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RECONSTRUCTION OF DIFFUSION COEFFICIENTS IN THE PROBLEM OF CARBONITRIDING

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The uniqueness of the determination of carbon and nitrogen diffusion coefficients is found for the process of carbonitriding with complete and abbreviated information on the concentration fields.

Introduction. The process of steel carbonitriding [1] is described under some additional conditions by a nonlinear system of parabolic equations linked by the diffusion coefficients $D_i = D_i(u_1, u_2)$, $i = 1, 2$, where u_1 and u_2 are carbon and nitrogen concentrations, respectively. The coefficients depend on the solution of the system (u_1 and u_2). Linear representations [2] or experimental formulas are used for the functions D_i. However, these approximations are not known for all technological materials. Therefore, the inverse problem [3] of determining D_i from indirect measurements of diffusion fields arises.

The question of the uniqueness of a solution of this problem is of basic importance, first of all, because the answer to it provides information sufficient for unique determination of the sought coefficients, assuming that all the initial data are perfectly accurate. Because of this, regularizing operators of searching for approximations [4] can be used with inaccurate input data.

From studies carried out within the general theory of parabolic equations [5, 6] and referred to the same equation, it can be concluded that even with complete information on the solution of the boundary-value problem in the region of its definition, the coefficients in the equation cannot, strictly speaking, be determined uniquely.

1. **Reconstruction of Carbon and Nitrogen Diffusion Coefficients with Complete Information on the Concentration Fields.** Let the functions $u_1(x, t)$, $u_2(x, t) \in C^{2,1}(\overline{Q})$, which are a solution of the boundary-value problem, be known in the domain $\overline{Q} \equiv [0, l \times [0, \hat{t}]$. The problem is as follows:

$$\frac{\partial u_1}{\partial t} = \frac{\partial}{\partial x}\left(D_1(u_1, u_2)\frac{\partial u}{\partial x}\right),$$

$$\frac{\partial u_2}{\partial t} = \frac{\partial}{\partial x}\left(D_2(u_1, u_2)\frac{\partial c}{\partial x}\right), \quad 0 < x < l, \quad 0 < t \le \hat{t}, \tag{1.1}$$

$$u_1(x, 0) = u_{10}(x), \quad u_2(x, 0) = u_{20}(x), \quad 0 \le x \le l,$$

$$u_1(l, t) = f_1(t), \quad u_2(l, t) = f_2(t), \quad 0 \le t \le \hat{t},$$

$$D_1(u_1, u_2)\frac{\partial u_1}{\partial x}\Big|_{x=0} = \beta_1(u_1, u_2)(u_1 - u_{10\,\mathrm{cr}})|_{x=0}, \quad 0 \le t \le \hat{t}, \tag{1.2}$$

$$D_2(u_1, u_2)\frac{\partial u_2}{\partial x}\Big|_{x=0} = \beta_2(u_1, u_2)(u_2 - u_{20\,\mathrm{cr}})|_{x=0}, \quad 0 \le t \le \hat{t},$$

where $f_i(t)$, $i = 1, 2$, $u_{10}(x)$, $u_{20}(x)$, $u_{10\mathrm{cr}}(t)$, $u_{20cr}(t)$, $\beta_i(u_1, u_2)$, $i = 1, 2$, are known functions of their arguments.

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Theorem 1. Let $u_1(x, t)$, $u_2(x, t) \in C^{2,1}(\overline{Q})$ *be known in* $\overline{Q}$. *Also let* $f_i(t)$, $i = 1, 2$, *on* $[0, t]$, $u_{10}(x)$, $u_{20}(x)$ *on* $[0, l]$, *and* $\beta_i(z, z_2)$, $i = 1, 2$, $z_1 \in [u_{1\min}, u_{1\max}]$, $z_2 \in [u_{2\min}, u_{2\max}]$ *be known.*

Also let $\partial u_1/\partial x \geq \alpha_1 > 0$, $\partial u_2/\partial x \geq \alpha_2 > 0$, $|\partial(u_{1,6}u_2)/\partial(x, t)| \neq 0$ *in* $\overline{Q}$. *Then* $D_1(u_1, u_2)$, $D_2(u_1, u_2)$ *are determined uniquely.*

Proof. The theorem will be proved as follows.

