Optimisation Approach to Minimize the Effects of Technological Disasters

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Abstract. It is known that the concentration of the pollutant can be reduced by adding a reagent, which increase the rate of pollutant’s decomposition. In framework of the optimization approach, the problem of decreasing of the pollutant’s concentration is reduced to the multiplicative control problem for a nonlinear model of reaction-diffusion-convection. In the model under consideration, the reaction coefficient rather arbitrarily depends on both the concentration of the pollutant and the spatial variable.

1. Introduction. Boundary value problem
During a long period the interest for the studying of boundary value and control problems for linear and nonlinear heat-and-mass transfer models hasn’t waned (see [1–15]). The main application of control problems is the search for effective mechanisms for controlling physical fields in continuous media.

The present paper is devoted to theoretical substantiation of soil research methods in the area of real space. It is supposed to use a reagent to increase the rate of decomposition of a harmful substance in water or air. Spread of pollutant is described using the reaction-diffusion-convection equation under mixed boundary conditions. It is assumed that the reaction coefficient rather arbitrarily depends on the concentration of the substance and the spatial variable. This makes it possible to take into account the uneven distribution of the reagent in the corresponding domains. It is possible that the reagent can also change the rate of decomposition of the pollutant from its concentration. Operator construction of the reaction coefficient used in this paper allows one to simulate such situations.

In bounded domain \( \Omega \subset R^3 \) with boundary \( \Gamma \), consisting of two parts: \( \Gamma_D \) and \( \Gamma_N \), the following boundary value problem for the nonlinear reaction-diffusion-convection equation is considered:

\[
-\lambda \Delta \phi + \mathbf{u} \cdot \nabla \phi + k(\phi, \mathbf{x})\phi = f \quad \text{in} \quad \Omega,
\]

\[
\phi = \psi \quad \text{on} \quad \Gamma_D, \quad \frac{\partial \phi}{\partial n} = \chi \quad \text{on} \quad \Gamma_N.
\]

Here function \( \phi \) represents the concentration of the pollutant, \( \mathbf{u} \) is a velocity vector, \( f \) is a volume sources density, \( \lambda \) is a constant diffusion coefficient, \( k(\phi, \mathbf{x}) \) is a reaction coefficient. Below, we will refer to the problem (1), (2) for given functions \( k, f, \chi \) and \( \psi \) as Problem 1.

Global solvability and uniqueness of solution to problem 1 follow from results [12]. In this paper, we prove principle of minimum and maximum for the concentration \( \phi \) under additional conditions on the initial data of problem 1.

Further for Problem 1 the problem of multiplicative control is formulated and researched. It is assumed that the reaction coefficient has the form of the product \( k(\phi, \mathbf{x}) = \beta(\mathbf{x})k_0(\phi) \). The role of controls in the problem is played by \( \beta(\mathbf{x}) \).

We also note that that in addition to the search of efficient mechanisms of control of physical processes in continuous medium, the study of control problems has also other applications. In the
framework of the optimisation approach a number of inverse problems are reduced to control ones. In particular, inverse coefficient problems are reduced to the multiplicative control problems (see [15–18] about the correctness of this approach).

Below we will use the Sobolev functional spaces $H^s(D), s \in R$. Here $D$ means either a domain $\Omega$ or some subset $Q \subset \Omega$, or the boundary $\Gamma$ or its part $\Gamma_0 \subset \Gamma$. By $\|s \|_{L_2}, |s|_{s,0}$ and $\langle \cdot , \cdot \rangle_{s,0}$ we denote the norm, seminorm and the scalar product in $H^s(Q)$, respectively. The norms and the scalar product in $L^2(Q), L^2(\Omega)$ and $L^2(\Gamma_N)$ will be denoted, correspondingly, by $\|s \|_{L_2}, |s|_{s,0}$ and $\langle \cdot , \cdot \rangle_{s,0}, \|s \|_{\Gamma_N}$ and $\langle \cdot , \cdot \rangle_{\Gamma_N}$.

Let $L^p_0(D) = \{k \in L^p(D); k \geq 0\}, p \geq 3/2$, $Z = \{v \in L^4(\Omega)^3; \div v = 0 \ in \ \Omega, v \cdot n|_{\Gamma_N} = 0\}$.

