

NUMERICAL SOLUTION OF AN INVERSE PROBLEM
OF DETERMINING THE PARAMETERS OF A SOURCE
OF GROUNDWATER POLLUTION

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Abstract The article deals with an inverse problem of determining parameters of groundwater pollution sources. We test three ways to solve the problem on the simulated data for a simple case of contamination. We discover that, in the presence of noise in the data of the inverse problem, the first method does not produce satisfactory recovery results, while the second and third ones are comparable in accuracy of the recovery of required parameters. Taking into account the ease of implementation, the speed of computing and parallelization feasibility the second method of solving the inverse problem is found to be most preferable. We also propose a method of finding pollution parameters in general case.

Key words: inverse problem, groundwater pollution, Volterra integral equation of the 1-st kind

AMS Mathematics Subject Classification: 35K20, 35R30

1 Introduction

Groundwater plays a highly important role in the water cycle in nature and maintaining the balance of ecosystems. It is a source of clean drinking water for many communities [12]. 75% of the Earth's surface is covered by water, of which 97% of the world's water is salty. Of the remaining three percent, two are presented as glaciers, so for the human needs only 1% of world reserves of water is suitable. This amount of water is in the form of surface water and groundwater, which accounts for 96% of the reserves.

General problem of environment pollution is closely related to the problem of groundwater contamination because ground water interacts closely to atmosphere, ground surface and surface water sources [13]. Purification of groundwater pollution is very expensive, so the main method of protection is prevention, that is, identification of pollution sources and their power, as well as the development of measures to prevent the contaminants getting into groundwater. This applies in particular to the pollution of groundwater by industry and urban settlements that have more or less local character [13, 14]. Contamination of groundwater can occur both from point and distributed sources. In order to determine sources, forms and dynamics of groundwater contamination it requires using of mathematical modeling. There are two approaches to the mathematical modeling of groundwater dynamics: direct and inverse. The direct approach assumes that by solving master equations we calculate unknown parameter such as speed, pressure, impurity concentration, etc. after the initial moment of time at

which they are known. The inverse approach involves calculation of values of physical parameters that are unknown at the initial moment of time or at the boundary of the motion.

Inverse problems for groundwater were considered in [15]-[30]. In particular, [26] studies a one-dimensional inverse problem of finding function of pollution source depending on time and location. The authors reduce the problem to one-dimensional parabolic equation with a time dependent coefficient and separable source function.

It is important to note that inverse problems formulated for groundwater are parabolic. In this regard, it is necessary to highlight the work [31], whose authors have made an outstanding contribution to the theory and numerical methods for the solution of parabolic inverse problems.

There is large quantity of data on the flow, structure and pollution of groundwater by various industrial wastes in some areas of the Republic of Kazakhstan. Analysis of the data and forecast on its basis is usually conducted by methods of information technology (see., for example, [1]-[11]). In this paper, we provide a simple method of data processing, based on the theory and numerical solution of inverse problems. The paper proposes three methods for the solution of the inverse problem under study. We test the methods using simulated data and chose one of them, based on the criteria of the ease of implementation, computing speed and feasibility of parallelization.

2 Problem statement

The propagation of groundwater contamination is described by the following equation:

$$RC_t = DC_{xx} - \nu C_x, \quad (1)$$

where $C(x, t) = \tilde{C}(x, t) - C_0$, \tilde{C} is concentration of a substance entered into the groundwater, C_0 is an average background value of the concentration of the substance, D is diffusion coefficient, R is retardation factor ($R \geq 1$), ν is the velocity of groundwater.

We assume that at the initial time, the concentration of contaminant in groundwater is equal to C_0 , i.e.

$$C(x, 0) = 0. \quad (2)$$

We assume that at $x = 0$ the impact on groundwater is described by the following boundary condition

$$-(DC_x - \nu C)|_{x=0} = \nu f(t). \quad (3)$$

We assume that at a large enough distance from the point of observation of the concentration of the substance does not change

$$C_x \rightarrow 0 \quad (x \rightarrow \infty). \quad (4)$$

For a known function $f(t)$ and the values D , R and ν it is not difficult to calculate a function $C(x, t)$ that is a solution of direct problem (1)-(4).

