Moscow University Physics Bulletin
Vol. 46, No. 6, pp. 27–30, 1991

Vestnik Moskovskogo Universiteta. Fizika
UDC 536.758;539.201

ON THE UNIQUENESS OF THE SOLUTION TO THE INVERSE CARBONITRIDING PROBLEM

V. B. Glasko, I. E. Stepanova, and S. A. Yurasov

The problem of uniqueness of the determination of diffusion coefficient from data on the concentration field is investigated for carbonitriding models. For a more general inverse problem the uniqueness is proved for the normal solution with respect to the polynomial coefficients of the parabolic system of equations.

1. The technological steel carbonitriding process [1] is described, under some additional conditions, by a nonlinear system of parabolic equations interrelated via the diffusion coefficients, which depend on the system solution, namely, on the concentration of carbon (u_1) and nitrogen (u_2): $D_i = D_i(u_1,\, u_2)$. For the functions D_i use is made of linear representations [2] or experimental formulas. However, these approximations are not known for all technological processes. There arises a problem of determining D_i from data of indirect measurements of diffusion fields, which belongs to the class of inverse problems [3]. The uniqueness of the solution to such a problem is of fundamental importance first of all because in this case some additional conditions can be set that would be sufficient for the unique determination of the sought coefficients under the assumption that all initial data are absolutely exact. When the solution is unique, one can use regularizing operators to construct approximations [4] for inexact input data.

The investigations carried out from the standpoint of the general theory of parabolic equations [5, 6] and related to a single equation suggest a conclusion that, generally speaking, even with complete information about the solution to the boundary value problem in its domain, it is impossible to determine uniquely the equation coefficients. In the present paper the problem of uniqueness is considered primarily within the framework of models close to those used in carbonitriding problems when the input information about the concentration field is not complete.

For the sake of vividness, we shall consider a spatially one-dimensional boundary value problem: $0 \leqslant x \leqslant l$, $0 \leqslant t \leqslant \hat{t}$.

2. First of all we consider the generally accepted linear model for the coefficients D_i:

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

where $\overline{a}_{0,i}$, $\overline{a}_{1,i}$ and $\overline{a}_{2,i}$ are some functions of the process temperature [1]. At not very high temperatures the interaction between the processes is neglected ($D_i = \overline{a}_{0,i}$), and the problem splits into two independent problems. At a high temperature T, which is regarded as a parameter, we shall distinguish between the following two modifications. Modification (α): the case $\overline{a}_{1,i} = \overline{a}_{2,i} \equiv \overline{a}_{1,i}$ when the interaction is determined by the sum of the concentrations. Here the vectors $\mathbf{p}_\alpha = \{\overline{a}_{0,i};\, \overline{a}_{1,i}\}$, $i = 1,\, 2$, with constant components for a fixed temperature, are regarded as unknown quantities. Modification (β): $\overline{a}_{1,i} \neq \overline{a}_{2,i}$ but the values of $\overline{a}_{0,i}$ are assumed to be known from indirect observations of uncoupled diffusion fields. In this case the unknown quantity is $\mathbf{p}_\beta = \{\overline{a}_{1,i};\, \overline{a}_{2,i}\}$, where the components are also constant.

Note that the parameters $\overline{a}_{0,i}$ for modification (β) can also be determined uniquely in the case when $\overline{a}_{0,i} = \overline{a}_{0,i}(u_i)$ with not too stringent restrictions on the class of such functions [7] and even with incomplete information about the diffusion fields: it is sufficient that, along with the ordinary boundary conditions of the second and third kind [8], the concentrations at one of the end points be set as functions of time: $u_i(0,\, t) = \varphi_i(t)$. Within the framework of the above models, for given initial concentrations and boundary conditions of any type, the diffusion process is described by the system of equations

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

Denote the set of values of $\mathbf{p}_\alpha$ (or $\mathbf{p}_\beta$) by M_p and the set of solutions $\mathbf{u} = (u_1, u_2)$ to system (2) by M_u for chosen additional conditions, and let $\mathbf{p}_\alpha \in M_p$ (or $\mathbf{p}_\beta \in M_p$). It is clear that the condition $\mathbf{u} \in M_u$ ensures the existence of solution for the inverse problem.

