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Analysis of some identification problems for the reaction-diffusion-convection equation

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Abstract. Identification problems for a linear stationary reaction–diffusion–convection model, considered in the bounded domain under Dirichlet boundary condition, are studied. Using an optimization method these problems are reduced to respective control problems. The reaction coefficient and the volume density of substance source play the role of controls in this control problem. The solvability of the direct and control problems is proved, the optimality system, which describes the necessary optimality conditions, is derived and the numerical algorithm is developed.

1. Introduction. Statement and solvability of the boundary value problem

Much attention has been given in recent years to the formulation and study of new classes of problems for heat and mass transfer models. The control problems are examples of such problems. There is a number of books [1–3] and papers [4–12] devoted to the theoretical studies of the control problems for models of heat and mass transfer.

Along with control problems, an important role in applications is played by identification problems for heat and mass transfer models. The unknown densities of boundary or distributed sources or the coefficients, involved in the differential equations or the boundary conditions for the heat and mass transfer models under study, are recovered in these problems using the additional information concerning the solution of the original boundary value problem. It is important that the identification problems can be reduced to corresponding extremum problems using a certain choice of the minimized cost functional. Based on this approach, there arise inverse extremum problems. They can be studied using well-known constrained minimization methods. The application of this approach to heat and mass transfer models was described in [13–17]. The papers [18–22], where an analogous approach was used for solving similar inverse problems arising in the study of thermal processes occurring in the Earth's mantle and in technical gas dynamics, should be also mentioned.

In this paper we consider the following boundary value problem for the stationary reaction–diffusion–convection equation:

$$-\operatorname{div}(\lambda\nabla C)+u\cdot\nabla C+kC=f \quad \text{in} \quad \Omega, \quad C\big|_{\Gamma}=\psi. \tag{1}$$

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Here Ω is a bounded domain in R^d, $d = 2.3$ with boundary Γ, $C(x)$ is the substance concentration, $\lambda = \lambda(x) > 0$ is the diffusion coefficient, $u = u(x)$ is the fluid velocity, function $k = k(x)$ is the reaction coefficient, function f describes the density of volume sources.

Below we shall use Sobolev function spaces $H^s(D), s \in R$. Here, D denotes Ω, its boundary Γ, or certain subdomain $Q \subset \Omega$. By $\|\cdot\|_{s,\Omega}$, $|\cdot|_{s,\Omega}$, and $(\cdot,\cdot)_{s,\Omega}$, we denote the respective norm, seminorm, and scalar product in $H^s(\Omega)$. Expressions $\|\cdot\|_Q$, $\|\cdot\|_{1,Q}$, $(\cdot,\cdot)_Q$ and $(\cdot,\cdot)_{1,Q}$ denote the norms and scalar products in $L^2(Q)$ and $H^1(Q)$, respectively. If $Q = \Omega$ we omit index Ω, setting $\|\cdot\|_\Omega = \|\cdot\|$, $\|\cdot\|_{1,\Omega} = \|\cdot\|_1$, and $(\cdot,\cdot)_\Omega = (\cdot,\cdot)$. Let $X = \{\eta \in H^1(\Omega) : \eta|_\Gamma = 0\}$. The duality relation between X and its dual X^* is denoted by $\langle\cdot,\cdot\rangle$. Let us define $Z = \{u \in H^1(\Omega)^3 : \operatorname{div} u = 0\}$, $L^2_+(\Omega) = \{k \in L^2(\Omega) : k \ge 0 \text{ in } \Omega\}$, $L^\infty_{\lambda_0}(\Omega) = \{\lambda \in L^\infty(\Omega) : \lambda \ge \lambda_0 \text{ in } \Omega\}$, where $\lambda_0 = \text{const} > 0$. We can recall that by Poincare' inequality [3] the following relation holds:

$$\left|C\right|^2_{1,\Omega} \ge \delta\left\|C\right\|^2_{1,\Omega} \forall C \in X$$

where $\delta = \text{const} > 0$.

