining the compactum $\hat{D}$ are not to be necessarily consistent. In the latter case, $\rho^* = \inf_{\hat{D}} \rho^2 v(Az, v) > \delta$, and it cannot be claimed that $z_\delta \to \hat{z}$ conforms to the exact solution of the problem for $\delta \to 0$.

Another possibility of stating the problem correctly lies in using the concept of a stabilizer [4] $\Omega(z)$ and in applying the Tikhonov smoothing functional:

$$z_\delta = \operatorname{arginf} \{\rho_V^2 (Az,\ v) + \alpha (\delta)\, \Omega (z)\}, \tag{5}$$

where $\alpha(\delta)$ is chosen, for example, from the condition $\rho_V^2(Az, v) = \delta^2$, if z^α is the element minimizing the functional (5) at an arbitrary $\alpha > 0$. Such a statement of the problem does not call for a priori limitations, determining the compactum, and the latter is obtained algorithmically.

Since the diffusion coefficient is determined unambiguously by the set of parameters in the linear model (1), we can select the function as a stabilizer in the considered problem:

$$\Omega_0 (z) \equiv \sum_{i=1}^{2} \sum_{k=0}^{1} a_{ki}^2. \tag{6}$$

As follows from [4], in this case any algorithm solving the problem (5) turns out to be regularizing. We realized exactly such an algorithm to perform the mathematical experiment.

4. The computational experiment, whose results are given below, is aimed not only at illustrating the efficiency of the realized algorithm of the problem solution, but also at gaining an answer to the basic question concerning a practical solution of the problem, viz., to what accuracy δ must the physical fields be measured in order to obtain the sought parameters of the object to the required accuracy ε? Apparently, this is a question of planning the physical measurements, and it cannot be answered with the help of a priori mathematical computations in view of unboundedness of the inverse operator A^{-1}, characteristic of inverse problems.

In the mathematical experiment, we chose the following additional conditions concretizing the problem (2):

$$\begin{gathered} u_1 (x,\ 0) = u_{10};\quad u_2 (x,\ 0) = u_{20},\quad u_{i0} = \text{const},\quad i = 1,\ 2,\quad 0 \leqslant x \leqslant l; \\ \frac{\partial u_1}{\partial x} (0,\ t) \quad \frac{\partial u_2}{\partial x} (0,\ t) = 0;\quad D_1 (u_1,\ u_2) \frac{\partial u_1}{\partial x} (l,\ t) = \beta_1 (u_{\text{vic.}1} - u_1 (l,\ t)), \\ D_2 (u_1,\ u_2) \frac{\partial u_2}{\partial x} (l,\ t) = \beta_2 (u_{\text{vic.}2} - u_2 (l,\ t)), \end{gathered} \tag{7}$$

where

$$\begin{gathered} u_{10} = 0{,}15\%;\ u_{20} = 0\%;\ D_1 = (\bar{a}_{0,1} + \bar{a}_{1,1} (u_1 + u_2)) \exp \left(- \frac{131\,000}{RT} \right) \text{m}^2/\text{s}\ ]; \\ D_2 = (\bar{a}_{0,2} + \bar{a}_{1,2} (u_1 + u_2)) \exp \left(- \frac{131\,000}{RT} \right) \text{m}^2/\text{s}\ ];\quad \beta_1 = \beta_2 = 1{,}36 \cdot 10^{-5} \times \\ \times \exp \left(- \frac{46420}{RT} \right) [\text{m/sec}],\ R = 8{,}31\ \text{J/(mole·K)}),\ T = 1203\,\text{K},\ l = 10^{-2}\ \text{m}, \\ \hat{t} = 4{,}5\text{ч},\ u_{\text{vic.}1} = 1{,}0\%,\ u_{\text{vic.}2} = 0{,}25\%. \end{gathered}$$

For calculating the concentration fields at requisite points with each z in the framework of a variational problem, we employed the implicit difference scheme with an approximation error $O(h^2 + \tau)$, where h is the step along the coordinate and τ is the step in time. As the system is nonlinear, a dual iteration process was realized, on each new temporal layer, with initial values taken from the preceding temporal layer. A natural structure of the external iteration procedure is defined by the equations

$$u_2^{(s)} \Rightarrow L_1 (u_1,\ u_2^{(s)}) = 0 \Rightarrow u_1^{(s+1)} \Rightarrow L_2 (u_1^{(s+1)},\ u_2) = 0 \Rightarrow u_2^{(s+1)}. \tag{8}$$

The internal iteration procedure solving each of the two equations, isolated on the s-th step, with respect to u_1 or u_2 corresponds to a simple iteration method, where on each s-th step the coefficients are taken from the preceding iteration. The above-mentioned implicit scheme refers to a system linearized on the (s, k)-step of the double cycle.