By $T = \{h \in H^1(\Omega); \rho|_{\Gamma_D} = 0\}$ we denote the main (and test) functional space for a concentration $\rho$.

Let the following conditions hold:

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

(ii) open sets $\Gamma_D$ and $\Gamma_N$ of $\Gamma$ satisfy conditions: $\Gamma = \Gamma_D \cup \Gamma_N, \Gamma_D \cap \Gamma_N = \emptyset$. Further, the surface measure $\Gamma_0$ is positive, and the boundary $\partial\Gamma_D$ of the set $\Gamma_D$ consists of finitely many closed Lipschitz curves;

(iii) $f \in L^2(\Omega), \chi \in L^2(\Gamma_N)$;

(iv) for any function $w \in T$, the embedding $k(w, \cdot) \in L^p_+(\Omega)$ is true for some $p \geq 3/2$, where $p$ does not depend on $w$; and on any sphere $B_r = \{w \in T; \|w\|_{1,\Omega} \leq r\}$ of radius $r$ the following inequality takes place:

$$\|k(w_1, \cdot) - k(w_2, \cdot)\|_{L^p(\Omega)} \leq L \|w_1 - w_2\|_{L^2(\Omega)} \ \forall w_1, w_2 \in T.$$ 

Here $L$ is the constant, which depends on $r$, but does not depend on $w_1, w_2 \in B_r$.

Let us also remind that the condition (iv) describes the reaction coefficient $k$ of Problem 1 or on the spatial variable $x \in \Omega$. For example,

$$\tilde{k}_1 = \phi^2 \ (or \ \tilde{k}_1 = \phi^2(\rho)) \ in \ subdomain \ Q \subset \Omega \ or \ \tilde{k}_1 = k_0(x) \in L^{3/2}(\Omega\setminus Q) \ in \ \Omega\setminus Q.$$ 

From a physical point of view, the coefficient $\tilde{k}_1$ corresponds to the situation, when the substance’s decomposition rate is proportional to the square (or cube) of substance’s concentration in a subdomain $Q \subset \Omega$ and outside $Q$ the rate of the chemical reaction depends only on a spatial variable (see [14,15]). Below we will just write $k(\rho)$, while emphasizing the nonlinear dependence of reaction coefficient on the concentration.

**Remark 1.1.** Below, for simplicity, we will write $k(\rho)$ instead of $k(\rho, x)$, except for those cases where dependence on $x$ plays no less important role than nonlinear dependence of these coefficients on $\rho$.

Let us also remind that, by the Sobolev embedding theorem, the space $H^1(\Omega)$ is embedded into the space $L^6(\Omega)$ continuously at $s \leq 6$ and compactly at $s < 6$ and, with a certain constant $C_s$, depending on $s$ and $\Omega$, we have the estimate

$$\|\varphi\|_{L^s(\Omega)} \leq C_s \|\varphi\|_{L^1(\Omega)} \ \forall \varphi \in H^1(\Omega).$$

The following technical lemma holds (see [10]).

**Lemma 1.1.** Under the conditions (i), (ii), $u \in Z, k_1 \in \tilde{L}^p_+(\Omega), p \geq 3/2$, there exist positive constants $C_0, \delta_0, \gamma_1$, which depend on $\Omega$ or depend on $\rho$ or depend on $\Omega, \Gamma_N$, such that the following relations hold:

$$|1(\lambda \varphi, \eta)| \leq C_0 \|\varphi\|_{L^1(\Omega)} \|\eta\|_{L^1(\Omega)}, \ |(u \cdot \nabla \varphi, \eta)| \leq \gamma_1 \|u\|_{L^4(\Omega)} \|\varphi\|_{L^1(\Omega)} \|\eta\|_{L^1(\Omega)},$$

$$|\langle \lambda^2 \varphi, \eta \rangle| \leq C_0 \|\varphi\|_{L^1(\Omega)} \|\eta\|_{L^1(\Omega)} \|\eta\|_{L^1(\Omega)},$$

$$|\langle \chi, h \rangle| \leq \gamma_2 \|\chi\|_{L^P(\Gamma_N)} \|h\|_{L^1(\Omega)} \ \forall \chi \in L^2(\Gamma_N), \ h \in H^1(\Omega),$$

$$|u \cdot \nabla \varphi, \varphi| = 0 \ (\lambda \varphi, \nabla \varphi) \geq \lambda_0 \|\varphi\|_{L^2} \ \forall \varphi \in T, \lambda_0 = \delta \lambda_0.$$
\[(\lambda \nabla \varphi, \nabla h) + (k(\varphi)\varphi, h) + (u \cdot \nabla \varphi, h) = (f, h) + (\chi, h)_{\Gamma_N} \quad \forall h \in T, \varphi|_{\Gamma_D} = \psi. \quad (7)\]

**Definition 1.1.** The function \(\varphi \in H^1(\Omega)\), satisfying \((7)\), will be called a weak solution of Problem 1. To prove the solvability of Problem 1, we need the following lemma [10].

