Optimization Approach in Modelling the Effects of Technological Disasters

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Abstract. In present paper the applying of an optimization approach in modeling the effects of technological disasters are studied. Mathematical models of the pollutants propagation in the water or in air, based on the convection-diffusion-reaction equation are used. The problems of recovering the diffusion and reaction coefficients by the pollutant concentration measured in a certain subdomain are studied. In framework of optimization approach these problems are reduced to the multiplicative control problems. Solvability of considered control problems are proved and the local stability estimates are obtained. The recovering of the diffusion coefficients and the reaction from the measured concentration makes it possible to realistically estimate the intensity of the diffusion of pollutants and the effectiveness of the processes aimed at the decomposition of the pollutant (reaction coefficient).

1. Introduction

In present paper the problems of recovering the diffusion and reaction coefficients included in the convection-diffusion-reaction equation which are measured substance concentration in some control subdomain are studied.

Recovering the diffusion coefficient allows us to estimate the diffusion propagation of the pollutant. Unlike convection, where we can know the rose of winds or the directions and velocities of currents, the diffusion process is more hidden. In turn, the recovery of the reaction coefficient will allow us to find out how the pollutant decomposes, both without interfering with the process, and under the influence of reagents that destroy pollutants.

In frame work of optimization approach (see [1-3]) the inverse coefficient problems reduced to the multiplicative control problems. The role of controls in these problems is played by the desired coefficients. In present paper the solvability of two-parameter multiplicative control problem is proved. For considered control problem the optimality system is derived. Based on analysis of this system the local stability estimates of optimal solutions are obtained and numerical algorithm for solution of control problem is constructed. Along with the study of extremum problems in this work, a qualitative analysis of the boundary value problems solution was carried out and its applications were shown.

We note that the interest in the study of boundary value and extremum problems for linear, semi-linear and non-linear models of mass transfer is only increasing. Note here both recent works [4-12] and earlier works [13-19].
2. Statement of the boundary value problem

We study the following admixture transfer model:
\[ -\text{div}(\lambda \nabla \varphi) + \mathbf{u} \cdot \nabla \varphi + k \varphi = f \quad \text{in} \quad \Omega, \quad \varphi|_\Gamma = \psi \]  
considered in a bounded domain \( \Omega \) in the space \( \mathbb{R}^d, d=2,3 \) with Lipschitz boundary \( \Gamma \). Here \( \lambda = \lambda(\mathbf{x}) > 0 \) is a variable diffusion coefficient, \( \mathbf{u} = \mathbf{u}(\mathbf{x}) \) is the velocity concentration in the fluid, \( k = k(\mathbf{x}) \geq 0 \) is a quantity characterizing disintegration of pollutant by chemical reactions, \( f = f(\mathbf{x}) \) is a volume source density, \( \psi(\mathbf{x}) \) is a function given on boundary \( \Gamma \).

As usual we will use the functional spaces \( H^1(\Omega), H^s(\Omega), L^\infty(\Omega), L^2_+(\Omega) = \{ k \in L^2(\Omega): k \geq 0 \} \), \( Z = \{ \mathbf{u} \in H^1(\Omega): \text{div} \mathbf{u} = 0 \} \), \( V = \{ \varphi \in H^1(\Omega): \varphi|_{\Gamma} = 0 \} \) and sets \( H^s_{\lambda_0}(\Omega), L^s_{\lambda_0}(\Omega), \lambda_0 = \text{const} > 0 \) while studying problem (1) and corresponding identification problem. The properties of these spaces and denotations can be found in [19].

Let the following conditions hold:
(i) \( \Omega \) is a bounded domain in \( \mathbb{R}^3 \) with boundary \( \Gamma \in C^{0,1} \);
(ii) \( \lambda \in H^s_{\lambda_0}(\Omega), \lambda_0 = \text{const} > 0, s > d/2, k \in L^2(\Omega), f \in L^2(\Omega), \varphi \in H^{1/2}(\Gamma) \).

We define the weak solution of problem (1) as the function \( \varphi \in V \) satisfying the identity
\[ (\lambda \nabla \varphi, \nabla \varphi) + (\mathbf{u} \cdot \nabla \varphi, \lambda \varphi) + (k \varphi, h) = (f, h) \quad \forall h \in V. \]  

The following theorem holds (see in details [19]).