We shall say that the diffusion fields are degenerate in a subregion Q if $\partial^2 u_i/\partial x^2 \equiv 0$ or $\frac{\partial}{\partial x}\Big((u_1, u_2)\times \frac{\partial u_i}{\partial x}\Big) \equiv \alpha \frac{\partial^2 u_i}{\partial x^2}$ in this subregion for some α, $i = 1, 2$.

Theorem 1. *Let $u \in M_u$ be known in some neighborhood ω_{M_0} of any point $M_0(x_0, t_0) \in Q$ and let the diffusion fields be nondegenerate. Then the solutions to the inverse problems $\mathbf{u}_\omega \to \mathbf{p}_\alpha$, $\mathbf{u}_\omega \to \mathbf{p}_\beta$ are unique.*

To prove the **Theorem 1**, for instance, in the case (α) we consider the function $F(\mathbf{p}_\alpha) \equiv \iint\limits_{\omega_{M_0}} \big(L_1^2(\overline{u}) + L_2^2(\overline{u})\big)\, d\sigma$. It is clear that $\inf F(\mathbf{p}_\alpha) = 0$, and any solution to the inverse problem is a solution to the variational problem.

We can now note that

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

$$p_{11}^{(i)} = \iint\limits_{\omega_{M_0}} \Big(\frac{\partial^2 u_i}{\partial x^2}\Big)^2 d\sigma, \quad p_{22}^{(i)} = \iint\limits_{\omega_{M_0}} \Big(\frac{\partial}{\partial x}\Big((u_1+u_2)\frac{\partial u_i}{\partial x}\Big)\Big)^2 d\sigma,$$

$$p_{12}^{(i)} = \iint\limits_{\omega_{M_0}} \frac{\partial^2 u_i}{\partial x^2}\frac{\partial}{\partial x}\Big((u_1+u_2)\frac{\partial u_i}{\partial x}\Big)\, d\sigma, \quad q_1^{(i)} = \iint\limits_{\omega_{M_0}} \frac{\partial u_i}{\partial t}\frac{\partial^2 u_i}{\partial x^2}\, d\sigma,$$

$$q_2^{(i)} = \iint\limits_{\omega_{M_0}} \frac{\partial u_i}{\partial t}\frac{\partial}{\partial x}\Big((u_1+u_2)\frac{\partial u_i}{\partial x}\Big)\, d\sigma, \quad r_i = \iint\limits_{\omega_{M_0}} \Big(\frac{\partial u_i}{\partial t}\Big)^2 d\sigma, \quad i = 1, 2.$$

In this case the critical points are found from the systems

$$\partial F/\partial \overline{a}_{k,i} = 0, \; k = 0, 1; \; i = 1, 2,$$

which split into uncoupled subsystems for $i = 1, 2$. By virtue of the obvious conditions $p_{11}^{(i)} \geqslant 0$, $\Delta_i = p_{11}^{(i)}p_{22}^{(i)} - p_{12}^{(i)} \geqslant 0$, the point of global extremum can be non-unique only in the case of the exact relations $p_{11}^{(i)} = 0$ or $\Delta_i = 0$ meaning, as can easily be seen, that the fields are degenerate.

In the case (β) the proof is analogous.

Note that the degeneracy conditions result either in the splitting of the equations for the diffusion fields u_1 and u_2 into independent subsystems, or (by analogy with [5]) in a specific structure of the equations incompatible with the conditions of problem (2). On the other hand, the stated uniqueness conditions are of local character and can be related to an arbitrarily small neighborhood of the point.

3. Another concept of the structure of D_i, following from physico-technological data, consists in that the mutual effect of the diffusion fields can be determined by a relatively small additional term to the "basic" coefficient $\overline{a}_{0,i}$. The asymptotic model

$$D_i(u_1, u_2) = \overline{a}_i(u_i) + \varepsilon\delta_i(u_j), \quad i = 1, 2; \; j = 1, 2; \; j \neq i, \tag{3}$$

where ε is a small parameter, corresponds to this case.