**Lemma 1.2.** Assume that the assumption (i) holds. Then for any function \(\psi \in H^{1/2}(\Gamma_D)\) there is function \(\varphi_0 \in H^1(\Omega)\), such that \(\varphi_0 = \psi \) on \(\Gamma_D\) and with some constant \(C_1\), depending on \(\Omega\) and \(\Gamma_D\), the estimate \(\|\varphi_0\|_{1, \Omega} \leq C_1 \|\psi\|_{1/2, \Gamma_D}\) holds.

In addition to (iv), we will assume that the nonlinearity \(k(\varphi)\varphi\) is monotone in the following sense:

(v) \((k(\varphi_1)\varphi_1 - k(\varphi_2)\varphi_2, \varphi_1 - \varphi_2) \geq 0\) for all \(\varphi_1, \varphi_2 \in H^1(\Omega)\);

Also, let the functions \(k(\varphi)\) be bounded in the sense that there exist positive constants \(A_1, B_1\) depending on \(k\) such that

(vi) \(\|k(\varphi)\|_{L^\infty(\Omega)} \leq A_1 \|\varphi\|_{1, \Omega} + B_1\) for all \(\varphi \in H^1(\Omega)\) as \(p \geq 3/2, r \geq 0\).

The following theorem holds (see in details [12]).

**Theorem 1.1.** Assume that the assumptions (i)–(v) hold. Then, there exists an unique weak solution \(\varphi \in H^1(\Omega)\) of Problem 1 and the following estimate is true:

\[
\|\varphi\|_{1, \Omega} \leq M_{\varphi} \equiv C_c C_2 \|\sigma\|_{\Omega} + C_{\gamma} \|\eta\|_{\Gamma_N} + C(C_0 C_1 + \gamma \Gamma_1 C_1) \|u\|_{L^2(\Omega)} + C_{\max}^{1/2} + C_{\max}^{1/2} + C_{\max}^{1/2} + C_{\max}^{1/2}, \quad (8)
\]

Here the constant \(C_2\) is introduced in (3), \(C_0, \gamma_1, \gamma_2, \lambda_1\) and \(C_1\) are constants from Lemmas 1.1 and 1.2, respectively.

Using some concepts of [19], let us prove maximum and minimum principle for concentration \(\varphi\). Let \(\psi_{\min}, \psi_{\max}, f_{\min}, f_{\max}\) be positive numbers and let, in addition to (i)–(vi), the following condition holds:

(vii) \(\psi_{\min} \leq \psi \leq \psi_{\max} \) a.e. on \(\Gamma_D, f_{\min} \leq f \leq f_{\max} \) a.e. in \(\Omega\) and \(\chi = 0\) on \(\Gamma_N\).

**Lemma 1.3.** Assume that the assumptions (i)–(vii) hold. Then for the weak solution \(\varphi \in H^1(\Omega)\) of Problem 1 the following maximum and minimum principle holds:

\[
m \leq \varphi \leq M \quad \text{a.e. in } \Omega, \quad M = \max\{|\psi_{\max}, M|\}, \quad m = \min\{|\psi_{\min}, m|\}. \quad (9)
\]

Here the constants \(M\) and \(m\) are found from the relations \(k(M)M = f_{\max}\) and \(k(m)m = f_{\min}\).

