Leading coefficient’s recovering problem for nonlinear convection–diffusion–reaction equation

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Abstract. The problem of diffusion coefficient identification for a nonlinear convection–
diffusion–reaction equation, in which reaction coefficient has a rather common dependence on
substance’s concentration and on spatial variable is considered.

1. Introduction. The boundary value problem

Inverse problems’ research for linear and nonlinear heat-and-mass transfer models has been
an urgent issue during a long period of time. One of the main problems is an identification
problem for unknown densities of boundary and distributed sources or of model’s differential
equations’ coefficients or boundary conditions with the help of additional information about
system’s conditions, which is described by the model. The studying of such inverse problems can
be reduced to the studying of corresponding extremal problems using the optimization method
[1]. A number of papers is dedicated to the description of this method for heat-and-mass transfer
and other hydrodynamic models (e.g. see [2–11]).

In this paper the diffusion coefficient’s identification problem is studied for the nonlinear
convection-diffusion-reaction equation in the case, when the reaction coefficient has a rather
common dependence on substance’s concentration and on spatial variable, is considered. The
inverse coefficient problems for nonlinear heat-and-mass transfer models were considered in [5, 6]
and [9, 10], also for semilinear convection-diffusion-reaction equation these problems were studied
in [12, 13].

See [12–17] on studying of boundary value and extremum problems for the semilinear
convection-diffusion-reaction model.

In a bounded domain $\Omega \subset \mathbb{R}^3$ with the boundary $\Gamma$ the following boundary value problem is
considered

$$-\text{div}(\lambda(x)\nabla \varphi) + u \cdot \nabla \varphi + k(\varphi, x)\varphi = f \text{ in } \Omega, \quad \varphi = \psi \text{ on } \Gamma.$$  (1)

Here function $\varphi$ means polluting substance’s concentration, $u$ is a given vector of velocity, $f$ is
a volume density of external sources of substance, $\lambda(x)$ – a diffusion coefficient, function $k(\varphi, x)$ is
a reaction coefficient, $\psi$ is a given boundary function. This problem (1) will be called Problem
1 below.

In this paper, firstly, a Problem 1’s global solvability is proved in a general case. An
identification problem of the diffusion coefficient $\lambda(x)$ is reduced to the multiplicative control
problem. It’s solvability is proved for the common type reaction coefficient. For concrete
reaction coefficients, as a rule, with a power dependence on the concentration, such as $k(\varphi, x) = \beta_1(x)\varphi^2 + \beta_2(x)\varphi^2 + \beta_3(x)$, the optimality systems for extremum problem are obtained.

While studying Problem 1 and optimal control problems, Sobolev spaces will be used: $H^s(\Omega)$, $s \in \mathbb{R}$, $L^r(\Omega)$, $1 \leq r \leq \infty$, where $D$ is either a domain $\Omega$ or its boundary $\Gamma$. Inner products in $L^2(\Omega)$ and $H^1(\Omega)$ are denoted by $(\cdot, \cdot)$, $\cdot, \cdot$ is a constant, which depends on $x$, $\varphi$, $\psi$, and $\eta$, and $\beta$ is a rule, with a power dependence on the concentration, such as

$$(k \varphi, x) = \beta_1(x)\varphi^2 + \beta_2(x)\varphi^2 + \beta_3(x),$$

the optimality systems for extremum problem are obtained.

Let $D(\Omega)$ be the space of infinitely differentiable, finite functions in $\Omega$, $H^1(\Omega)$ be the closure of $D(\Omega)$ in $H^1(\Omega)$, $H^{-1}(\Omega) = H_0^1(\Omega)^*$. The Poincare-Friedrichs inequality holds:

$$|\varphi|_{1, \Omega} \geq \delta|\varphi|_{1, \Omega} \forall \varphi \in H^1_0(\Omega),$$

where $\delta = \text{const} > 0$, $L^p_+(\Omega) = \{k \in L^p(\Omega) : k \geq 0\}$, $p \geq 3/2$, $H^s_0(\Omega) = \{h \in H^s(\Omega) : h \geq \lambda_0 > 0\}$, $s \geq 0$.

Let us denote $\mathbf{Z} = \{\mathbf{v} \in L^4(\Omega) : \text{div}\mathbf{v} = 0 \text{ in } \Omega\}$.