Let us suppose that the following conditions take place:

(i) $\Gamma \in C^{0,1}$, $\lambda \in L^\infty_{\lambda_0}(\Omega)$, $\lambda_0 = \text{const} > 0$, $u \in Z$;

(ii) $k \in L^2_+(\Omega)$, $f \in L^2(\Omega)$.

We will begin with a brief study of unique solvability of the boundary value problem (1). Let us multiply the equation in (1) by test function $\eta \in X$, integrate over Ω and apply Green's formula. Proceeding as in [17], we obtain

$$a_k(C,\eta) \equiv (\lambda\nabla C, \nabla\eta) + (u\cdot\nabla C, \eta) + (kC, \eta) = (f, \eta) \quad \forall \eta \in X. \tag{2}$$

Here we use notation

$$(\lambda\nabla C, \nabla\eta) = \int_\Omega \lambda\nabla C\cdot\nabla\eta dx,\ (u\cdot\nabla C, \eta) = \int_\Omega (u\cdot\nabla C)\eta dx,\ (kC, \eta) = \int_\Omega kC\eta dx.$$

We shall call solution $C \in H^1(\Omega)$ of the problem (2) a weak solution of the problem (1).

A simple analysis shows that bilinear form $a_k(\cdot,\cdot)$ which is defined in (2) is continuous and coercive on X and the following inequality takes place:

$$a_k(C,C) \ge \delta\lambda_0\left\|C\right\|^2_{1,\Omega}\ \forall C \in X.$$

Based on this fact and using the Lax-Milgram theorem one can prove the following theorem concerning the existence of the unique weak solution of the problem (2).

Theorem 1. Let the conditions (i) take place. Then the following assertions hold:

1) The bilinear form $a_\lambda : X \times X \to R$ given in the left hand of (2) is continuous and coercive on X with coercitivity constant $\lambda_* = \delta_0\lambda_0$.

2) For any pair (k, f), satisfying conditions (ii), the problem (2) has a unique solution $C \in X$ and this solution satisfies the estimate

$$\|C\|_{1,\Omega} \le \lambda_0^{-1}\|f\|_\Omega. \tag{3}$$

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2. Statement and solvability of control problem. Optimality system

We recall that the boundary value problem (1) contains four variable parameters: diffusion λ, velocity u, reaction coefficient k and source density f. All these functions must be provided for the solution of the problem (1.1) in order to be unique. However there appear situations in practice when some of mentioned functions are unknown and one has to determine them using the additional information about the solution. For example one can use values $C_d(x)$ of concentration C measured in points of some set $Q \in \Omega$.

Get us consider the situation when reaction coefficient k and density f are unknown, and one should determine them together with solution C of (1). This identification problem is studied by applying an optimization method [3]. According to this method the problem is reduced to a corresponding inverse extremum problem (see details in [15-17]). Following this method, we divide the set of input data in the problem (1) into two groups. One consists of fixed data, namely, invariable functions λ and u. The other group consists of two distributed controls, namely, functions k and f. Assume that controls k and f change over sets K_1 and K_2 satisfying the following conditions:

(j) $K_1 \subset Z,\ K_2 \subset L^2(\Omega)$ are nonempty convex closed subsets.

Let us denote $K = K_1 \times K_2,\ u = (k, f)$ and define operator $F = X \times K \to X^*$ acting by

$< F(C,u), \eta >= a_k(C,\eta) - (f,\eta).$

Let $I : X \to R$ be arbitrary weak lower semicontinuous cost functional. We consider the following constrained minimization problem:

$$(\alpha_0/2)I(C) + (\alpha_1/2)\|k\|_\Omega^2 + (\alpha_2/2)\|f\|_\Omega^2 \to \inf,\ F(C,u) = 0,$$
$$(C,u) \equiv (C,k,f) \in X \times K. \tag{4}$$

As the admissible cost is functional we choose one of the following:

$$I_1(C) = \|C - C_d\|_Q^2 = \int_Q |C - C_d|^2 dx, \quad I_2(C) = \|C - C_d\|_{1,Q}^2.$$

Here $C_d \in L^2(Q)$ (or $C_d \in H^1(Q)$) is a given function in Q. We assume in addition to (j) that the following conditions hold:

(jj) $\alpha_0 > 0$, $\alpha_1 \geq 0$, $\alpha_2 \geq 0$ and K_1, K_2 are bounded sets or $\alpha_1 > 0,\ \alpha_2 > 0.$

The following theorem can be proved.