In case the function $f(t)$ is unknown we will assume that we have accessible measurements of the concentration of pollution in some remote point $x = x_0$:

$$C(x_0, t) = g(t). \quad (5)$$

Thus, we can formulate an inverse problem: according to measurements (5), determine the unknown function $f(t)$ if it is known that the reduced concentration $C(x, t)$ satisfies the conditions of direct problem (1)-(4) and the parameters D , R and ν are known.

3 Equivalent statements, existence and uniqueness of the solution of the inverse problem

We apply the Laplace transformation to the variable t . Then equation (1) transforms into:

$$\hat{C}_{xx} - \frac{\nu}{D}\hat{C}_x - \frac{R}{D}p\hat{C} = 0, \quad (6)$$

where $\hat{C}(p) = \mathcal{L}[C(t)]$ and p is a parameter of the Laplace transformation. Boundary conditions take the form

$$-(D\hat{C}_x - \nu\hat{C})|_{x=0} = \nu\hat{f}(p), \quad \hat{C}_x \rightarrow 0 \quad (x \rightarrow \infty). \quad (7)$$

Additional information takes the following form:

$$\hat{C}(x_0, p) = \hat{g}(p). \quad (8)$$

We find the solution of equation (6) in general form

$$\hat{C}(x, p) = A_1 e^{\lambda_1 x} + A_2 e^{\lambda_2 x}, \quad \text{where} \quad \lambda_{1,2} = \frac{1}{2} \left[\frac{\nu}{D} \pm \sqrt{\frac{\nu^2}{D^2} + 4\frac{R}{D}} \right].$$

According to the second boundary condition (7) $A_1 = 0$. (8) leads to

$$\hat{C}(x, p) = \hat{g}(p) e^{\lambda_2(x-x_0)}.$$

Substituting this expression into the first boundary condition (7) we obtain the relationship between the Laplace images of functions $f(t)$ and $g(t)$:

$$\hat{g}(p) = 2ae^{ab} \frac{e^{-b\sqrt{a^2+p}}}{a + \sqrt{a^2+p}} \hat{f}(p), \quad \text{where} \quad a = \frac{\nu}{\sqrt{RD}}, \quad b = x_0 \sqrt{\frac{R}{D}}. \quad (9)$$

The inverse Laplace transformation [32, p. 221] for equation (9) leads to the relationship

$$g(t) = \int_0^t K(t-s)f(s)ds, \quad (10)$$

where

$$K(t) = 2ae^{ab} \left[\frac{1}{\sqrt{\pi t}} e^{-\frac{b^2}{4t}} - ae^{ab+a^2t} \operatorname{erfc} \left(\frac{b}{2\sqrt{t}} + a\sqrt{t} \right) \right] e^{-a^2t}.$$

We find that the solution of inverse problem (1)-(5) is equivalent to the solution of the Volterra integral equation of the 1st kind (10).

It should be noted that the Volterra equation of the 1st kind (10) cannot be reduced to the Volterra equation of the 2nd kind by conventional methods (see., e.g., [33]), because $K(0) = 0$ and any derivative of the kernel also equals to zero at $t = 0$. Thus, the numerical solution of (10) is an ill-posed problem (see., e.g., [34]).

Consider the function $K(t)$. It is obvious that there is some punctured neighborhood of $t = 0$, where $K(t) \neq 0$. Then, according to the Titchmarsh's theorem [35] (see also [36]), if the solution of equation (10) exists, it is unique. Due to the equivalence of inverse problem (1)-(5) to the solution of integral equation (10), the existence of the solution of inverse problem (1)-(5) leads to its uniqueness. To the best of our knowledge, the theorem of the existence of solutions of integral equation (10) in general form is still not proven.

However, for practical applications, the contamination could well be approximated by a function [14]

$$f(t) = \beta e^{-\alpha t}, \quad (11)$$

where the parameters α (1/d) and β (m³/d) characterize the intensity of groundwater contamination at $x = 0$.