**Proof.** Let us first prove that \(\varphi \leq m\) a.e. in \(\Omega\). For this purpose, we introduce the function \(\bar{\varphi} = \max\{\varphi - M, 0\}\). It clear that \(\varphi \in T\) and the following equality hold:

\[
(\bar{\varphi}, \nabla \bar{\varphi}) = (\nabla \bar{\varphi}, \nabla \bar{\varphi}), \quad (u \cdot \nabla \varphi, \bar{\varphi}) = (u \cdot \nabla \varphi, \bar{\varphi}) = 0.
\]

With this in mind, setting \(h = \bar{\varphi} \) in \((7)\), we obtain

\[
\lambda (\nabla \bar{\varphi}, \nabla \bar{\varphi}) + (k(\bar{\varphi})\bar{\varphi}, \bar{\varphi}) = (f, \bar{\varphi}). \quad (10)
\]

By \(Q_M \subset \Omega\) we denote the subdomain \(\Omega\), where \(\varphi > M\). It clear that

\[
(k(\bar{\varphi})\bar{\varphi}, \bar{\varphi}) = (k(\bar{\varphi})\bar{\varphi}, \bar{\varphi})_{Q_M} = (k(\bar{\varphi} + M, \bar{\varphi}), \bar{\varphi})_{Q_M}
\]

and by (v) for all functions \(\varphi_1 = \bar{\varphi} + M\) and \(\varphi_2 = M\) form \(H^1(\Omega)\) the following inequality holds:

\[
0 \leq (k(\bar{\varphi} + M)(\bar{\varphi} + M) - k(M)M, \bar{\varphi}) = (k(\bar{\varphi} + M)(\bar{\varphi} + M) - k(M)M, \bar{\varphi})_{Q_M}, \quad (11)
\]

since \(\bar{\varphi} = 0\) in \(\Omega \setminus \overline{Q_M}\).

Subtracting \((k(M)M, \bar{\varphi})\) from both sides of \((10)\), we obtain

\[
\lambda (\nabla \bar{\varphi}, \nabla \bar{\varphi}) + (k(\bar{\varphi} + M)(\bar{\varphi} + M) - k(M)M, \bar{\varphi})_{Q_M} = (f - k(M)M, \bar{\varphi})_{Q_M}. \quad (12)
\]

By Lemma 1.1 and \((11)\), from \((12)\) we come to the estimate

\[
\lambda \|\bar{\varphi}\|^2_{1, \Omega} \leq (f - k(M)M, \bar{\varphi})_{Q_M}.
\]

From this estimate it follows that if \(M\) is chosen from the condition \((9)\), then \(\bar{\varphi} = 0\).

We set \(\bar{\varphi} = \min\{\varphi - m, 0\}\). It clear that \(\bar{\varphi} \in T\). We will assume that in the subdomain \(Q_M \subset \Omega\) and on the part \(\Gamma^1_M \subset \Gamma_N\) the inequality \(\varphi < m\) is true.

Arguing as above, we come to the equality

\[
\lambda (\nabla \bar{\varphi}, \nabla \bar{\varphi}) + (k(\bar{\varphi} + m)(\bar{\varphi} + m) - k(m)m, \bar{\varphi})_{Q_M} = (f - k(m)m, \bar{\varphi})_{Q_M},
\]

from which we derive the estimate

\[
\lambda \|\bar{\varphi}\|^2_{1, \Omega} \leq (f - k(m)m, \bar{\varphi})_{Q_M}.
\]

From the obtained estimate, as above, it follows that \(\bar{\varphi} = 0\) for \(m\) from \((9)\).
Remark 1.2. The parameters $M$ and $m$, in view of the monotonicity $k(\varphi)\varphi$ are defined in a unique way. For degree coefficients, these parameters are easy to calculate. For example, if $k(\varphi) = \varphi^2$, then $M = \int_{\max}^{1/3}$ and $m = \int_{\min}^{1/3}$.

2. Multiplicative control problem

When studying the problem, we will assume that the function $k(\varphi, x)$ satisfies the condition

\[(\text{viii})\; k(\varphi, x) = \beta(x)k_0(\varphi), \quad \text{where} \; \beta(x) \in H^3(\Omega), \; k_0(\varphi) \in L^2_\varphi(\Omega) \; \text{for all} \; \varphi \in H^1(\Omega).\]

By condition (viii) as $p > 2$ and in any ball $B_r = \{ \varphi \in H^1(\Omega): \| \varphi \|_{L^\varphi} \leq r \}$ of radius $r$ the inequality holds:

\[
\| k_0(\varphi_1) - k_0(\varphi_2) \|_{L^\varphi} \leq L_2 \| \varphi_1 - \varphi_2 \|_{L^\varphi} \quad \forall \varphi_1, \varphi_2 \in B_r.
\]

Here the constant $L_2$ depends on radius $r$ and does not depend on concrete $\varphi_1, \varphi_2 \in B_r$.

