OPTIMAL CONTROL METHOD FOR ESTIMATION OF UNKNOWN PARAMETERS OF GROUNDWATER CONTAMINATION

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Abstract
A problem of source functions identification for contaminant transport equation is considered. The optimal control formulation for steady-state and transient partial differential equations was used. The conjugated problems were constructed. For minimization of according functionals the gradient method was used. The direct and conjugate problems were solved by means of the difference method for every gradient step. To demonstrate the efficiency of the developed mathematical facilities results of numerical experiments are represented.

Introduction
During last time there has been increasing appearance of problems coupled to determination of unknown parameters of different sources of groundwater contamination. Such problems arise in a monitoring system of large industrial objects, sites of storage and burial of different wastes (including radioactive ones), where, as a rule, regular observations on the groundwater contamination are performed. But observations can only state a fact of contaminant entering into groundwater and, as a rule, don't allow to determine a contaminant source location and its power. Using of according mathematical and program facilities to solve reverse problems, that are problems of reconstruction of some process parameters under existing information about solution, seems to be a promising way for such kind of problems. In the time being there are a lot of reliable methods for groundwater contaminant transport modeling and forecasting. Besides, there are a great amount of field data accumulated on wastes disposal sites, ash-storage, burial sites etc. So it is necessary to develop and extend reliable software for reverse problems. In this investigation the problem of unknown source function determination, when information about contaminant concentration levels is available, was formulated as the optimal control problem for contaminant transport equation in plane. Existence of reliable methods and software for modeling and forecasting of contaminant transport in plane is a necessary condition for successful solution of such problems. A numerical algorithm for optimal control problem solving is developed. This algorithm is based on the according functional minimization by means of the gradient method, for every step of which direct and conjugate problems to be solved. For direct and conjugate problems solving the finite-difference method is used.

Methods
In modeling of contaminant transport with a plane flow of groundwater it is necessary to solve, at least, a system of equations: equation for determination of velocity distribution of groundwater flow (Bussinesq equation) and contaminant transport equation. Let consider a problem of a source function reconstruction for the Bussinesq equation under existing field of concentration.

Contaminant concentration $C(x_1, x_2, t)$ to be determined from an equation

$$\frac{\partial C}{\partial t} = \sum_{i=1}^{2} \frac{\partial}{\partial x_i}\left(D \frac{\partial C}{\partial x_i} \right) - \sum_{i=1}^{2} \frac{\partial (v_i C)}{\partial x_i} + U(x_1, x_2, t) \qquad (1)$$

where $U(x_1, x_2, t)$ - source function, to be determined, D - diffusive coefficient, v_i - velocity components.

Let seek a solution interior to the rectangular domain $\Omega = \{x = (x_1, x_2);\ 0 \le x_1 \le L_1, 0 \le x_2 \le L_2\}$ under $0 < t \le T$. Along the appropriate domain boundaries the next conditions, for instance, may be prescribed.

$$\left.\frac{\partial C}{\partial x_1}\right|_{x_1 = 0} = \left.\frac{\partial C}{\partial x_1}\right|_{x_1 = L_1} = 0,\ D\left.\frac{\partial C}{\partial x_2}\right|_{x_2 = 0} = v_2 C,\ \left.C\right|_{x_2 = L_2} = Q, \tag{2}$$

where Q - given function.

The initial condition is prescribed in the form

$$C(x,0) = \varphi(x),\ x \in \Omega \tag{3}$$

At some time moment T measurements of concentration field interior to the domain was performed. These measurements can be performed in some separate points and then can be extended for entire domain.

The problem is reduced to seeking of minimum of the next functional:

$$J(U) = \int_0^{L_1}\int_0^{L_2} \left(C(x,T;U) - Z(x)\right)^2 dx_1 dx_2, \tag{4}$$

where $Z(x)$ - given in Ω function (is constructed on the basis of observations data), U - control function, which belongs to some Hilbert space H. We shall consider $C(x_1, x_2, t)$ and $U(x_1, x_2, t)$ as solutions of the reverse problem.

For finding of minimum of the functional we'll use the gradient method (1).

Increment of the functional (4) can be written as follows

$$\Delta J(U) = J(U+h) - J(U) =$$

$$= \int_0^{L_1}\int_0^{L_2} 2\left(C(x,T;U) - Z(x)\right)\Delta C dx_1 dx_2 + \alpha(U,h),$$

where $\Delta C = C(x,t;U+h) - C(x,t;U)$, $h(x)$ - increment of control , $\alpha(U,h$)- infinitesimal with respect to $\|h\|_H \to 0$.

