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OPTIMIZATION APPROACH FOR IDENTIFICATION PROBLEMS FOR STATIONARY EQUATION OF ADMIXTURE TRANSFER

Abstract. The identification problem for the stationary admixture transfer equation considered in bounded domain with a Dirichlet condition imposed on the boundary of the domain is studied. By applying an optimization method this problem is reduced to the control problem in which the role of controls is played by variable coefficients of diffusion and chemical reaction. Solvability of the control problem is proved, the optimality system, which describes necessary conditions of an extremum is derived, the stability estimates for optimal solutions are established and the efficient numerical algorithm for solving the control problem is developed.

Keywords mass transfer model, diffusion-reaction equation, variable coefficients of diffusion and reaction, identification problem, control problem.

1. Introduction

In recent years, much attention has been paid to the formulation and study of new classes of problems for heat and admixture transfer models. Control problems can be stated as examples of such problems. Among theoretical studies of the indicated problems for linear and nonlinear models of heat and admixture transfer, we note [1–4].

Along with control problems, an important role in applications is played by identification problems for heat and mass transfer models. In the latter problems, unknown densities of boundary or distributed sources or the coefficients involved in the differential equations or the boundary conditions for the model under study are recovered from additional information about the solution of the original boundary value problem. Importantly, with a certain choice of the minimized cost functional, identification problems can be reduced to corresponding extremum problems. Following this approach, control problems arise there. They can be can studied using well-known constrained minimization methods. This approach as applied to heat and mass transfer models was described in [5 – 11].

The goal of this paper is to develop a theory for the uniqueness and stability analysis of inverse extremum problems for a linear admixture transfer model defined by the variable diffusivity and quantity characterizing disintegration of pollutant by chemical reactions. This model is considered in a bounded domain Ω with a Dirichlet condition specified on the boundary Γ.

2. Statement of the boundary value problem

We study the following admixture transfer model:

$$-div(\lambda\nabla\varphi)+k\varphi=f \quad \text{in} \quad \Omega, \quad \varphi|_{\Gamma}=0 \tag{1}$$

considered in a bounded domain Ω in the space $\mathbf{R}^d$, d=2,3 with Lipschitz boundary Γ. Here $\lambda\equiv\lambda(\mathbf{x})>0$ is a variable diffusion coefficient, $k\equiv k(\mathbf{x})\geq 0$ is a quantity characterizing disintegration of pollutant by chemical reactions, $f\equiv f(\mathbf{x})$ is a volume source density.

As usual we will use the functional spaces $H^1(\Omega)$, $H^s(\Omega)$, $L^\infty(\Omega)$, $L^2_+(\Omega)=\{k\in L^2(\Omega): k\geq 0\}$, $V=\{\varphi\in H^1(\Omega):\varphi|_\Gamma=0\}$ and sets $H^s_{\lambda_0}(\Omega)$, $L_{\lambda_0}(\Omega)$, λ_0=const>0 while studying problem 1 and corresponding identification problem. The properties of these spaces and denotions can be found in

[6]. Assuming that $\Gamma\in C^{0,1}$, $\lambda\in H^s_{\lambda_0}(\Omega)$, $k\in L^2_+(\Omega)$, $f\in L^2(\Omega)$ we define the weak solution of problem (1) as the function $\varphi\in V$ satisfying the identity

$$(\lambda\nabla\varphi,\nabla h)+(k\varphi,h)=(f,h)\quad\forall h\in V. \tag{2}$$

3. Statement of the identification problem, reduction to an extremum problem, and necessary optimality conditions

The boundary value problem (1), considered in Section 2, involves three functional parameters, namely, the diffusivity λ, the decay coefficient k and the function f describing the source density. The boundary value problem (1) contains a number of parameters that must be given to ensure the uniqueness of the solution. In practice, situations can arise when some of the parameters are unknown. For this reason, we need additional information about the solution φ of problem (1). As this information we can use, for example, concentration $\varphi_d(x)$ measured in some subdomain $Q\subset\Omega$ (see fig. 1). Let coefficients λ and k be unknown functions and we must determine these functions along with the solution φ of problem (1). For the study of this identification problem we apply optimization method and reduce solution of this problem to the corresponding extremum problem (see [6]).

Following this method, as distributed controls we will choose the functions λ and k, which are changed in some sets K_1 and K_2.