**Theorem 1.** If conditions (i), (ii) holds there exists a unique weak solution of (1) and the following estimate takes place:
\[ ||\varphi||_1 \leq C(||\lambda||_1 + ||f||_{L^2}) \]  

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 four functional parameters, namely, the diffusivity \( \lambda \), the decay coefficient \( k \), the function \( f \) describing the source density and the function \( \psi \) given on boundary. 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 \( \varphi \) of problem (1). As this information we can use, for example, concentration \( \varphi(\mathbf{x}) \) measured in some subdomain \( Q \subset \Omega \) (see fig. 1). Let coefficients \( \lambda \) and \( k \) be unknown functions and we must determine these functions along with the solution \( \varphi \) 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 [19]).

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

![Figure 1. The geometry of the domain.](image-url)
More concretely, we assume that the following conditions take place:

(i) \( K_1 \subset H^1_0(\Omega), \lambda > 0, s > d/2, K_2 \subset L^2(\Omega) \) are nonempty 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 by formula

\[
\langle F(\varphi, \lambda, k, f), h \rangle = (\lambda \varphi, h) + (u \cdot \varphi, h) + (k \varphi, h) - (f, h) \quad \forall h \in V
\]

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

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

\[
\frac{\mu_0}{2} I(\varphi) + \frac{\mu_1}{2} \|\varphi\|^2_\Omega + \frac{\mu_2}{2} \|k\|^2 \to \inf, \quad F(\varphi, u, f) = 0, \quad (\varphi, u) \in V \times K.
\]

Here, \( \mu_0, \mu_1, \mu_2 \) are nonnegative parameters that specify the relative importance of each of the terms in (4). Another purpose of introducing \( \mu \) is to ensure the uniqueness and stability of solutions of particular extremum problems.

As admissible cost functionals, we use

\[
I_1(\varphi) = \|\varphi - \varphi_d\|^2_\Omega = \int_\Omega |\varphi - \varphi_d|^2 \, dx = \int_\Omega r(\varphi - \varphi_d)^2 \, dx, \quad I_2(\varphi) = \|\varphi - \varphi_d\|^2_\Omega.
\]

Here \( \varphi_d \in L^2(Q) \) is a given function in \( Q \), \( r = \chi_Q \) is the characteristic function of \( Q \), and \( \varphi_d \in L^2(\Omega) \) is a function that is equal to \( \varphi_d \) 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 \((\varphi, u)\) 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 (j), let the following condition hold:

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

**Theorem 2.** Let conditions (i), (ii) and (jj) hold and \( I: V \to \mathbb{R} \) be a weakly semicontinuous below cost functional and \( Z_{ad} \) be a nonempty set. Then problem (4) has at least one solution \((\varphi, u) \in V \times K\).

Note that Theorem 2 remains valid for the functionals \( I_1 \) and \( I_2 \), since they are nonnegative and weakly lower semicontinuous, while \( Z_{ad} \) is not empty.

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 [20, 21]), we introduce a Lagrange multiplier \( \eta \in V \) which is interpreted as an “adjoint” concentration.

Additionally, the Lagrangian \( \mathcal{E}: V \times K \times L^2(\Omega) \to \mathbb{R} \) is defined as

\[
\mathcal{E}(\varphi, u, f, \eta) = J(\varphi, u) + \langle F(\varphi, u, f), \eta \rangle = (\mu_0/2) \|\varphi\|^2_\Omega + (\mu_1/2) \|\lambda\|^2_\Omega + (\mu_2/2) \|k\|^2 + \langle F(\varphi, u, f), \eta \rangle.
\]

The result of [21, p. 79] implies the following assertion.