Equations (1.1) will be integrated with respect to x between 0 and x:

$$D_1(u_1, u_2)\frac{\partial u_1}{\partial x}(x, t) - D_1(u_1, u_2)\frac{\partial u_1}{\partial x}\Big|_{x=0} = \int_0^x \frac{\partial u_1}{\partial t}(\xi, t)\, d\xi,$$

$$D_2(u_1, u_2)\frac{\partial u_2}{\partial x}(x, t) - D_2(u_1, u_2)\frac{\partial u_2}{\partial x}\Big|_{x=0} = \int_0^x \frac{\partial u_2}{\partial t}(\xi, t)\, d\xi.$$

Since $D_1\partial u_1/\partial x|_{x=0}$, $D_2\partial u_2/\partial x|_{x=0}$ and $\partial u_1/\partial x$, $\partial u_2/\partial_x \geq \alpha_0$ ($\alpha_0 = \max\limits_{i=1,2} \alpha_i$) are known, then

$$D_1(u_1, u_2) = \frac{\int_0^x \frac{\partial u_1}{\partial t}(\xi, t)\, d\xi}{\frac{\partial u_1}{\partial x}}, \quad D_2(u_1, u_2) = \frac{\int_0^x \frac{\partial u_2}{\partial t}\, d\xi}{\frac{\partial u_2}{\partial x}}. \tag{1.3}$$

The expressions in the right-hand sides of equalities (1.3) are known, and therefore D_1 and D_2 can be found as functions of x and t. Since $I = |\partial(u_1; u_2)/\partial(x, t)| \neq 0$ in $\overline{Q}$, x and t can be expressed uniquely in terms of u_1 and u_2: $x = x(u_1, u_2)$, $t = t(u_1, u_2)$ (from the theorem of the implicit function). Thus, $D_1(u_1, u_2)$ and $D_2(u_1, u_2)$ have been determined.

2. Determination of Diffusion Coefficients with Abbreviated Information on the Concentration Fields. Let us consider the conventional linear model for the coefficients D_i:

$$D_i = \overline{a}_{0,i} + \overline{a}_{1,i}u_1 + \overline{a}_{2,i}u_2, \tag{2.1}$$

where $\overline{a}_{0,i}$, $\overline{a}_{1,i}$, $\overline{a}_{2,i}$, $i = 1, 2$, are some functions of the process temperature [1]. When the temperatures are not too high, the interaction of the processes is neglected ($D_i = \overline{a}_{0,i}$) and the problem is divided into two independent problems. At a high temperature T, assumed to be a parameter, two modifications will be distinguished: α) $\overline{a}_{1,i} = \overline{a}_{2,i} \equiv \overline{a}_{1,i}$, where the interaction is determined by the sum of the concentrations; in this case the sought quantity is considered to be $p_\alpha = \{\overline{a}_{0,i}, \overline{a}_{1,i}\}$, $i = 1, 2$, with the components constant at fixed T; β) $\overline{a}_{1,i} \neq \overline{a}_{2,i}$, but the values of $\overline{a}_{0,i}$ are considered to be known from indirect observations of the diffusion fields; in this case the sought quantity is $p_\beta = \{\overline{a}_{1,i}, \overline{a}_{2,i}\}$, $i = 1, 2$, where the components are also constant.

It should ne noted that in case (β), $\overline{a}_{0,i}$ can also be determined uniquely when $\overline{a}_{0,i} = \overline{a}_{0,i}(u_i)$, without too strict a limitation imposed on the class of these fucntions [7] and even with abbreviated information on the diffusion fields. In this case it is sufficient that apart from ordinary boundary conditions of the second or third kind, the concentrations $u_i(0, t) = \varphi_i(t)$, $i = 1, 2$, be prescribed as a time function at one of the ends.

