Mathematical Modelling of Production Localization with Risks of Technological Disaster

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Abstract. In the present paper the propagation of pollutants due to a technological disaster is simulated. This will allow us at the design stage to identify areas of the terrain where the concentration of harmful substances will be increased in the event of an accident. For this purpose, theoretical and numerical analysis of boundary value and extremum problems for the reaction-diffusion-convection model is carried out.

1. Introduction

Mathematical modeling of production localization with risks of technological disaster should serve the safety of people who live near such industries due to economic necessity or historically. We assume that a technological disaster is possible. In this case, a pollutant is emitted and we simulate its propagation. For this purpose, we use linear, semi-linear and non-linear reaction-diffusion-convection models (see [1-12]). Based on a qualitative analysis of solutions to the corresponding boundary value problems, we construct effective numerical algorithms for solving boundary value problems. The graph of the numerical solution of the boundary value problem will show exactly in which areas of space the pollution will exceed the permissible limits. When designing the respective facility, these areas will be designated as uninhabitable.

Obviously, both in the analytical and in the numerical solution of the boundary value problem, we must know all of its initial data. We can know the wind rose, the location of the pollution source and the intensity of the pollution release. In other words, we know the velocity vector and the density of the source of pollution in the mass transfer model (see [1,8,9]). At the same time, the diffusion coefficient and the reaction coefficient are much more difficult to determine. We propose to restore these coefficients by the substance concentration measured in a certain subdomain. For this purpose, a pollutant of safe concentration is released at the facility. In the framework of the optimization approach the considered inverse problem is reduced to the two-parameter multiplicative control problem (see [6, 8, 12-15]).

The present paper is devoted to the development of numerical algorithms for solving multiplicative control problems for a linear reaction-diffusion-convection model. Let us note papers [8, 16, 17], in which the numerical algorithms for solving of the multiplicative control problem for the mass-transfer model are studied. Separately, we note the papers [16, 17], devoted to numerical algorithms for recovering constant diffusion and reaction coefficients. In this article, special attention is paid to the...
Discussion of the results of numerical experiments on the reconstruction of the variable diffusion coefficient.

2. Boundary value and extremum problems

In a bounded domain $\Omega \subseteq \mathbb{R}^d$, $d=2,3$ with Lipschitz boundary $\Gamma$ we consider the following admixture transfer model:

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

(1)

Here $\lambda=\lambda(x) > 0$ is a variable diffusion coefficient, $u = u(x)$ is the velocity vector, $k = k(x) \geq 0$ is a reaction coefficient, $f = f(x)$ is a volume source density. For given functions $\lambda$, $u$, $k$ and $\psi$ problem (1) has a unique weak solution (see [1]). However, in practice, situations often arise when one or more of the given functions of problem (1) are unknown. In such situations, we need additional information about the solution $\varphi$ of problem (1).

In this paper, we consider the problem of finding the coefficients $\lambda$ and $k$ along with the solution $\varphi$ of problem (1) by concentration $\varphi_d(x)$ measured in some subdomain $Q \subseteq \Omega$. In framework of the optimization approach, this problem is reduced to a two-parameter multiplicative control problem (see [6, 8, 12-15]).

Let us assume that the multiplicative controls $\lambda$ and $k$ can change in some sets $K_1$ and $K_2$ and the following conditions hold:

(j) $K_1 \subseteq H^1_0(\Omega)$, $\lambda_{\Omega} > 0$, $s > d/2$, $K_2 \subseteq L^2(\Omega)$ 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

$$F(\varphi, \lambda, k, f, h) = (\lambda \nabla \varphi \cdot \nabla h) + (u \cdot \nabla \varphi, h) + (k \varphi, h) - (f, h) \quad \forall h \in V$$

(3)

where $\varphi \in V$ is the weak solution of problem (2).

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

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

(4)

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.

We use the following cost functionals:

$$I_1(\varphi) = \| \varphi - \varphi_d \|^2_{0, \Omega} = \int_{\Omega} |\varphi - \varphi_d|^2 \, dx, \quad I_2(\varphi) = \| \varphi - \varphi_d \|^2_{0, \partial Q}.$$  

(5)

Here $\varphi_d \in L^2(Q)$ is a given function in $Q$, $r = r_Q$ is the characteristic function of $Q$, and $\tilde{\varphi}_d \in L^2(\Omega)$ is a function that is equal to $\varphi_d$ in $Q$ and vanishes outside of $Q$.