We shall assume that the coefficients $\overline{a}_i(u_i) > 0$ are known and are determined uniquely [7] (along with the diffusion fields $u_i \equiv u_{0i}(x, t)$) by Eqs. (2) with the following conditions:

$$\overline{a}_i(u_i)\frac{\partial u_i}{\partial x}\Big|_{x=0} = \psi_i(t), \quad \psi_i|_{t=0} > 0, \quad u_i|_{x=0} = \chi_i(t),$$
$$\frac{\partial u_i}{\partial x}\Big|_{x=l} = 0, \quad u_i|_{t=0} = \varphi_i(x), \tag{4}$$

which are compatible in the classical sense. Note that for the chosen $\psi_i(t)$ we have $\frac{\partial u_{0i}}{\partial x}\Big|_{x=0} \geqslant \gamma > 0$. The existence of such regimes for boundary conditions of the third kind in carburizing and nitriding problems was demonstrated in [9]. The unknown function turns out to be $\boldsymbol{\delta}(\mathbf{u}) = \{\delta_1(u_2), \delta_2(u_1)\}$.

Using the estimates from [10] of solutions to parabolic systems for sufficiently smooth functions $\overline{a}_i$, δ_i, ψ_i, and φ_i, one can show that in the case (3) the diffusion fields have the following asymptotic structure:

$$u_i(x, t) = \sum_{k=0}^{1} \varepsilon^k u_{ki}(x, t) + O(\varepsilon^2), \qquad i = 1, 2. \tag{5}$$

The field $\partial u_i/\partial x$ has a similar structure.

Denote by N_δ the set of vector functions $\boldsymbol{\delta}(\mathbf{u})$ continuously differentiable on the positive semi-axis $[0, +\infty)$. Let N_u be the set of the functions $\mathbf{u}_1 \equiv \{u_{11}(x, t), u_{12}(x, t)\}$ defined for each $\delta \in N_\delta$, by virtue of representation (5), by system (2) for the same values of ψ_i and φ_i in (4). It can be shown that $u_{1i}(t)$ satisfy for $x = 0$ the boundary conditions

$$\Big(\overline{a}_i(u_{0i})\frac{\partial u_{1i}}{\partial x} + \overline{a}_i'(u_{0i})\frac{\partial u_{0i}}{\partial x}u_{1i}\Big)\Big|_{x=0} = -\delta(u_j)\frac{\partial u_{0i}}{\partial x}\Big|_{x=0}. \tag{6}$$

Theorem 2. *Let $u_{1i}(x, t) \in N_u$, $i = 1, 2$, and let $\chi_i(t)$ be continuous monotonically increasing functions with range $\Delta \equiv [u_{i,\min}, u_{i,\max}]$. Then for given $\frac{\partial u_i}{\partial x}\Big|_{x=0} = \psi_i(t)$ and $u_{1i}|_{x=0} = \varphi_{1i}(t)$ the functions $\delta_1(u_2)$ and $\delta_2(u_1)$ are uniquely determined on the closed interval Δ.*

Indeed, according to [6], the functions $\delta_1^*(t) \equiv \delta_1(\chi_2(t))$, $\delta_2^*(t) \equiv \delta_2(\chi_1(t))$ are uniquely defined under the condition $\frac{\partial u_{0i}}{\partial x}\Big|_{x=0} \neq 0$, which is implied by the condition $u_{1i} \in N_u$. However, under the indicated restrictions on $\chi_i(t)$, the inverse functions $t_j = t_j(u)$, $\delta_i^*(t_i(u)) = \delta_i(u_j)$, $j \neq i$; $i, j = 1, 2$, are defined on the closed interval Δ.

4. In conclusion we state the result for the linear model, which, in a sense, generalizes (1) and at the same time extends the fact established in [6] to the system of two equations.