Within the above models at preset initial concentrations and with boundary conditions of any type, the diffusion process is described by the system of equations

$$L_i(u_1, u_2) \equiv \frac{\partial u_i}{\partial t} - \frac{\partial}{\partial x}\left[D_i(u_1, u_2)\frac{\partial u_i}{\partial x}\right] = 0,$$

$$x, t \in Q \equiv (0, l) \times (0, \hat{t}), \quad i = 1, 2. \tag{2.2}$$

Let us denote the set of values of p_α (or p_β) by M_p and the set of solutions of system (2.2) under the chosen additional conditions $p_\alpha \in M_p$ (or $p_\beta \in M_p$) by M_u. It is clear that the condition $\boldsymbol{u} \in M_u$ ensures the existence of a solution of the inverse problem.

Diffusion fields are called degenerated in a subregion Q if $\partial^2 u_i/\partial x^2 \equiv 0$ or $\partial/\partial x[(u_1+u_2)\partial u_i/\partial x] \equiv \alpha\partial^2 u_i/\partial x^2$, $i = 1, 2$, for some $\alpha \neq 0$.

Theorem 2. *Let $u \in M_u$ be known in a vicinity ω_{M_0} of any point $M_0(x_0, t_0 \in Q$ and in ω_{M_0} the diffusion fields not be degenerate. Then a solution of the inverse problems $\mathbf{u}_\omega \to \mathbf{p}_\alpha$, $\mathbf{u}_\omega \to \mathbf{p}_\beta$ is unique.*

Proof. For example, in case (α) let us consider the function $F(\mathbf{p}_\alpha) \equiv \int\int_{\omega M_0} [L_1^2(\mathbf{u}) + L_2^2(\mathbf{u})]d\sigma$. It is obvious that inf $F(\mathbf{p}_\alpha) = 0$ and any solution of the inverse problem is a solution of the variational problem. Now, it can be noted that

$$F(\mathbf{p}_\alpha) = \sum_{i=1}^{2} (p_{11}^{(i)} \bar{a}_{0,i}^2 + 2p_{12}^{(i)} \bar{a}_{0,i} \bar{a}_{1,i} + p_{22}^{(i)} \bar{a}_{1,i}^2 - 2q_1^{(i)} \bar{a}_{0,i} - 2q_2^{(i)} \bar{a}_{1,i} + r_i),$$

$$p_{11}^{(i)} = \int_{\omega}\int_{M_0} \left(\frac{\partial^2 u_i}{\partial x^2}\right)^2 d\sigma, \quad p_{12}^{(i)} = \int_{\omega}\int_{M_0} \frac{\partial^2 u_i}{\partial x^2} \frac{\partial}{\partial x}\left[(u_1 + u_2)\frac{\partial u_i}{\partial x}\right] d\sigma,$$

$$p_{22}^{(i)} = \int_{\omega}\int_{M_0} \left\{\frac{\partial}{\partial x}\left[(u_1 + u_2)\frac{\partial u_i}{\partial x}\right]\right\}^2 d\sigma,$$

and the terms containing no $\bar{a}_{k,i}$, $k = 0, 1$, $i = 1, 2$, are denoted by r_i.

Then the critical points are determined from systems separated in i: $\partial F/\partial\bar{a}_{k,i} = 0$, $k = 0, 1$, $i = 1, 2$. Because of the obvious inequalities $p_{11}^{(i)} \geq 0$, $\Delta_i = p_{11}^{(i)}p_{22}^{(i)} - [p_{12}^{(i)}] \geq 0$, the point of the global extremum can be nonunique only when the exact equalities $p_{11}^{(i)} = 0$ or $\Delta_i = 0$ are satisfied. It can be easily seen that they mean degeneration of the fields. For case (β) the proof is similar. It should be noted that the conditions of degeneration result either in decomposition of the diffusion field for u_1 and u_2 into independent fields or (similarly to [5]) in a specific structure for them that is inconsistent with the conditions of problem (2.2). On the other hand, the formulated conditions of uniqueness are local and can be referred to an infinitesimal neighborhood of a point.

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