Let us mention that power functions $k(\varphi, x)$ is not an ordinary function of $\varphi$ and $x$, but $k$ is an operator, acting from $H^1(\Omega) \to L^p_+(\Omega)$, where $p \geq 3/2$ and satisfying the following conditions:

(i) $\Omega$ is a bounded domain in $\mathbb{R}^3$ with boundary $\Gamma \in C^{0,1}$;

(ii) $u \in \mathbf{Z}, f \in L^2(\Omega)$;

(iii) $\lambda \in H^2_0(\Omega), \psi \in H^{1/2}(\Gamma)$.

In the present paper the reaction coefficient $k(\varphi, x)$ is not an ordinary function of $\varphi$ and $x$, but $k$ is an operator, acting from $H^1(\Omega) \to L^p_+(\Omega)$, where $p \geq 3/2$ and satisfying the following conditions:

(1) for any $w_1, w_2 \in B_r = \{w \in H^1(\Omega) : \|w\|_{1, \Omega} \leq r\}$ the estimate takes place:

$$||k(w_1, \cdot) - k(w_2, \cdot)||_{L^p(\Omega)} \leq L\|w_1 - w_2\|_{L^4(\Omega)},$$

where $L$ is a constant, which depends on $r$, but doesn’t depend on $w_1, w_2$;

(2) with a certain $s \geq 0$ the estimate holds

$$||k(w, \cdot)||_{L^p(\Omega)} \leq C_{1p}\|w\|_{1, \Omega}^{1/2} \forall w \in H^1(\Omega),$$

(3) $k(\varphi, \cdot)\varphi$ satisfies the monotonicity condition

$$(k(\varphi_1)\varphi_1 - k(\varphi_2)\varphi_2, \varphi_1 - \varphi_2) \geq 0 \quad \varphi_1, \varphi_2 \in H^1(\Omega).$$

Let us mention that power functions $k(w) = w^2$ and $k(w) = w^2|w|$ from [19, 20] also satisfy the conditions (1)–(3) (see [16]).

Further let us make an example of the operator $k(\varphi, x)$, satisfying (1)–(3) and not being an ordinary function of $(\varphi, x)$: $k(\varphi) = \varphi^2$ in a subdomain $Q \subset \Omega$ and $k(\varphi) = k_0$ in $\Omega \setminus Q$, where $k_0 \in L^{3/2}_+(\Omega)$.

The following Green’s theorem will be used (see [11, p. 128] for more details about it):

$$\int_{\Omega} (\Delta \varphi, \eta) - (\varphi, \Delta \eta) - (\partial \varphi / \partial n, \eta)\Gamma \quad \forall \varphi \in H^1(\Omega), \eta \in H^1(\Omega),$$

$$(u \cdot \nabla \varphi, \eta) = -(u \cdot \nabla \eta, \varphi) \quad \forall u \in \mathbf{Z}, \varphi, \eta \in H^1_0(\Omega).$$

Here and below $\langle \cdot, \cdot \rangle_{\Omega}$ means the relation of duality between $H^{1/2}(\Gamma)$ and $H^{-1/2}(\Gamma)$.

Let us denote bilinear forms $a_u$ and $a_0$: $H^1_0(\Omega) \times H^1_0(\Omega) \to \mathbb{R}$ by formulæ

$$a_u(\varphi, \eta) = \int_{\Omega} (u \cdot \nabla \varphi, \eta)dx, a_0(\varphi, \eta) = \lambda(\nabla \varphi, \nabla \eta) + a_u(\varphi, \eta) + (k_0 \varphi, \eta).$$

(5)
Due to (6)–(8) and property (2) we show that the operator $A$ have the following properties:

1) the operator $A$ is bounded and semicontinuous, i.e. the form $(A(u + \lambda v), w)$ is continuous in $\lambda \in \mathbb{R}$ for all $u, v, w \in V$;

2) the operator $A$ is monotone, i.e. $(A(u) - A(v), u - v) \geq 0$ for all $u, v \in V$;

3) $(A(u), v) / \|v\|_V \to +\infty$ at $\|v\|_V \to \infty$.

Then the mapping $A : V \to V^*$ is surjective, i.e. for any $l \in V^*$ there is such $u \in V$ that $A(u) = l$.