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:

(ii) $\mu_0 > 0$, $\mu_1 \geq 0$, $\mu_2 \geq 0$ 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.

On solvability of problem (4) see in [8].

3. Derivation of the optimality system

Let us derive the optimality system for problem (4). According to the general theory of extremum problems (see [18]), we introduce a Lagrange multiplier $\eta \in V$ which is interpreted as an “adjoint” concentration.

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

$$L(\varphi, u, f, \eta) = J(\varphi, u) + \langle F(\varphi, u, f), \eta \rangle = (\mu_0/2) f(\varphi) + (\mu_1/2) \| \lambda \|_u^2 + (\mu_2/2) \| k \|_k^2 + \langle F(\varphi, u, f), \eta \rangle.$$  

(6)
The result of [18, p. 79] implies the following assertion.

**Theorem 3.1.** Let under the assumptions $\Omega$ is a bounded domain in $\mathbb{R}^3$ with boundary $\Gamma \in C^0$, $\lambda \in H_{0}^{1}\left(\Omega\right)$, $\lambda_{0}=\text{const}>0$, $s>0$, $l_{0} \in L_{1}(\Omega)$, $f \in L_{2}(\Omega)$, $\psi \in H^{1}(\Gamma)$ and (j), (ii) the solution $\left(\hat{\phi}, \hat{u}\right) \in V \times K$ be a local minimizer in problem (4), and let the cost functional $I\left(\cdot\right): V \rightarrow \mathbb{R}$ be continuously differentiable with respect to $\varphi$ at the point $\hat{\phi}$. Then there exists a unique Lagrange multiplier $\eta \in V$ such that the Euler-Lagrange equation takes place

$$
E'_{\varphi}\left(\hat{\phi}, \hat{u}, f, \eta\right) = 0 \quad \text{in} \quad V^* 
$$

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

$$
\begin{align*}
\left\langle E_{\lambda}\left(\hat{\phi}, \hat{u}, f, \eta\right), \lambda - \hat{\lambda} \right\rangle &= \mu_{1}\left(\lambda - \hat{\lambda}\right)_{\Omega} + \left(\lambda - \hat{\lambda}\right) \nabla \phi \cdot \nabla \eta \geq 0 \quad \forall \lambda \in K_{1}, \\
\left\langle E_{k}\left(\hat{\phi}, \hat{u}, f, \eta\right), k - \hat{k} \right\rangle &= \mu_{2}\left(k - \hat{k}\right)_{\Omega} + \left(k - \hat{k}\right) \hat{\phi} \cdot \hat{\eta} \geq 0 \quad \forall k \in K_{2}.
\end{align*}
$$

It follows from (6) that

$$
\left\langle F'_{\varphi}\left(\hat{\phi}, \hat{u}, f\right), \tau, \eta\right\rangle = \left\langle F'_{\varphi}\left(\hat{\phi}, \hat{u}, f\right), \tau, \eta\right\rangle = \left(\lambda \nabla \tau, \nabla \eta\right) + \left(\mu_{0}/2\right) \left(F_{\varphi}'\left(\hat{\phi}, \hat{u}, f\right), \tau, \eta\right) \quad \forall \tau \in V.
$$

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

$$
\left(\lambda \nabla \tau, \nabla \eta\right) + \left(\mu_{0}/2\right) \left(F_{\varphi}'\left(\hat{\phi}, \hat{u}, f\right), \tau\right) = 0 \quad \forall \tau \in V.
$$

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 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. Results of numerical experiments

Numerical experiments confirmed the effectiveness of the numerical algorithm described in [15, 19]. In papers [16, 17] the indicated algorithm showed good results for the case when the sought parameters are constants. In this work, the case was considered when it is required to restore an unknown parameter depending on a spatial variable. Discretization of boundary value problems is carried out using the finite differences method, and the solution of the optimality system is based on the Newton method [20]. The algorithm was tested using the Scilab software package [21].