**Theorem 3.** Under the assumptions (i), (ii) and (jj) let the element \((\varphi, u) \in V \times K\) be a local minimizer in problem (4), and let the cost functional \( I(\cdot): V \to \mathbb{R} \) be continuously differentiable with respect to \( \varphi \) at the point \( \hat{\varphi} \). Then there exists a unique Lagrange multiplier \( \eta \in V \) such that the Euler-Lagrange equation takes place

\[
\mathcal{E}'(\varphi, u, f, \eta) = F'(\varphi, u, f), \eta + \mu_0/2 F'(\varphi) = 0 \quad \text{in} \quad V^*
\]

and the minimum principle \( \mathcal{E}(\varphi, u, f, \eta) \leq \mathcal{E}(\hat{\varphi}, u, f, \eta) \) \( \forall u \in K \) holds which is equivalent to the inequalities

\[
\left\{ \begin{array}{l}
\langle \mathcal{E}(\varphi, u, f, \eta), \lambda - \hat{\lambda} \rangle = \mu_1(\hat{\lambda}, \lambda - \hat{\lambda}), \Omega + (\hat{\lambda} - \lambda \nabla \hat{\varphi}, \nabla \eta) \geq 0 \quad \forall \lambda \in K_1, \\
\langle \mathcal{E}(\varphi, u, f, \eta), k - \hat{k} \rangle = \mu_2(k, k - \hat{k})_\Omega + (\hat{k} - k \nabla \hat{\varphi}, \nabla \eta) \geq 0 \quad \forall k \in K_2.
\end{array} \right.
\]

It follows from (6) that
\[ \left\langle F'_\varphi \left( \hat{\varphi}, \hat{u}, f \right), \eta, \tau \right\rangle = \left\langle F'_\varphi \left( \hat{\varphi}, \hat{u}, f \right), \eta, \tau \right\rangle = \left( \lambda \nabla \tau, \nabla \eta \right) + \left( \dot{u} \cdot \nabla \tau, \eta \right) + \left( \dot{k} \tau, \eta \right) \quad \forall \tau \in V. \quad (10) \]

From (10), we conclude that the Euler–Lagrange equation (7) is equivalent to the identity
\[ \left( \lambda \nabla \tau, \nabla \eta \right) + \left( \dot{u} \cdot \nabla \tau, \eta \right) + \left( \dot{k} \tau, \eta \right) = -\left( \mu_0 / 2 \right) \left\langle I'_\varphi \left( \hat{\varphi} \right), \tau \right\rangle \quad \forall \tau \in V. \quad (11) \]

Identity (11) is a weak formulation of a boundary value problem for the adjoint concentration \( \eta \). 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 the 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 \( F_{ad} \subset L^2(\Omega) \). Denote by \( (\varphi, u, f) = (\varphi, \lambda, k) \in V \times K \) an arbitrary solution of problem (4) with a given function \( f = f_i \in F_{ad} \). Let \( (\varphi, u, f) = (\varphi, \lambda, k) \in V \times K \) denote the solution of the problem
\[ \frac{\mu_0}{2} \left( \hat{\varphi} \right) + \frac{\mu_1}{2} \left\| \lambda \right\|_{L^2(\Omega)}^2 + \frac{\mu_2}{2} \left\| k \right\|_{L^2(\Omega)}^2 \rightarrow \inf \quad F(\varphi, u, f) = 0, \quad (\varphi, u) \in V \times K, \quad (12) \]

which is obtained from (4) by replacing \( I \) with a close functional \( \tilde{I} \) and by replacing \( f_i \) with a close function \( \tilde{f} = f_i \in F_{ad} \). Assuming that \( K_1 \) and \( K_2 \) are bounded sets, the functions \( \varphi \) satisfy the estimates
\[ \left\| \varphi \right\| \leq M_\varphi = C_0 \sup_{f_i \in F_{ad}} \left\| f \right\|, \quad C_0 = \left( \delta_i \lambda_i \right)^{-1}, \quad i = 1, 2, \quad (13) \]

where \( \delta_i = \text{const} > 0, \lambda_i = \text{const} > 0 \) are certain constants. Clearly, \( M_\varphi \rightarrow 0 \) if the sets \( K_1, K_2 \) and \( F_{ad} \) are all bounded.