Let us multiply the equation in (1) by $h \in H^1(\Omega)$ and integrate over $\Omega$, applying the formula (3). Then this will be obtained:

$$\langle \lambda \nabla \varphi, \nabla h \rangle + (k(\varphi, x)\varphi, h) + (u \cdot \nabla \varphi, h) = (f, h) \quad \forall h \in H_0^1(\Omega).$$

(9)

The function $\varphi \in H^1(\Omega)$, which satisfies (9), will be called a weak solution of problem 1. To prove the solvability of (9), represent the function $\varphi$ in the form

$$\varphi = \tilde{\varphi} + \varphi_0,$$

(10)

where $\tilde{\varphi} \in H_0^1(\Omega)$ is an unknown function and the function $\varphi_0 \in H^1(\Omega)$ satisfies the conditions

$$\varphi_0 = \psi \text{ on } \Gamma, \quad \|\varphi_0\|_{1,\Omega} \leq C_\Gamma \|\psi\|_{1/2,\Gamma}.$$ 

Substituting (10) into (9) we obtain

$$\langle \lambda \nabla \tilde{\varphi}, \nabla h \rangle + (k(\tilde{\varphi} + \varphi_0, x)(\tilde{\varphi} + \varphi_0), h) + (u \cdot \nabla (\tilde{\varphi} + \varphi_0), h) =$$

$$= (f, h) - (\lambda \nabla \varphi_0, \nabla h) - (u \cdot \nabla \varphi_0, h) \quad \forall h \in H_0^1(\Omega).$$

(11)

Adding to both sides of (11) the term $-k(\varphi_0, x)\varphi_0, h)$, we obtain

$$\langle \lambda \nabla \tilde{\varphi}, \nabla h \rangle + (k(\tilde{\varphi} + \varphi_0, x)(\tilde{\varphi} + \varphi_0), h) + (u \cdot \nabla (\tilde{\varphi} + \varphi_0), h) =$$

$$= (f, h) - (k(\varphi_0, x)\varphi_0, h) - (\lambda \nabla \varphi_0, \nabla h) - (u \cdot \nabla \varphi_0, h) \quad \forall h \in H_0^1(\Omega).$$

For the proof of problem (9)'s solvability introduce a nonlinear operator $A : H_0^1(\Omega) \to H^{-1}(\Omega)$ by formula

$$(A(\tilde{\varphi}), h) \equiv \langle \lambda(x)\nabla \tilde{\varphi}, \nabla h \rangle + (k(\tilde{\varphi} + \varphi_0, x)(\varphi_0 + \tilde{\varphi} - k(\varphi_0)\varphi_0), h) + (u \cdot \nabla \tilde{\varphi}, h) \quad \forall h \in H_0^1(\Omega).$$

Due to (6)–(8) and property (2) we show that the operator $A$ is continuous:

$$|(A(\tilde{\varphi}_1) - A(\tilde{\varphi}_2), h)| \leq (\|\lambda\|_{2,\Omega} + \gamma_p L\|_4 \|\tilde{\varphi}_1\|_{1,\Omega} + \gamma_p C_{1p} C_s (\|\tilde{\varphi}_1\|_{1,\Omega}^s + C_{1p}^s \|\psi\|_{1/2,\Gamma}^s) +$$

$$+ \gamma_p C_{1p} C_s (\|\tilde{\varphi}_2\|_{1,\Omega}^s + C_{1p}^s \|\psi\|_{1/2,\Gamma}^s).$$
the group of controls, which consists of function $\lambda$, two groups: the group of fixed data, where functions $\phi$ are considered problem is reduced to the solving of the control problem.

By definition, $A(0) = 0$, then from (12) at $\tilde{\phi}_2 = 0$ follows the boundedness of operator $A$.

The monotonicity of the operator $A$ follows from property (2) and (8). From monotonicity of $k(\varphi, \cdot) \varphi$ and (8) follows that $3)$ is true.

Arguing further as in [16, 17], we are coming to the next theorem

**Theorem 2.** Let conditions $(i)$–$(iii)$ and $(1)$–$(3)$ hold. Then there is a unique weak solution $\varphi \in H^1(\Omega)$ of the problem 1 and the following holds

$$\|\varphi\|_{1, \Omega} \leq C_s(\|f\|_{\Omega} + C_T(\|\lambda\|_{L^\infty(\Omega)} + \gamma\|u\|_{L^1(\Omega)})\|\psi\|_{1/2, \Gamma} + \gamma_p C_1 p_{\phi}\|\psi\|_{1/2, \Gamma} + C_T\|\psi\|_{1/2, \Gamma}.$$  

2. Optimal control problem

There are a lot of situations in practice, when some parameters of Problem 1 are unknown and it’s required to determine them together with the solution $\varphi$ according to some information about the solution. On the capacity of the mentioned information about solution, the values $\varphi^d(x)$ of the concentration $\varphi$ are often taken, which can be measured in points of some set $Q \subset \Omega$.