Theorem 2. Under assumptions (i), (j) and (jj) the control problem (4) for $I = I_m, m = 1,2$ has at least one solution $(\hat{C},\hat{u}) \equiv (\hat{C},\hat{k},\hat{f})$, which is an element of $X \times K_1 \times K_2$.

3. The optimality system. Numerical algorithm

The following stage of studying the control problem is the derivation of the optimality system for the problem (4). The Lagrange principle for extremum problems (see [3, p. 341]) is used for this purpose. Using this principle and techniques of [3,17] we can prove the following theorem.

Theorem 3. Let us suppose that, under conditions of Theorem 2, triple $(\hat{C},\hat{k},\hat{f}) \in X \times K_1 \times K_2$ is a solution of the problem (4) and let $I(C)$ continuously be a Frechét differentiable functional with respect to C at point $\hat{C}$. Then there is unique non-zero Lagrange multiplyer $\theta \in X$, so that the Euler–Lagrange equation

$$F_C'(\hat{C},\hat{u})^*\theta + (\alpha_0/2)I_C'(\hat{C}) = 0$$

holds in X^* which is equivalent to the identity

$$\lambda(\nabla\tau,\nabla\theta) + (\hat{u}\cdot\nabla\tau,\theta) + (k\tau,\theta) = -(\alpha_0/2)\left\langle I_C'(\hat{C}),\tau\right\rangle \quad \forall\tau\in X \tag{5}$$

and the minimum principle holds which is equivalent to the pair of variational inequalities

$$\alpha_1(\hat{k},k-\hat{k}) + ((k-\hat{k})C,\theta) \geq 0 \quad \forall u\in K_1, \tag{6}$$

$$\mu_2(\hat{f},f-\hat{f}) - (f-\hat{f},\theta) \geq 0 \quad \forall f\in K_2. \tag{7}$$

The direct problem (2), the adjoint problem (5) together with the variational inequalities (6), (7) form the optimality system that describes the necessary optimality conditions. The optimality system plays an important role when studying control problems. Based on the analysis of the optimality system one can apply fundamental properties of solutions to the control problem (see in more details in [13,15,17]). Besides, on the base of the optimality system, the efficient numerical algorithm can be developed for solving the control problem (4). If, in particular, to apply the simple iteration method to the optimality system (2) (5), (6), (7) then one can derive the following iteration algorithm:

$$a_k(C^n,h) \equiv (\lambda\nabla C^n,\nabla h) + (u\cdot\nabla C^n,h) + (k^nC^n,h) = (f^n,h) \quad \forall h\in X, \tag{8}$$

$$\lambda(\nabla\tau,\nabla\theta^n) + (u\cdot\nabla\tau,\theta^n) + (k^nC,\theta^n) = -(\alpha_0/2)\left\langle I_T(T^n),\tau\right\rangle \quad \forall\tau\in X, \tag{9}$$

$$\alpha_1(k^{n+1},k-k^n) + ((k-k^{n+1})\cdot C^n,\theta^n) \geq 0 \ \forall k\in K_1, \tag{10}$$

$$\alpha_2(f^{n+1},f-f^n) - (f-f^n,\theta^n) \geq 0 \forall f\in K_2. \tag{11}$$

The proposed algorithm consists of finding k^{n+1} and f^{n+1} for given k^n and f^n by sequentially solving problems (8), (9), (10) and (11). The separate paper of the authors will be devoted to study of the properties of the corresponding algorithm and the analysis of the results of computational experiments on the base of this algorithm.

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