Numerical study of the inverse problem for the diffusion-reaction equation using optimization method

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Abstract. The model of transfer of substance with mixed boundary condition is considered. The inverse extremum problem of identification of the main coefficient in a nonstationary diffusion-reaction equation is formulated. The numerical algorithm based on the Newton-method of nonlinear optimization and finite difference discretization for solving this extremum problem is developed and realized on computer. The results of numerical experiments are discussed.

1. Introduction

The modern machine-building production, based on use of a large variety of materials, technological processes and the large range of products, creates the large quantity of various pollution. There are many methods to control industrial environmental pollution, for example, rational placement of sources of pollution, their localization, cleaning of emissions mathematical modeling, etc. One of the widespread methods is the method of mathematical modeling of the process of transfer pollution [1].

The application of the method of mathematical modeling for studying the distribution process of pollution necessitates the construction and study of the mathematical models describing distribution of pollution in the studied area. The mentioned models contain a number of parameters, which values have to be given for unambiguous finding the solution of boundary value problems. In practice, situations can arise when some of the parameters are unknown and they are to be found along with the solution of the boundary problem. Such problems belong to the class of the inverse problems of identification of unknown density of sources or the coefficients entering used models of transfer pollution. In the latter problems, the 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 revealed from additional information on the solution of the original boundary value problem. It is important that with a certain choice of the minimized cost the functional identification problems can be reduced to corresponding extremum problems. Following this approach, there arise inverse extremum problems, which can be studied using well known constrained minimization methods. This approach as applied to heat and mass transfer models was described in [1-10] for nonstationary models and in [11-23] for stationary heat and mass transfer models. We should also mention papers [24, 25] where the optimization method is applied for solving the related problems of technical gasdynamics.

In this work we consider the problem of identification of the main coefficient in the parabolic nonlinear diffusion-reaction equation considered at mixed boundary condition, using the additional information on the solution of the initial boundary value problem. The study of this problem can be reduced to the study of the corresponding extremum problem for a certain cost functional [3]. We develop an effective numerical algorithm, based on Newton-method of nonlinear optimization [26] and finite difference discretization of solving this extremum problem, and discuss some results of numerical experiments.

We study the following initial boundary value problem for the nonlinear nonstationary parabolic equation with mixed boundary conditions:

$$\begin{gathered}\frac{\partial\varphi}{\partial t}=\frac{\partial}{\partial x}\left(\lambda\frac{\partial\varphi}{\partial x}\right)-k\varphi+f,\quad (x,t)\in\Omega,\quad x\in(a,b),\\ \varphi(x,0)=\psi(x),\quad \lambda\frac{\partial\varphi}{\partial x}(a,t)=\chi_1(t),\quad \varphi(b,t)=\chi_2(t),\quad t\in[0,T]\end{gathered},\tag{1}$$

which is considered in a bounded domain $\Omega=\{(x,t): a<x<b,\quad 0<t<T\}$. Here $\lambda\equiv\lambda(x)>0$ is the variable diffusion coefficient, $k=\mathrm{const}\geq 0$ is a quantity characterizing disintegration of substance by chemical reactions, $f=f(x,t)$ is the volume source density, $\psi(x)$ is a function given in the initial condition, $\chi_1(t)$, $\chi_2(t)$ are functions given at $x=a$ and $x=b$.

2. Statement of Control Problem

The initial 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 solution φ of problem (1). For this information we can use, for example, concentration $\varphi_d(x_d,t)$ measured in some set $Q\subset\Omega$. We assume that coefficient λ is an unknown function and we must determine this function together with solution φ of problem (1).

For the study of this identification problem we apply optimization method and reduce solving this problem to the corresponding extremum problem (see [1, 19]). Assuming that $\mathrm{Q}=\{(x_d,t),\quad 0<t<T\}$ where x_d is fixed we introduce the following cost functional:

$$J(\lambda)=\int_0^T(\varphi(x_d,t)-\varphi_d(t))^2\,dt\,.$$

Our inverse extremum problem consists of finding two functions φ and λ so that the following conditions take place:

$$\begin{gathered}\frac{\partial\varphi}{\partial t}=\frac{\partial}{\partial x}(\lambda\frac{\partial\varphi}{\partial x})-k\varphi+f,\quad (x,t)\in\Omega,\quad x\in(a,b),\\ \varphi(x,0)=\psi(x),\quad \lambda\frac{\partial\varphi}{\partial x}(a,t)=\chi_1(t),\quad \varphi(b,t)=\chi_2(t),\quad t\in[0,T],\end{gathered}\tag{2}$$

$$J(\lambda)=\int_0^T(\varphi(x_d,t)-\varphi_d(t))^2\,dt\to\inf\,,\ (\varphi,\lambda)\in H^1(\Omega)\times H^s(\Omega)\,.\tag{3}$$

So far there are many works devoted to the theoretical analysis of the inverse extremum problems for the equations of a parabolic type. About solvability of related control problems it is possible to read in works [4, 10], where the existence and uniqueness of solutions of the extremum problems under some restrictions on initial data were proved.