It is easy to show that conditions (vii) describe a particular case function $k(\varphi)$ satisfying (iv). Really, (see also [14]):

\[
\| \beta(k_0(\varphi_1) - k(\varphi_2)) \|_{L^{3/2}(\Omega)} \leq \| \beta \|_{L^6(\Omega)} \| k_0(\varphi_1) - k_0(\varphi_2) \|_{L^2(\Omega)} \leq C_0 \| \beta \|_{L^1(\Omega)} \| \varphi_1 - \varphi_2 \|_{L^4(\Omega)}.
\]

To formulate the control problem, we divide the set of initial data of Problem 1 into two groups: a group of fixed data, where we assign the functions $u, k_0(\varphi), f, \chi$ and $\psi$, and a control group, where we assign the function $\beta$, assuming that it can change in some set $K$ satisfying the condition

\[(j) \; K \subset L^2_\varphi(\Omega) \text{ is a nonempty convex closed bounded set.}\]

We introduce the space $Y = T^* \times H^{1/2}(\Gamma_d)$ and introduce an operator $F = (F_1, F_2): H^1(\Omega) \times K \rightarrow Y$ by formulae:

\[
\langle F_1(\varphi, u), h \rangle = (\lambda \nabla \varphi, \nabla h) + (\beta(x)k_0(\varphi)\varphi, h) + (u \cdot \nabla \varphi, h) + (\lambda \alpha(\varphi, x)\varphi, h)_{\Gamma_N} - (f, h) - (\chi, h)_{\Gamma_N},
\]

\[
F_2(\varphi) = \varphi|_{\Gamma_d} - \psi
\]

and rewrite (7) in the form $F(\varphi, \beta) = 0$. Considering this equality as a conditional constraint on the state $\varphi \in H^1(\Omega)$ and the control $\beta \in K$, we formulate the following conditional minimization problem:

\[
J(\varphi, \beta) \equiv \frac{\mu_0}{2} I(\varphi) \rightarrow \inf_{\varphi \in H^1(\Omega) \times K} F(\varphi, \beta) = 0, (\varphi, \beta) \in H^1(\Omega) \times K.
\]

Here $I: H^1(\Omega) \rightarrow R$ -- functional, полунепрерывный снизу относительно слабой сходимости.

The set of possible pairs for the problem (14) is denoted by $Z_{ad} = \{(\varphi, \beta) \in H^1(\Omega) \times K: F(\varphi, \beta) = 0, J(\varphi, \beta) < \infty\}$.

We use the following cost functionals [10]:

\[
I_1(\varphi) = \| \varphi - \varphi^d \|_2^2 + \int_0^1 | \varphi - \varphi^d |^2 dx, \quad I_2(\varphi) = \| \varphi - \varphi^d \|_2^2.
\]

Here a function $\varphi^d \in L^2(Q)$ denotes a desired concentration field, which is given in a subdomain $Q \subset \Omega$.

Using approaches [14], the following theorem is proved.

Theorem 2.1. Assume that the assumptions (i)–(vi), (viii) and (j) take place. Let $I: H^1(\Omega) \rightarrow R$ be a weakly semicontinuous below functional and let $Z_{ad} \ni 0$. Then there is at least one solution $(\varphi, \beta) \in H^1(\Omega) \times K$ of the control problem (14).

Remark 2.1. The functionals in (15) satisfy the conditions of Theorem 2.1.

The next stage in the research of the extremal problem is the derivation of an optimality system, which provides valuable information about additional properties of optimal solutions. On the basis of its analysis, one can establish, in particular, the uniqueness and stability of optimal solutions (see details, for example, in [10–16]. A separate article by the authors will be devoted to the research of the uniqueness and stability of optimal solutions. Specifically, for optimal solutions to problem (14), the bang-bang property will be established (see [20,21]).

3. Conclusion

In this article, a boundary value problem and a control problem for a nonlinear reaction-diffusion-convection model are studied. The proposed construction of the reaction coefficient makes it possible to study the effectiveness of the effect of the reagent on the rate of pollutant’s decomposition. From an applied point of view, the results of this article are close [22,23].
4. References

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