In this paper, we present the results of numerical experiments for a special case of problem (4), when it is necessary to restore only the parameter $\lambda$ and the concentration $\varphi$. Having restored the diffusion coefficient $\lambda$, we can simulate the propagation of pollutants due to a technological disaster. We assume that the concentration of the pollutant is maximum at the center of the considered domain $\Omega$ and decreases toward the boundary $\Gamma$ of $\Omega$. In this regard, the density of pollution sources is described by the formula $f = 2\lambda \left(y - y^2 + x - x^2\right) + k \left(x - x^2\right) \left(y - y^2\right)$. The reaction coefficient is constant in all domain ($k=0.5$), and the pollutant is absent on boundary $\Gamma$, i.e. $\psi=0$ on $\Gamma$. The transfer of the pollutant within the domain is carried out only by diffusion, since there is no convection in the study domain (i.e. $u=(0,0)$). The role of additional information on the solution $\varphi$ of problem (1) is played by the function $\varphi_{0}(x)$, obtained by solving of problem (1), where $\lambda_{0} = \sin(\pi y)$. The information about the solution $\varphi$ of problem (1) is known throughout the domain $\Omega$ (i.e. $Q=\Omega$), the domain $\Omega$ being a unit square (see figure 1) on which a uniform grid is introduced.
Uniqueness and stability of solution of extremum problem (4) depends on choice of regularization parameters $\mu_0$ and $\mu_1$. In the course of the researches, the parameter $\mu_0$ was selected to be 1 and the effect of the parameter $\mu_1$ on the solution of the problem (4) is studied. Figure 2 and figure 3 graphs 

$$ E_0 = \sqrt{\| \phi - \phi_d \|^2 / \| \phi_d \|^2} $$ \quad \text{and} \quad 

$$ E_1 = \sqrt{\| \lambda - \lambda_d \|^2 / \| \lambda_d \|^2} $$

show the effect of the regularization parameter $\mu_1$ on the accuracy of solution $\phi$ and the parameter $\lambda$ recovery. The graphs show that the values of the functions $\lambda$ and $\phi$ will be closest to the desired ones if $\mu_1 < 10^{-6}$.

**Figure 2.** Graph of function $E_0$ versus regularization parameter $\mu_1$.

**Figure 3.** Graph of function $E_1$ versus regularization parameter $\mu_1$.

Using the value $\mu_1 = 10^{-8}$, then a range of values was determined for the initial approximation $\lambda_0$ (Newton method parameter influencing the convergence of the method). In figure 4 and figure 5 graphs $E_0$ and $E_1$ show that in order to converge the solution to the desired value, the initial approximation $\lambda_0$...
must be selected from the range [0.3;0.6]. Since the Newton method has quadratic convergence, it took from 4 to 6 iterations to obtain a solution to the coefficient inverse extremum problem.

![Graph of function $E_0$ depending on the choice of the initial approximation.](image1)

![Graph of function $E_1$ depending on the choice of the initial approximation.](image2)

**Figure 4.** Graph of function $E_0$ depending on the choice of the initial approximation.  
**Figure 5.** Graph of function $E_1$ depending on the choice of the initial approximation.

Given the results of the studies, in figure 6 and figure 7 shows graphs of the reconstructed function $\varphi$ and parameter $\lambda$ for the regularization parameter $\mu=10^{-8}$ and the initial approximation $\lambda_0=0.4$.

![Restored solution $\varphi$.](image3)

![Restored parameter $\lambda$.](image4)

**Figure 6.** Restored solution $\varphi$.  
**Figure 7.** Restored parameter $\lambda$.

5. **Conclusion**

In this work, the main attention is paid to the problem of restoring the diffusion coefficient depending on the spatial variable. For this inverse problem the efficient numerical algorithm was developed and implemented, using the Scilab software package. The influence of the regularization parameter on the solution of the considered inverse problem is studied. Having restored the diffusion coefficient, we can simulate the propagation of pollutants due to a technological disaster. Having identified areas with increased pollution, we recommend making them non-residential at the design stage (see also [19]).

6. **References**

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