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3. Numerical Algorithm

In the work the optimality system was obtained. 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 initial 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 the control problem (2), (3). The simplest numerical algorithm can be obtained by applying a simple iteration method for solving the optimality system. Direct and adjoint problems entering the optimality system can be solved by finite difference discretization method using Scilab [27].

4. Numerical Experiments

Now we should discuss some results of numerical experiments. Concentration of substance φ_d is the analytically given function $\varphi = (x - x^2)(t - t^2)$. We will take functions $f = (1-2t)(x - x^2) + 2(t - t^2) + 0.01(x - x^2)(t - t^2)$, $\psi(x) = 0$, $\chi_1(t) = -(t - t^2)$, $\chi_2(t) = 0$, diffusion coefficient λ=1 and coefficient k=0.01.

The results of the numerical solution of the inverse extremum problem (2), (3) will be presented below. The surface of restored function φ is shown in Figure 1 (right). The received surface coincides with the analytically given function presented in Figure 1 (left). Figure 2 shows restored function λ (dotted line) and required function λ (solid line). Figure 1 and Figure 2 show the case when area Q coincides with Ω.

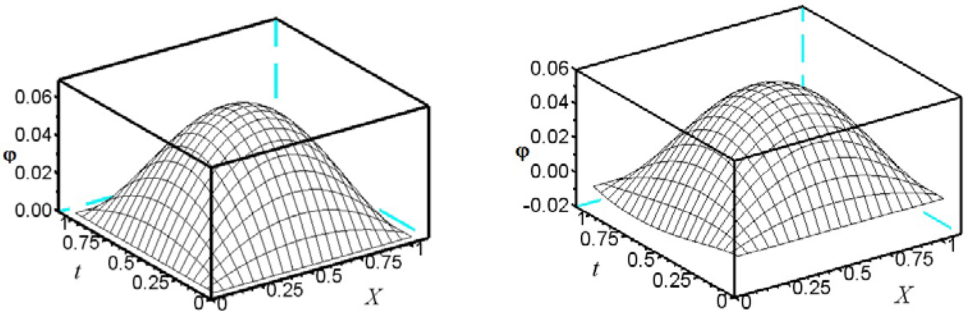

Figure 1. Analytically given function φ (left) and restored function φ (right)

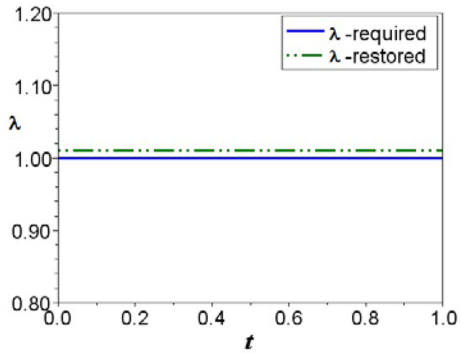

Figure 2. Required (solid line) and restored functions λ (dotted line)

Figure 3 shows restored function φ and required (solid line) and restored functions λ (dotted line) for the case, when observations in the research area are made at one point of the research area in the course of time. The results of calculations were obtained for a case when a source of additional information is the measurements of concentration measured at point x=0.5. The presented graphics show that the developed algorithm of the numerical solution of the inverse extremum problem allows even at a small amount of information a qualitative restoration of the required functions for the non-stationary parabolic equation.

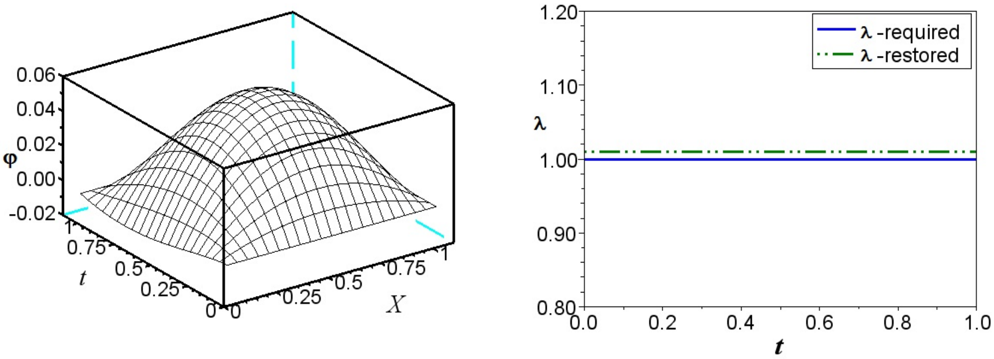

Figure 3. Restored function φ on the left and required (solid line) and restored functions λ (dotted line) on the right