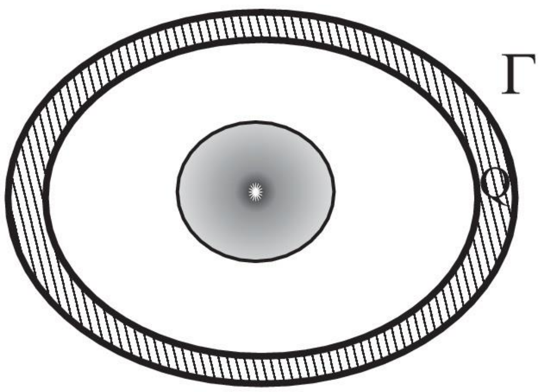

Fig. 1. The geometry of the domain

More concretely, we assume that the following conditions take place:

(*i*) $\Gamma\in C^{0,1}$, $f\in L^2(\Omega)$;

(*ii*) $K_1\subset H^s_{\lambda_0}(\Omega)$, $\lambda_0>0$, $s>d/2$, $K_2\subset L^2_+(\Omega)$ are convex closed sets.

Setting $K=K_1\times K_2$, $u=(\lambda,k)$, we introduce an operator $F:V\times K\times L^2(\Omega)\to V^*$ acting according to the formula

$$\langle F(\varphi,\lambda,k,f),h\rangle=(\lambda\nabla\varphi,\nabla h)+(k\varphi,h)-(f,h)\quad\forall h\in V \tag{3}$$

where $\varphi\in V$ is the weak solution of problem (1).

Let $I:V\to\mathbf{R}$ be a weakly lower semicontinuous cost functional. Consider the extremum problem:

$$\frac{\mu_0}{2}I(\varphi)+\frac{\mu_1}{2}\|\lambda\|_s^2+\frac{\mu_2}{2}\|k\|^2\to\inf,\quad F(\varphi,u,f)=0,\quad(\varphi,u)\in V\times K. \tag{4}$$

Here, μ_0, μ_1, μ_2 are nonnegative parameters that specify the relative importance of each of the terms in (4). Another goal of introducing μ_1 is to ensure the uniqueness and stability of solutions of particular extremum problems.

As admissible cost functionals, we use

$$I_1(\varphi)=\|\varphi-\varphi_d\|_Q^2=\int_Q|\varphi-\varphi_d|^2d\mathbf{x}=\int_\Omega r(\varphi-\tilde{\varphi}_d)^2d\mathbf{x},\quad I_2(\varphi)=\|\varphi-\varphi_d\|_{1,Q}^2. \tag{5}$$

Here $\varphi_d\in L^2(Q)$ is a given function in Q, $r=\chi_Q$ is the characteristic function of Q, and $\tilde{\varphi}_d\in L^2(\Omega)$ is a function that is equal to φ_d in Q and vanishes outside of Q. It is well known, that each of the functionals in (5) is weakly lower semicontinuous. The set of admissible pairs (φ, u) for problem (4) is defined as $Z_{ad}=\{(\varphi,u)\in V\times K: F(\varphi,u,f)=0,\quad J(\varphi,u)<\infty\}$. In addition to ($ii$), let the following condition hold:

(iii) $\mu_0>0$, $\mu_1\geq 0$, $\mu_2\geq 0$ and K_1 and K_2 are bounded sets or $\mu_l>0$, l=0,1,2 and the functional I is bounded from below.

Theorem 1. Let I:$V\to\mathbf{R}$ be a weakly lower semicontinuous cost functional; conditions (i), (ii), and (iii) hold; and Z_{ad} be a nonempty set. Then problem (4) has at least one solution $(\varphi,u)\in V\times K$.

Note that Theorem 1 remains valid for the functionals I_1 and I_2, since they are nonnegative and weakly lower semicontinuous, while Z_{ad} is not empty. Therefore, the following result holds.

Theorem 2. Let conditions (i) and (ii) be satisfied, $\mu_0>0$ and $\mu_l>0$ or $\mu_0>0$ and $\mu_l\geq 0$; and K_l be bounded sets, l=1,2. Then problem (4) for $I=I_m$, m=1,2 has at least one solution $(\varphi,u)\in V\times K$.

Let us derive necessary optimality conditions for problem (4). For this purpose, the extremal principle is applied to smooth convex extremum problems. According to the general theory of extremum problems (see [13, 14]), we introduce a Lagrange multiplier $\eta\in V$ which is interpreted as an “adjoint” concentration. Additionally, the Lagrangian £: $V\times K\times L^2(\Omega)\times V\to\mathbf{R}$ is defined as

$$£(\varphi,u,f,\eta)\equiv J(\varphi,u)+\langle F(\varphi,u,f),\eta\rangle\equiv(\mu_0/2)I(\varphi)+(\mu_1/2)\|\lambda\|_s^2+(\mu_2/2)\|k\|^2+\langle F(\varphi,u,f),\eta\rangle. \quad (6)$$

The result of [13, p. 79] implies the following assertion.