Suppose the function $g(t)$ in the interval $[0, T]$ satisfies conditions:

$$g'(t) + \alpha g(t) = \beta K(t), \quad g(0) = 0, \quad (12)$$

where α and β are certain constants. Then the solution of inverse problem (1)-(5) in the interval $[0, T]$ exists and is given by (11).

Indeed, the solution of Cauchy problem (12) can be written in the form

$$g(t) = \int_0^t K(s) \beta e^{-\alpha(t-s)} ds,$$

that coincides with (10) after the change of variables $\tau = t - s$.

It is obvious that the problem of determining of the constants α and β can be formulated as follows: Find the constants α and β , if the function $g(t)$ is known, and we know that it satisfies to the conditions of problem (12).

4 Numerical solution of the inverse problem

Showed below variants of the numerical solution of the inverse problem have been tried on simulated data, i.e. some values of the constants α and β that are possible in practice were chosen. Then using function $f(t)$ of form (11) the function $g(t)$ had been computed, and then a multiplicative random error term was added to it.

$$g_\delta(t_k) = g(t_k) \left(1 + \xi_k \frac{P}{100} \right),$$

where ξ_k is a random variable normally distributed on the interval $[-1, 1]$, and P is percentage error value.

Since real data has an error the data smoothing procedure is needed. Based on the properties of the smoothing procedure (good removal of a high-frequency components [37]), we chose the following two methods for the numerical experiments:

1) moving average

$$\tilde{g}(t_i) = \frac{1}{2N+1} \sum_{l=-N}^N g_\delta(t_{i+l})$$

2) smoothing with a Gaussian kernel:

$$\tilde{g}(t_i) = \frac{1}{2N+1} \sum_{l=-N}^N G\left(\frac{g_\delta(t_i) - g_\delta(t_{i+l})}{b}\right) g_\delta(t_{i+l}) \Big/ \sum_{l=-N}^N G\left(\frac{g_\delta(t_i) - g_\delta(t_{i+l})}{b}\right),$$

where

$$G(t) = \frac{1}{0.37\sqrt{2\pi}} e^{-\frac{t^2}{2(0.37)^2}}$$

and b is the parameter determined by the width of the smoothing window. In this paper, we chose $N = 5$, $b = (2N + 1)\tau$, where $\tau = 1$ day is the time step, with which we know the function $g(t)$.

We ran a large number of numerical experiments. The results and conclusions were made based on the following pair of test exact solution of the inverse problem:

$$\alpha = 3.0 \cdot 10^{-2}, \quad \beta = 5.0.$$

Data error of the inverse problem was $P = 3\%$. $D = 10$ (m²/d), $R = 1$, $\nu = 1$ (m/d), $x_0 = 100$ (m).

In order to calculate the function $K(t)$ it is necessary to calculate the function $\text{erfc}(t)$. To do this, we used the expression [38]:

$$\text{erfc}(t) = e^{-t^2} \epsilon(t), \tag{13}$$

where

$$\begin{aligned} \epsilon(t) &= \tau e^{\eta(\tau)}, \quad \tau = 1/(1 + 0.5t), \\ \eta(\tau) &= -1.26551223 + 1.00002368\tau + 0.37409196\tau^2 + 0.09678418\tau^3 \\ &\quad - 0.18628806\tau^4 + 0.27886807\tau^5 - 1.13520398\tau^6 + 1.48851587\tau^7 \\ &\quad - 0.82215223\tau^8 + 0.17087277\tau^9. \end{aligned}$$

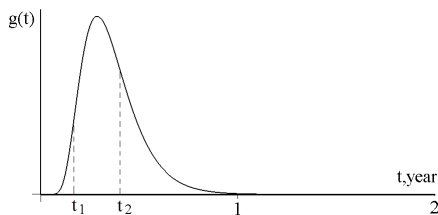
In view of (13) the expression for $K(t)$ can be rewritten:

$$K(t) = 2a \cdot e^{-\left(\frac{b}{2\sqrt{t}} - a\sqrt{t}\right)^2} \left[\frac{1}{\sqrt{\pi t}} - a\epsilon\left(\frac{b}{2\sqrt{t}} + a\sqrt{t}\right) \right].$$

4.1 The first method of numerical solving

Since the data $g(t)$ must satisfy (12), we offer the following algorithm:

- Step 1: Select the interval $[\tau_1, \tau_2]$ (see. Fig. 1) from which we take data to recover the parameters α and β ;

Figure 1: Function $g(t)$.