For gradient finding a conjugate problem(2) to (1)-(3) is used, where $\Psi(x_1, x_2, t)$- sufficiently smooth function.

$$-\frac{\partial \Psi}{\partial t} = \sum_{i=1}^{2} \frac{\partial}{\partial x_i}\left(D\frac{\partial \Psi}{\partial x_i}\right) + \sum_{i=1}^{2} v_i \frac{\partial \Psi}{\partial x_i} \tag{5}$$

$$\left.\left(D\frac{\partial \Psi}{\partial x_1} + v_1\Psi\right)\right|_{x_1 = 0} = \left.\left(D\frac{\partial \Psi}{\partial x_1} + v_1\Psi\right)\right|_{x_1 = L_1} = 0, \tag{6}$$

$$\left.\frac{\partial \Psi}{\partial x_2}\right|_{x_2 = 0} = 0,\quad \left.\Psi\right|_{x_2 = L_2} = 0,\quad 0 \le t < T,$$

$$\Psi(x,T) = 2\left(C(x,T) - Z(x)\right),\ x \in \Omega. \tag{7}$$

Then gradient can be written as $J'(U) = \Psi(x,t)$.

To solve the boundary problems (1)-(3) and (5)-(7) the finite-difference method on non-uniform grid is used (3).

After finding of solutions of direct and conjugate problems new control according the gradient method can be found from formula

$$U_{ij}^{k\,s+1} = U_{ij}^{k\,s} - \lambda_s \Psi_{ij}^{k\,s},\ s = 0,1,2...,\ k = \overline{1, N_T - 1} \tag{8}$$

where i, j - vary with all interior nodes of the grid domain $\Omega_{h_i h_j}$, k - time moment, $(N_T + 1)$- the number of grid nodes in the direction t, λ_s- step coefficient, which is chosen under condition $|\ J(U^{s+1})\ | \langle |\ J(U^s)\ |$.

The next conditions is a criterion to stop of the iteration process (8)

$$\max_{ijk} \left| \Psi_{ij}^{ks} \right| \langle\ \varepsilon, \qquad \varepsilon\ \rangle\ 0.$$

In the case long-term operation of a source of contamination (as it is in the most of practical problems) it is advisable to consider the steady-state equation (1), which can be written in the form

$$\sum_{i=1}^{2} \frac{\partial}{\partial x_i} \left(D \frac{\partial C}{\partial x_i} \right) - \sum_{i=1}^{2} \frac{\partial (v_i C)}{\partial x_i} = U(x) \qquad (9)$$

The appropriate boundary conditions are adjoined to the equation (9).
Instead the functional (4) the next functional will be considered:

$$J(U) = \int_0^{L_1} \int_0^{L_2} \left(C(x;U) - Z(x) \right)^2 dx_1 dx_2 \qquad (10)$$

The conjugate equation can be written in the form

$$\sum_{i=1}^{2} \frac{\partial}{\partial x_i} \left(D \frac{\partial \Psi}{\partial x_i} \right) + \sum_{i=1}^{2} v_i \frac{\partial \Psi}{\partial x_i} = -2\left(C(x) - Z(x) \right) \qquad (11)$$

In this problem the functional gradient is determined by formula
$J'(U) = \Psi(x)$.
For the functional minimum finding we can use the gradient method again.

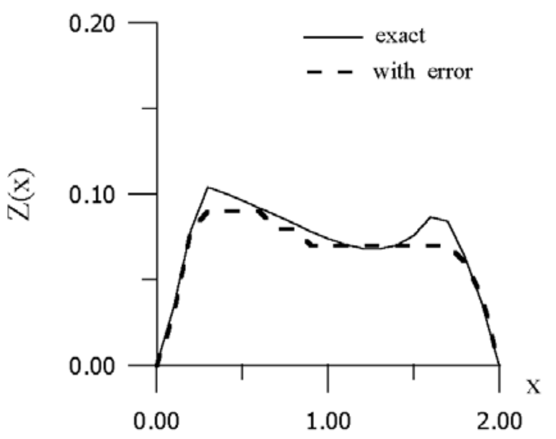
Results

According to problems formulated and algorithms developed the software was created and numerical calculations were carried out.

1. Let consider one-dimensional equation (1) under uniform boundary conditions of first kind and uniform initial condition.

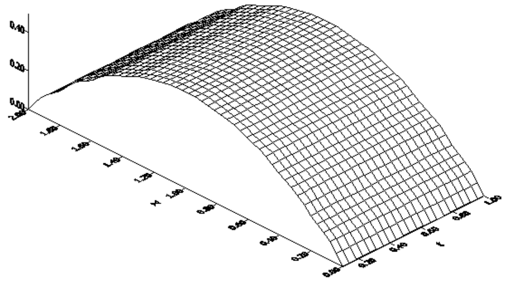
The next example was used as a test one. First the direct problem is solved under condition $0 \le x \le 2$, $T = 1$ for $D = 0.3$ $v = -1$. In numerical calculations 21 points in x direction and 11 points in t direction were used. The source function was prescribed in the form $U(x,t) = 1$ under $0.2 \le x \le 0.3$, $U(x,t) = 0.5$ under $1.6 \le x \le 1.7$ and $U(x,t) = 0$ for all rest points, $0 \langle\ t \le 1)$. Prescribed concentration $C(x,T) = Z(x)$ is given in Figure 1.