Theorem 3. Under the conditions of Theorem 2, let a pair $(\hat{\varphi},\hat{u})\in V\times K$ be a local minimizer in problem (4), and let the functional $I(\cdot):V\to\mathbf{R}$ be continuously differentiable with respect to φ at the point $\hat{\varphi}$. Then there exists a unique Lagrange multiplier $\eta\in V$ such that the Euler-Lagrange equation

$$£'_\varphi(\hat{\varphi},\hat{u},f,\eta)\equiv F'_\varphi(\hat{\varphi},\hat{u},f)^*,\eta+(\mu_0/2)I'_\varphi(\hat{\varphi})=0\quad\text{in}\quad V^* \quad (7)$$

holds and the minimum principle $£(\hat{\varphi},\hat{u},f,\eta)\leq £(\hat{\varphi},u,f,\eta)\quad\forall u\in K$ is valid and is equivalent to the variational inequalities

$$\left\langle £'_\lambda(\hat{\varphi},\hat{u},f,\eta),\lambda-\hat{\lambda}\right\rangle=\mu_1\left(\hat{\lambda},\lambda-\hat{\lambda}\right)_{s,\Omega}+\left(\left(\lambda-\hat{\lambda}\right)\nabla\hat{\varphi},\nabla\eta\right)\geq 0\quad\forall\lambda\in K_1, \quad (8)$$

$$\left\langle £'_k(\hat{\varphi},\hat{u},f,\eta),k-\hat{k}\right\rangle=\mu_2\left(\hat{k},k-\hat{k}\right)_{\Omega}+\left(\left(k-\hat{k}\right)\nabla\hat{\varphi},\nabla\eta\right)\geq 0\quad\forall k\in K_2. \quad (9)$$

It follows from (6) that

$$\left\langle F'_\varphi(\hat{\varphi},\hat{u},f)^*\eta,\tau\right\rangle=\left\langle F'_\varphi(\hat{\varphi},\hat{u},f)\tau,\eta\right\rangle=\left(\hat{\lambda}\nabla\tau,\nabla\eta\right)+\left(\hat{k}\tau,\eta\right)\quad\forall\tau\in V. \quad (10)$$

From (10), we conclude that the Euler–Lagrange equation (7) is equivalent to the identity

$$\left(\hat{\lambda}\nabla\tau,\nabla\eta\right)+\left(\hat{k}\tau,\eta\right)=-(\mu_0/2)\left\langle I'_\varphi(\hat{\varphi}),\tau\right\rangle\quad\forall\tau\in V. \quad (11)$$

Identity (11) is a weak formulation of a boundary value problem for the adjoint concentration η. Its form depends on a type of the cost functional I. The problem (11) is referred formally as the adjoint problem below. We emphasize that the direct problem (2), adjoint problem (11), and inequalities (8), (9) comprise an optimality system describing the necessary conditions for a minimum in problem (4). Below, based on an analysis of this optimality system, we formulate sufficient conditions on the input data under which the solution of problem (4) is unique and stable for particular cost functionals.

4. Stability estimates for solutions of control problems

Assume that the function f for the equation of state $F(\varphi,u,f)=0$ ranges over a set $F_{\mathrm{ad}}\subset L^2(\Omega)$. Denote by $(\varphi_1,u_1)=(\varphi_1,\lambda_1,k_1)\in V\times K$ an arbitrary solution of problem (4) with a given function $f=f_1\in F_{\mathrm{ad}}$. Let $(\varphi_2,u_2)=(\varphi_2,\lambda_2,k_2)\in V\times K$ denote the solution of the problem

$$\frac{\mu_0}{2}\tilde{I}(\varphi)+\frac{\mu_1}{2}\|\lambda\|_s^2+\frac{\mu_2}{2}\|k\|^2\to\inf,\quad F(\varphi,u,f_2)=0,\quad(\varphi,u)\in V\times K, \quad (12)$$

which is obtained from (4) by replacing I with a close functional $\tilde{I}$ and by replacing f_1 with a close function $\tilde{f} = f_2 \in F_{\text{ad}}$. Assuming that K_1 and K_2 are bounded sets, the functions φ_i satisfy the estimates

$$\|\varphi_i\|_1 \le M_\varphi = C_0 \sup_{f\in F_{\text{ad}}} \|f\|, \quad C_0 = (\delta_1\lambda_0)^{-1}, \quad i=1,2, \tag{13}$$

where δ_1=const>0, λ_0=const>0 are certain constants. Clearly, $M_\varphi<\infty$ if the sets K_1, K_2 and F_{ad} are all bounded.