Relying on the results of [9], we now establish sufficient conditions for the uniqueness and stability of the solution \( \left( \hat{\varphi}, \hat{\lambda}, \hat{k} \right) \) of the following control problem corresponding to the cost functional
\[ I_1(\varphi) = \left\| \varphi - \varphi_i \right\|_Q^2 \quad (14) \]

**Theorem 4.** Let under conditions (i), (ii) and (j), (jj) \( K_1, K_2 \) and \( F_{ad} \subset L^2(\Omega) \) are bounded sets. Let the triple \( (\varphi, \lambda, k) \in V \times K \times K \) be a solution of problem (14) corresponding to given functions \( \varphi_i \in L^2(Q) \) and \( f_i \in F_{ad} \), \( i = 1, 2 \), where \( Q \) is an arbitrary open bounded set. Let
\[ M_\varphi = M_\varphi + \max \left\{ \left\| \varphi_j \right\|_Q, \left\| \varphi_j \right\|_Q \right\} \quad (15) \]

and let the following conditions
\[ \mu_0 \left( 1 - \varepsilon \right) > 5 \mu_0 \gamma_0 C_0 M_\varphi, \quad \mu_2 \left( 1 - \varepsilon \right) > 5 \mu_0 \gamma_0 C_0 M_\varphi, \quad \mu_0 > 0, \quad (15) \]

be satisfied for some constant \( \varepsilon \in (0, 1) \), where \( M_\varphi \) is defined in (13). Then the following stability estimates hold:
\[ \left\| \varphi_i - \varphi_j \right\|_Q \leq \left\| \varphi_i - \varphi_j \right\|_Q + \beta \left( f_i - f_j \right) \quad (16) \]
\[ \left\| \lambda_i - \lambda_j \right\|_{L^2(\Omega)} \leq \sqrt{\mu_0 / \varepsilon \mu_\Delta}, \quad \left\| k_i - k_j \right\|_{L^2(\Omega)} \leq \sqrt{\mu_0 / \varepsilon \mu_\Delta} \quad (17) \]
\[ \left\| \varphi_i - \varphi_j \right\|_{L^2(\Omega)} \leq \left( \sqrt{\mu_0 / \varepsilon \mu_\Delta} + \gamma_1 \sqrt{\mu_0 / \varepsilon \mu_\Delta} \right) \Delta + \left\| f_i - f_j \right\|_{L^2(\Omega)} \quad (18) \]

Here \( \Delta \) and \( \beta \) are defined by
\[ \Delta = \left\| \varphi_i - \varphi_j \right\|_Q + \beta \left( f_i - f_j \right), \quad (19) \]
\[ \beta(\|f\|_{\Omega}) = a\|f\|_{\Omega} + b\|f\|_{\Omega}^2 = 2C_0M_0\|f\|_{\Omega} + 2C_0^2M_0^2M_0^{-1}\|f\|_{\Omega}^2. \]  

(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 \( \phi^n, \eta^n, \lambda^{n+1} \) and \( k^{n+1} \) for given \( \lambda^n \) and \( k^n \) by sequentially solving following problems

\[ (\lambda^n \nabla \phi^n, \nabla h) + (\mathbf{u} \cdot \nabla \phi^n, h) + (k^n \phi^n, h) = (f, h) \quad \forall h \in V, \]

\[ (\lambda^n \nabla \tau, \nabla \eta^n) + (\mathbf{u} \cdot \nabla \tau, \eta^n) + (k^n \eta^n, \tau) = -\left(\frac{1}{\mu_0} + \frac{1}{2}\right)\left(I_{\phi^n}, \tau\right) \quad \forall \tau \in V, \]

\[ \mu_1(\lambda^{n+1} - \lambda^n) + \left((\lambda - \lambda^{n+1}) \nabla \phi^n, \nabla \eta^n\right) \geq 0 \quad \forall \lambda \in K_1, \]

\[ \mu_2(k^{n+1} - k^n) + \left((k - k^{n+1}) \nabla \phi^n, \nabla \eta^n\right) \geq 0 \quad \forall k \in K_2. \]  

(21)

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

6. Conclusion

In this paper, boundary value and inverse coefficient problems for the linear mass transfer equation are formulated and studied. In the framework of optimization approach, the problem of restoring of diffusion and reaction coefficients is reduced to the two-parameter multiplicative control problem. From an applied point of view, the numerical solution of direct problems allows us to predict the propagation of pollutants in space during an accident at a hazardous production site. In calculating the economic efficiency of enterprises, life safety of people will be taken into account, and the prognosis of the propagation of pollutants will determine the location of safe places for people to live near hazardous industries. However, the solving of direct problems is possible when environmental parameters are known. The determination of diffusion and reaction coefficients is particularly difficult. In the framework of the proposed approach, these coefficients can be restored from the concentration of a substance measured in a certain subdomain.

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