Figure 1: Prescribed concentration



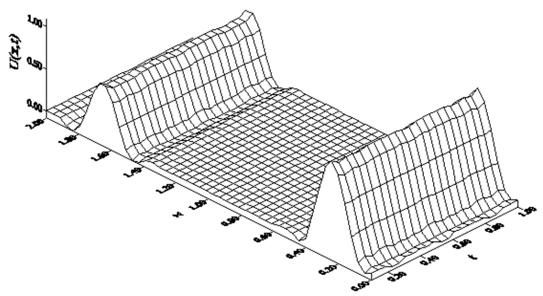
Then using $Z(x) = C(x,T)$ and assuming $U(x,t)=\phi(x,t)$, where $\phi(x,t)$ is an arbitrary initial control (graph for $\phi(x,t)$ function is given in Figure 2), we solved the reverse problem ($\varepsilon = 0.001$).

Figure 2: Initial control



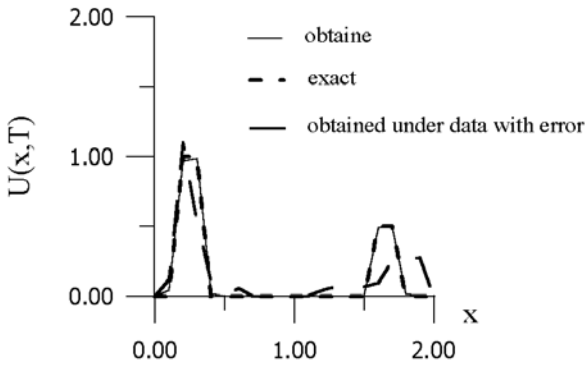
The control obtained, $U(x,t)$ is shown in Figure 3. As it is seen the source function may be reconstructed with a high accuracy.

Figure 3: Control obtained



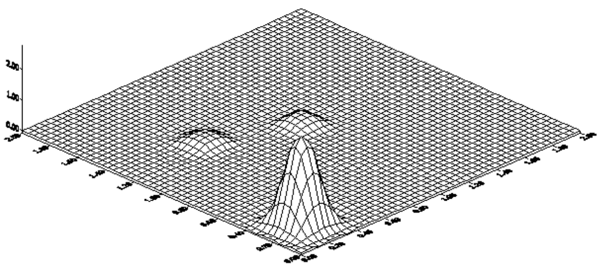
Under the previous problem conditions let consider a function $Z(x)$ with error in measurement (Figure 1). The computed function $U(x,T)$ is shown in Figure 4. In that case parameters of one source are determined accurately enough, while parameters of another source are determined with error due to error in function $Z(x)$.

Figure 4: Influence of error in $Z(x)$



2. Let consider a problem for two-dimensional steady-state transport equation (9). In numerical calculations in $\Omega = \{x = (x_1, x_2);\ 0 \le x_1 \le 2, 0 \le x_2 \le 2\}$ domain a uniform grid of 21x21 points was used. In computation $D = 0.75$, $v_1 = v_2 = -3$.
A test problem for unknown parameters determination (location and power) for three sources of contamination located interior to the domain was considered. Sources were chosen in such a way that one of them was much more powerful than others and masked their operation.
As in the previous problem first the direct problem with known source function was solved and then according a problem solution obtained the unknown source parameters were reconstructed. The function $U(x)$ computed is given in Figure 5.

Figure 5: Obtained control



In this problem the methods developed allowed to find unknown source parameters practically exact.

Conclusions
Developed mathematical and program facilities for determination of the unknown parameters of sources of groundwater contamination were approved for several test problems. The results of modeling demonstrate a high accuracy and reliability of the methods developed and can be used in solving of real ecological problems.

References
(1) F.P. Vasiliev, Numerical methods of extremal problems solving, Nauka, Moscow, USSR, (1980)
(2) J.L.Lions, Optimal control of systems governed by partial differential equations, Mir, Moscow, USSR, (1972)
(3) O.B.Stelya, L.P.Stelya, A combined three-dimensional model of flow and contaminant transport in saturated-unsaturated media. Visnyk Kyivs'kogo universytetu, phys.& math. sciences, **4,** 195, (1997)