Relying on the results of [12], we now establish sufficient conditions for the uniqueness and stability of the solution $(\hat{\varphi}, \hat{\lambda}, \hat{k})$ of the following control problem corresponding to the cost functional $I_1(\varphi) = \|\varphi - \varphi_d\|_Q^2$:

$$\frac{\mu_0}{2} I_1(\varphi) + \frac{\mu_1}{2}\|\lambda\|_{s,\Omega}^2 + \frac{\mu_2}{2}\|k\|_\Omega^2 \to \inf, \quad F(\varphi,u,f)=0, \quad (\varphi,u)\in V\times K. \tag{14}$$

Theorem 4. Assume that conditions (i) and (ii) hold and, additionally, K_1, K_2 and $F_{\text{ad}} \subset L^2(\Omega)$ are bounded sets. Let the triple $(\varphi_i,\lambda_i,k_i)\in V\times K_1\times K_2$ be a solution of problem (14) corresponding to given functions $\varphi_d^{(i)} \in L^2(Q)$ and $f_i\in F_{\text{ad}}$, i=1,2, where Q is an arbitrary open bounded set. Let $M_\varphi^0 = M_\varphi + \max\left(\|\varphi_d^{(1)}\|_Q, \|\varphi_d^{(2)}\|_Q\right)$ and let the following conditions

$$\mu_1(1-\varepsilon) > 5\mu_0\gamma_0^2 C_0^2 M_\varphi^0 M_\varphi, \quad \mu_2(1-\varepsilon) > 5\mu_0\gamma_1^2 C_0^2 M_\varphi^0 M_\varphi, \quad \mu_0>0, \tag{15}$$

be satisfied for some constant $\varepsilon\in(0,1)$, where M_φ is defined in (13). Then the following stability estimates hold:

$$\|\varphi_1-\varphi_2\|_Q \le \|\varphi_d^{(1)} - \varphi_d^{(2)}\|_Q + \beta(f_1 - f_2), \tag{16}$$

$$\|\lambda_1-\lambda_2\|_{s,\Omega} \le \sqrt{\mu_0/\varepsilon\mu_1}\,\Delta, \quad \|k_1-k_2\| \le \sqrt{\mu_0/\varepsilon\mu_2}\,\Delta, \tag{17}$$

$$\|\varphi_1-\varphi_2\|_{1,\Omega} \le M_\varphi\left(\gamma_0\sqrt{\mu_0/\varepsilon\mu_1} + \gamma_1\sqrt{\mu_0/\varepsilon\mu_2}\right)\Delta + \|f_1-f_2\|_\Omega, \tag{18}$$

Here Δ and β are defined by

$$\Delta = \|\varphi_d^{(1)} - \varphi_d^{(2)}\|_Q + \beta(f_1-f_2), \tag{19}$$

$$\beta(\|f\|_\Omega) = a\|f\|_\Omega + b\|f\|_\Omega^2 = 2C_0 M_\varphi^0\|f\|_\Omega + 2C_0^2 M_\varphi^0 M_\varphi^{-1}\|f\|_\Omega^2. \tag{20}$$

5. Numerical algorithm

The optimality system plays an important role in investigating properties of solutions of the control problem. On the basis of the analysis of optimality systems sufficient conditions for the input data which provide the uniqueness and stability of solutions to individual extremum problems can be formulated. Optimality system derived above can be used to design effective numerical algorithms for solving control problem (14). The simplest numerical algorithm can be obtained by applying simple iteration method for solving the optimality system. The n-th iteration of the algorithm consists in finding values φ^n, η^n, λ^{n+1} and k^{n+1} for given λ^n and k^n by sequentially solving following problems

$$\begin{gathered}
(\lambda^n\nabla\varphi^n, \nabla h) + (k^n\varphi^n, h) = (f,h) \quad \forall h\in V, \\
(\lambda^n\nabla\tau, \nabla\eta^n) + (k^n\eta^n, \tau) = -(\mu_0/2)\langle I'_\varphi, \tau\rangle \quad \forall\tau\in V, \\
\mu_1(\lambda^{n+1}, \lambda-\lambda^n)_{s,\Omega} + ((\lambda-\lambda^{n+1})\nabla\varphi^n, \nabla\eta^n) \ge 0 \quad \forall\lambda\in K_1, \\
\mu_2(k^{n+1}, k-k^n)_\Omega + ((k-k^{n+1})\nabla\varphi^n, \nabla\eta^n) \ge 0 \quad \forall k\in K_2.
\end{gathered} \tag{21}$$

Direct and adjoint problems in (21) can be solved by finite element method using FreeFem++.

The authors plan to devote a separate paper to studying the convergence of the algorithm and to the analysis of results of numerical experiments.

6. Conclusion

Summarizing, we have formulated identification problems for the linear diffusion–reaction equation. Using optimization method these problems were reduced to corresponding control problems. We have proved the solvability of these control problems, have derived the optimality system, which describes the necessary conditions of extremum, have established sufficient conditions on the input data under which the solutions of particular extremum problems are unique and stable. Based on analysis of optimality system we also developed the numerical algorithm of solving control problems. The properties of such an algorithm and numerical results will be analyzed elsewhere. The separate paper of the authors will be devoted to the analysis of results of numerical experiments.

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