The results of numerical experiments are given above, when the error in measurements of substance concentration is absent. When solving the applied problems of the main coefficient identification of non-stationary diffusion-reaction equation of substance concentration the given measurements are the main source of errors [3, 4]. It is caused by the features of concentration sensors functioning which are inevitable as a consequence of discrete nature of measurements, the accuracy of sensors indication, etcetera. In this regard the problem of identification of unknown coefficient λ with the indignant input data is of interest, that is, there is a need to investigate the resistance of the method for solution of the inverse problems to the errors of measurements.

For these experiments input data were perturbed according to formula $\varphi_d = \varphi + 2\delta(\text{rand}(1,1)\text{-}1/2))$, where $\delta = 0.1$, rand (1,1) – random number generator. As a result of calculations the following function graphs were received (Figure 4). The developed algorithm of the numerical solution of the inverse extremum problem allows a considerable approach of the numerical solution of φ (at the left) and λ (on the right) to the exact solution.

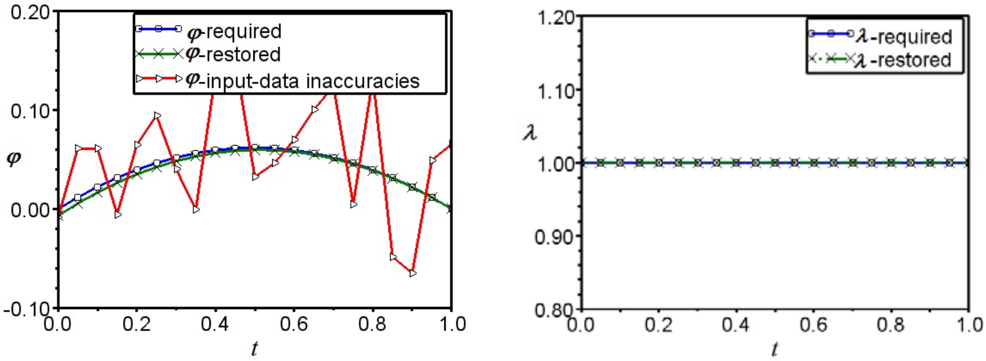

Figure 4. Function φ (left) and functions λ (right) with $\delta = 0.1$

In the next test (see Figure 5) the value $\delta = 0.01$ was choosed in the expression for function φ_d. As it follows from Figure 4 the error between exact and approximate solutions is essentially less than for the case when $\delta = 0.1$.

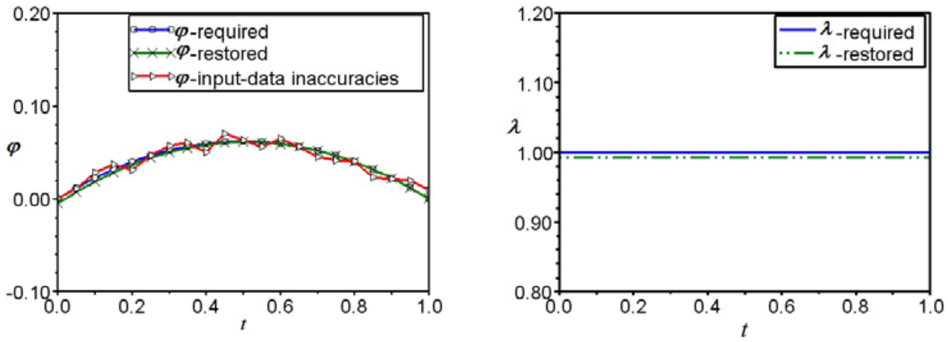

Figure 5. Function φ (left) and functions λ (right) with $\delta = 0.01$

5. Conclusion

In this work the problem of identification of the main coefficient in the nonlinear one-dimensional mass transfer model was formulated and studied. Our model has the form of nonlinear nonstationary diffusion-reaction equation with variable coefficient of the diffusion. This equation is considered to be in the bounded domain under mixed boundary condition. Based on the Newton method of nonlinear optimization we constructed the algorithm and developed a code for numerical solution of the coefficient inverse problem. The results of numerical experiments have shown the effectiveness of the used numerical algorithm and the code of numerical solution of the coefficient inverse problem for the mass transfer model under study.

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