Below we study the case, when the diffusion coefficient $\lambda(x)$ is unknown and should be searched together with the solution $\varphi$.

To solve this inverse problem the optimization method will be used, according to which the considered problem is reduced to the solving of the control problem.

In compliance with this method let’s divide the whole set of initial data of problem 1 into two groups: the group of fixed data, where functions $u$, $f$, $k(\varphi, x)$ and $\psi$ will be included, and the group of controls, which consists of function $\lambda(x)$, assuming that it can be changed in some set $K$.

Let us introduce the operator of the direct problem $F = (F_1, F_2) : H^1(\Omega) \times K \to Y = H^{-1}(\Omega) \times H^{1/2}(\Gamma)$ by the formulae

$$(F_1(\varphi, \lambda), h) = (\lambda(x)\nabla \varphi, \nabla h) + (k(\varphi, x)\varphi, h) + (u \cdot \nabla \varphi, h) - (f, h),$$

$$F_2(\varphi) = \varphi|_{\Gamma} - \psi.$$  

Then (9) can be rewritten in the following form:

$$F(\varphi, \lambda) = 0.$$  

Treating (13) as a conditional restriction on the state $\varphi \in H^1(\Omega)$ and on the control $\lambda \in K$, the problem of conditional minimization can be formulated as follows:

$$J(\varphi, \lambda) \equiv \frac{\mu_0}{2} I(\varphi) + \frac{\mu_1}{2} \|\lambda\|_{2, \Omega}^2 \to \inf, F(\varphi, \lambda) = 0, (\varphi, \lambda) \in H^1(\Omega) \times K.$$  

Here $I : H^1(\Omega) \to \mathbb{R}$ is a weakly semicontinuous below functional.

The set of possible pairs for problem (14) is denoted by $Z_{ad} = \{(\varphi, \lambda) \in H^1(\Omega) \times K : F(\varphi, \lambda) = 0, J(\varphi, \lambda) < \infty\}$ and let’s suppose that these conditions hold

$(j) K \subset H^2_0(\Omega)$ is a nonempty convex closed set;

$(jj) \mu_0 > 0$, $\mu_1 \geq 0$ and $K$ is a bounded set or $\mu_0 > 0$, $\mu_1 > 0$ and functional $I$ is bounded below.

The following cost functionals can be used in the capacity of the possible ones [11]:

$$I_1(\varphi) = \|\varphi - \varphi^d\|_{Y}^2 = \int_{\Omega} |\varphi - \varphi^d|^2 d\mathbf{x}, \quad I_2(\varphi) = \|\varphi - \varphi^d\|_{1, Q}^2.$$

$$+ \gamma_1 \|u\|_{L^1(\Omega)})\|\psi - \varphi^d\|_{1, \Omega}.$$  

(12)
Here $\varphi^d \in L^2(Q)$ (or $\varphi^d \in H^1(Q)$) is a given function in some subdomain $Q \subset \Omega$.

**Theorem 3.** Let conditions (i)--(iii), (1)–(3) and (j), (jj) hold, $I: H^1(\Omega) \to \mathbb{R}$ is a weakly semicontinuous below functional, and $Z_{ad}$ is nonempty set. Then there is at least one solution $(\varphi, \lambda) \in H^1(\Omega) \times K$ of optimal control problem (14).

**Proof.** Let $(\varphi_m, \lambda_m) \in Z_{ad}$ be a minimizing sequence for the functional $J$, for which the following is true:

$$\lim_{m \to \infty} J(\varphi_m, \lambda_m) = \inf_{(\varphi, \lambda) \in Z_{ad}} J(\varphi, \lambda) \equiv J^*.$$ 

That and the conditions of theorem for the functional $J$ from (14) imply the estimate $\|\lambda_m\|_{2, \Omega} \leq c_1$. From Theorem 2 follows directly that $\|\varphi_m\|_{1, \Omega} \leq c_2$, where constants $c_1, c_2$ don’t depend on $m$.