Let us set

$$\overline{a}_{0,i} \equiv a_{0,i}; \quad \overline{a}_{k,i} = \overline{a}_{k,i}(x, t), \quad k = \overline{0, 2}, \quad i = 1, 2, \tag{7}$$

in (1). We shall assume that $a_{k,i}(x, t) \in W_2^{1,0}(Q)$ and that the conditions (γ) are satisfied:

$$0 \leqslant \lambda_{k,i} \leqslant \overline{a}_{k,i}(x, t) \leqslant \overline{\lambda}_{k,i}; \quad \|\overline{a}_{k,i}\|_{W_2^{1,0}} \leqslant M_{k,i}, \quad k = \overline{0, 2},$$
$$i = 1, 2, \quad M_{k,i} \geqslant \widetilde{\lambda}_{k,i}\sqrt{lt},$$

where $\lambda_{k,i}$, $\widetilde{\lambda}_{k,i}$, and $M_{k,i}$ are some constants set a priori. The set of such collections of coefficients will be denoted as K_a, and let K_u be the corresponding set of solutions to system (2) for boundary conditions of the first kind and arbitrary initial functions compatible with them in the classical sense.

We denote $\mathbf{p} \equiv \{\overline{a}_{k,i}(x, t)\} \in K_a$ and introduce the norm $\|\mathbf{p}\|$ by the formula

$$\|\mathbf{p}\| \equiv (\mathbf{p}, \mathbf{p}) = \sum_{k=0}^{2}\sum_{i=1}^{2} \iint_Q \Big[\overline{a}_{k,i}^2 + \Big(\frac{\partial \overline{a}_{k,i}}{\partial x}\Big)^2\Big]\, dx\, dt. \tag{8}$$

We have

Theorem 3. *If K_a is a bounded closed convex set and if for the diffusion fields defined in Q we have $\mathbf{u} = \{u_1, u_2\} \in K_u$, then the corresponding set $\mathbf{p} = \{\overline{a}_{k,i}(x, t)\}$ (minimal with respect to the norm (8)) is unique.*

To prove **Theorem 3** one should consider the variational problem for a functional similar to $F(\mathbf{p})$ in **Theorem 1**, and then the analysis can be carried out by complete analogy with [10].

The assertion of the theorem can be restated in a local manner by replacing Q by ω_{M_0}. However, in contrast to the above **Theorems 1** and **2**, **Theorem 3** does not imply the solution uniqueness in the classical sense for the applied problem under consideration.

The authors express their gratitude to A. N. Tikhonov and V. D. Kal'ner for interest in this work and valuable advice.

REFERENCES

1. M. N. Leonidova, L. A. Shvartsman, and L. N. Shul'ts, *Physico-Chemical Foundations of Metal Interaction with Controlled Atmospheres* (in Russian), Moscow, 1980.
2. *Computer-Based Modeling and Automation of Processes of Chemicothermal Treatment of Motor-Car Components. Information Survey. Series 11. Motor-Car Construction Technology* (in Russian), Moscow, 1987.
3. A. N. Tikhonov, V. D. Kal'ner, and V. B. Glasko, *Mathematical Modeling of Technological Processes and the Inverse Problem Method in Machine Building* (in Russian), Moscow, 1990.
4. A. N. Tikhonov and V. Ya. Arsenin, *Methods for Solving Improperly Posed Problems* (in Russian), Moscow, 1986.
5. V. V. Frolov, *Inzh.-Fiz. Zhurn.*, vol. 29, no. 1, p. 808, 1975.
6. B. M. Budak and V. N. Vasil'eva, *Solution of Optimal Control Problems and Some Inverse Problems* (in Russian), p. 3, Moscow, 1974.
7. N. V. Muzylev, *Zh. Vychisl. Matem. i Matem. Fiziki*, vol. 20, no. 2, p. 388, 1980.
8. A. N. Tikhonov and A. A. Samarskii, *Equations of Mathematical Physics* (in Russian), Moscow, 1953.
9. V. D. Kal'ner, S. A. Yurasov, V. B. Glasko, N. I. Kulik, and Yu. K. Evseev, *Metalloved. i Termich. Obrabotka Metallov*, no. 1, p. 11, 1986.
10. O. A. Ladyzhenskaya, V. A. Solonnikov, and N. N. Ural'tseva, *Linear and Quasi-Linear Parabolic Equations* (in Russian), Moscow, 1967.

5 February 1991 Department of Mathematics