Concentrations for solving the inverse problem were specified from the conditions $u_i(x_s, \hat{t}) = \varphi_i(x_s)$, i = 1, 2, s = 1, 2 ..., and N (N = 100), where $\hat{t}$ is the time of process termination. This kind of indirect information on the diffusion coefficients is the most convenient for conducting the physical experiment. Here, in Eq. (5) we have

$$\rho_V^2(Az, v) \equiv \sum_{i=1}^{2} \sum_{s=1}^{N} \sigma_s [u_i(x_s, \hat{t}) - \varphi_i(x_s)]^2, \tag{9}$$

where σ_s are the weighing factors corresponding to the Simpson quadrature formula for an appropriate continuous analog of the functional

$$\rho_V^2(Az, v) \equiv \sum_{i=1}^{2} \|u_i(x, \hat{t}) - \varphi_i(x)\|^2_{L_2[0,l]}.$$

The performed mathematical experiment consists of two stages.

1. First, from the known linear functions $D_i(u_1, u_2)$, i = 1, 2 (version (α)) for steel marks [2] we obtained, with computer accuracy, the concentration fields on the set $\hat{\omega}_N \equiv \{(x_s, \hat{t})\}$ (s = 1, 2,...,N) at h = 10^{-4} m, τ = 0.45 h, $l = 10^{-2}$ m, and $\hat{t}$ = 4.5 h. In the version presented here, the assumed coefficients are:

$$D_1 = (0{,}04 + 0{,}08(u_1 + u_2)) \exp\left(-\frac{131\,000}{RT}\right) \cdot 10^{-4}\ \text{m}^2/\text{sec};$$

$$D_2 = (0{,}5 + 1{,}0(u_1 + u_2)) \exp\left(-\frac{131\,000}{RT}\right) \cdot 10^{-4}\ \text{m}^2/\text{sec}.$$

The inverse problem was solved by the above-described algorithm using the Rozenbrok [9] method, which is an analog of the method of conjugate gradients, and in the framework of the method of descent by a parameter on the following network of α:

$$\alpha_i = q\alpha_{i-1}, \quad \alpha_0 = 100, \quad q = 10^{-1}.$$

When initial approximations are assigned randomly with a 2% deviation from the exact solution, the problem solution is correct to $2 \cdot 10^{-3}$%.

Since the input data have no "experimental" error, the above-stated discrepancy is associated with a collective error of the approximations of computational procedures, and it indicates a maximum available accuracy of solving the inverse problem at the given parameters of the finite-difference scheme. The obtained result testifies to the efficiency of the algorithm, whose accuracy can be improved still more.

2. Knowing the limiting accuracy, we may also get an answer to the main question about the relation $\delta = \delta(\varepsilon)$. For this end, it suffices to reiterate the computational experiment with various random errors of the measure δ and to calculate the measure of solution deviation ε from accurate values of the coefficients. It is thus obtained relation $\varepsilon = \varepsilon(\delta)$, presented in graphically form, that will permit finding of the sought one.

To simulate experimental errors on the level of δ, the perturbed input data were computed from the equations:

$$\tilde{\varphi}_i(x_s) = \varphi_i(x_s) + \frac{\delta}{\sqrt{2}} \frac{\xi_{is}}{\sum_{s=1}^{N} \sigma_s \xi_{is}^2}, \quad i = 1, 2, \tag{10}$$

where ξ_{is} the value of a random quantity with a uniform distribution on the segment [−1, 1], then

$$\rho_V^2 = \sum_{i=1}^{2} \sum_{s=1}^{N} \sigma_s (\tilde{\varphi}_i(x_s) - \varphi_i(x_s))^2 = \delta^2.$$

A relative error of the result is estimated a posteriori, with the exact solution $\bar{a}_{k,i}$ of the problem in the experimental conditions known, from the equation

$$\varepsilon = \max_{k,i} \left| \frac{\delta a_{k,i}}{\bar{a}_{k,i}} \right|, \tag{11}$$

where $\delta a_{k,i} = \bar{a}_{k,i} - a_{k,i}$, $a_{k,i}$ are the solutions of the inverse problem obtained at the given δ.

The relation $\varepsilon = \varepsilon(\delta)$ is plotted in Fig. 1. The relation corresponds to the "admissible" range of ε (of up to 15%) and determines, specifically, a maximal possible measurement error (δ = 3%).

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NOTATION

$\mathbf{p}_\alpha$, vector of parameters in the model α; $\mathbf{p}_\beta$, vector of parameters in the model β; $L_i(u_1, u_2)$, i = 1, 2, operator of the system of partial differential equations for u_1 and u_2; M_p, set of the values of $\mathbf{p}_\alpha$ (or $\mathbf{p}_\beta$); M_u, set of the solutions $\mathbf{u} = (u_1, u_2)$; ω_{M_0}, neighborhood of the point M_0 with the coordinates (x_0, t_0); $\mathbf{u}_\omega \to \mathbf{p}_\alpha$, $\mathbf{u}_\omega \to \mathbf{p}_\beta$, mapping; $\int\int_{\omega M_0} f(x, t)d\sigma$, double Riemann integral of the function f(x, t) in the vicinity ω_{M_0} of the point $M_0(x_0, t_0)$; inf $F(\mathbf{p}_\alpha)$, exact lower bound of the function F dependent on the vector of parameters $\mathbf{p}_\alpha$; D, metric space of linear functions; V, metric space of concentration fields observed on the specified set of argument values; $\rho_V^2(Az, v)$, square of metric in the space V; $z_\delta \to \hat{z}$, convergence in metric of the space D; $\Omega(z)$, Tikhonov's stabilizer.

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