Then the weak limits $\varphi^* \in H^1(\Omega)$ and $\lambda^* \in K$ of some subsequences of the sequences \{\varphi_m\} and \{\lambda_m\} exist. Corresponding sequences will be also denoted by \{\varphi_m\} and \{\lambda_m\}. With this in mind it can be considered that

$$\varphi_m \to \varphi^* \in H^1(\Omega) \text{ weakly in } H^1(\Omega) \text{ and strongly in } L^s(\Omega), \ s < 6,$$

$$\lambda_m \to \lambda^* \in K \text{ weakly in } H^2(\Omega) \text{ and strongly in } L^\infty(\Omega).$$

Let’s show that $F(\varphi^*, \lambda^*) = 0$, i.e.

$$(\lambda, \nabla \varphi^*, \nabla h) + (k(\varphi^*, x)\varphi^*, h) + (u \cdot \nabla \varphi^*, h) = (f, h) \ \forall h \in H^1_0(\Omega).$$

And it should be taken into account that the pair $(\varphi_m, \lambda_m)$ satisfies the relations

$$(\lambda_m \nabla \varphi_m, \nabla h) + (k(\varphi_m, x)\varphi_m, h) + (u \cdot \nabla \varphi_m, h) = (f, h) \ \forall h \in H^1_0(\Omega), \ m = 1, 2, \ldots.$$ 

Let’s pass to the limit in (18) at $m \to \infty$. All linear summands in (18) turn into corresponding ones in (17).

From condition (1) follows that $k(\varphi_m, \cdot) \to k(\varphi^*, \cdot)$ strongly in $L^{3/2}(\Omega)$. Taking into account that $\varphi_m \to \varphi$ strongly in $L^3(\Omega)$ by (16), we obtain that

$$k(\varphi_m, \cdot)\varphi_m \to k(\varphi^*, \cdot)\varphi^* \text{ strongly in } L^1(\Omega)$$

and

$$(k(\varphi_m, x)\varphi_m, h) \to (k(\varphi^*, x)\varphi^*, h) \text{ at } m \to \infty \ \forall h \in H^1_0(\Omega).$$

From identity

$$(\lambda_m \nabla \varphi_m, \nabla h) - (\lambda^* \nabla \varphi^*, \nabla h) = ((\lambda_m - \lambda^*) \nabla \varphi_m, \nabla h) + (\lambda^* \nabla (\varphi_m - \varphi^*), \nabla h),$$

relations (16), (15) and Theorem 2 we obtain that $(\lambda_m \nabla \varphi_m, \nabla h) \to (\lambda^* \nabla \varphi^*, \nabla h)$ at $m \to \infty$ for all $h \in H^1_0(\Omega)$.

As the functional $J$ is weakly semicontinuous below on $H^1(\Omega) \times H^2(\Omega)$, then from aforesaid follows that

$$J^* = \lim_{m \to \infty} J(\varphi_m, \lambda_m) = \lim_{m \to \infty} J(\varphi_m, \lambda_m) \geq J(\varphi^*, \lambda^*) \geq J^*. \ ■$$

Let us $Y^* = H^1_0(\Omega) \times H^{-1/2}(\Gamma)$ is the dual space for $Y = H^{-1}(\Omega) \times H^{1/2}(\Gamma), \ where \ H^{-1/2}(\Gamma) = H^{1/2}(\Gamma)^*$. We introduce the Lagrange multiplier $y^* = (\theta, \zeta) \in Y^*$ and Lagrangian $L$ by formula

$$L(\varphi, \lambda, y^*) = J(\varphi, \lambda) + \langle y^*, F(\varphi, \lambda) \rangle.$$
concrete reaction coefficient.

\( \varphi \) is differentiable with respect to (14) is an element afforing a local minimum in problem

\( y^* = (\theta, \zeta) \in H^1_0(\Omega) \times H^{-1/2}(\Gamma) \) for wich Euler–Lagrange equation

\[
\langle \lambda \nabla \tau, \nabla \theta \rangle + 4((\beta_1 \varphi^2 \hat{\varphi} + \beta_2) \tau, \theta) + \langle \mu \cdot \nabla \tau, \theta \rangle + \langle \zeta, \tau \rangle \Gamma = -\langle \mu_1/2 \rangle \langle L_\varphi(\hat{\varphi}), \tau \rangle \forall \tau \in H^1(\Omega) \tag{19}
\]

and minimum principle \( L_\varphi'(\hat{\varphi}, \lambda, \theta, \hat{\varphi} - \lambda) \geq 0 \) holds for all \( \lambda \in K, \) which equivalent to the inequality

\[
\mu_1(\lambda, \lambda - \hat{\lambda})_2 - (\lambda - \hat{\lambda}) \nabla \hat{\varphi}, \nabla \theta \geq 0 \quad \forall \lambda \in K. \tag{20}
\]

The Problem 1’s weak formulation (9), Euler–Lagrange equation (19) and minimum principle (20) are the optimality system for the extremum problem (14). This system describes the first-order necessary optimality conditions for problem (14) and will be used for studying of the uniqueness and stability of solutions to problem (14) in future papers.

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