- Step 2: Select the time moments $t_{1,i} < t_{2,i}$ ($i = \overline{0, N}$) from the interval $[\tau_1, \tau_2]$;
- Step 3: Solve the system of equations

$$\begin{aligned} \tilde{g}_\delta(t_{1,i})\alpha - K(t_{1,i})\beta &= -\frac{1}{2\tau} [\tilde{g}_\delta(t_{1,i} + \tau) - \tilde{g}_\delta(t_{1,i} - \tau)], \\ \tilde{g}_\delta(t_{2,i})\alpha - K(t_{2,i})\beta &= -\frac{1}{2\tau} [\tilde{g}_\delta(t_{2,i} + \tau) - \tilde{g}_\delta(t_{2,i} - \tau)]. \end{aligned} \quad (14)$$

and obtain a set of values $\{\alpha_i, \beta_i\}$ ($i = \overline{0, N}$);

- Step 4: Calculate the mean values α_e and β_e , which are taken as the solution of the inverse problem.

In numerical experiments, $t_{1,0} = \tau_1$, $t_{2,0} = \tau_{1,0} + 20\tau$. Further each successive pair of $(t_{1,i}, t_{2,i})$ is obtained from the previous one by shifting one step $\tau = 1$ (day) to the right, $N = 150$.

Recovery results:

- Smoothing by moving average: recovered values – $\alpha_e = 3.18 \cdot 10^{-2}$ and $\beta_e = 5.86$; the relative error – 6 and 17 % respectively;
- Smoothing by Gaussian kernel: recovered values – $\alpha_e = 3.18 \cdot 10^{-2}$ and $\beta_e = 5.86$; the relative error – 6 and 17 % respectively.

Fig. 2 presents functions $g(t)$, $g_\delta(t)$ and $\tilde{g}_\delta(t)$, as well as the recovery results α_i and β_i ($i = \overline{0, N}$), with different smoothing options.

Smoothing with a Gaussian kernel gives a much smaller variation of values of α_i and β_i relative to the exact values. However, in both cases, the average values α_e and β_e are identical.

The disadvantage of the proposed method is that its implementation assumes numerical differentiation of data which is an ill-posed problem [39].

4.2 Second numerical method of solving

To reduce the influence of errors contained in $\tilde{g}_\delta(t)$, we modify the above-stated algorithm:

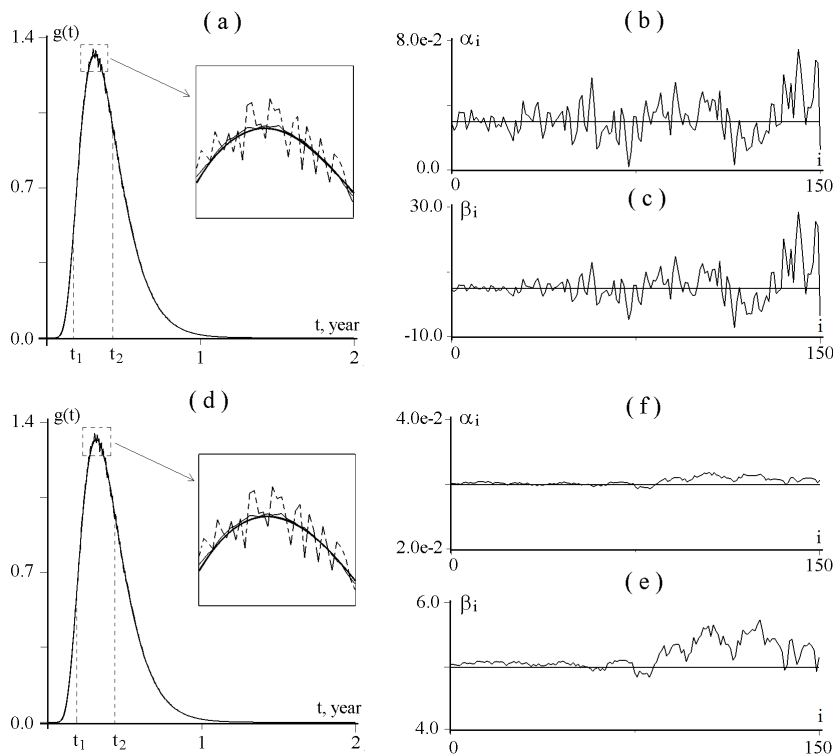


Figure 2: The functions $g(t)$, $g_\delta(t)$, and $\tilde{g}_\delta(t)$; the results of recovery α_i and β_i ($i = \overline{0, N}$). a) and d) $g(t)$ – solid line; $g_\delta(t)$ – dotted line; a) $\tilde{g}_\delta(t)$ – solid thin line, data smoothing by moving average; d) $\tilde{g}_\delta(t)$ – solid thin line, data smoothing by the Gaussian kernel. b,c) the results of the recovery of values of α_i and β_i ($i = \overline{0, N}$) in the interval $[\tau_1, \tau_2]$, using data smoothing by moving average, recovered values are shown by the dotted line, exact values – by the solid one. e,f) the results of the recovery of values of α_i and β_i ($i = \overline{0, N}$) in the interval $[\tau_1, \tau_2]$, using data smoothing by the Gaussian kernel, recovered values are shown by the dotted line, exact values – by the solid one.

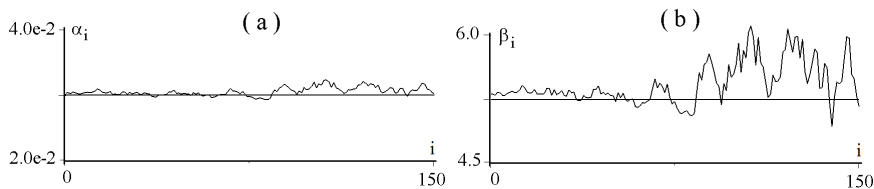


Figure 3: Results of recovery of α_i and β_i ($i = \overline{0, N}$). Recovered values are shown by the dotted line, the exact value – by the solid one.

- Step 1: Select the interval $[\tau_1, \tau_2]$ (see. Fig. 1), from which we take data to recover the parameters α and β ;
- Step 2: Choose time points $t_{1,i} < t_{2,i}$ and $t_{3,i} < t_{4,i}$, $t_{1,i} < t_{3,i}$, $t_{2,i} < t_{4,i}$, ($i = \overline{0, N}$) from the interval $[\tau_1, \tau_2]$;
- Step 3: Solve the system of equations

$$\begin{aligned}
 \int_{t_{1,i}}^{t_{2,i}} \tilde{g}_\delta(t) dt \cdot \alpha - \int_{t_{1,i}}^{t_{2,i}} K(t) dt \cdot \beta &= \tilde{g}_\delta(t_{1,i}) - \tilde{g}_\delta(t_{2,i}), \\
 \int_{t_{3,i}}^{t_{4,i}} \tilde{g}_\delta(t) dt \cdot \alpha - \int_{t_{3,i}}^{t_{4,i}} K(t) dt \cdot \beta &= \tilde{g}_\delta(t_{3,i}) - \tilde{g}_\delta(t_{4,i}).
 \end{aligned} \tag{15}$$

and get a set of values $\{\alpha_i, \beta_i\}$ ($i = \overline{0, N}$);

- Step 4: Calculate the mean values α_e and β_e , which are taken as the solution of the inverse problem.

In system (15), the integrals are calculated using the trapezoidal rule. In numerical experiments $t_{1,0} = \tau_1$, $t_{2,0} = t_{1,0} + 70\tau$, $t_{3,0} = \tau_1 + 50\tau$, $t_{4,0} = t_{3,0} + 70\tau$. Every next pair $(t_{1,i}, t_{2,i})$ and $(t_{3,i}, t_{4,i})$ are obtained from the previous ones by shifting one step $\tau = 1$ (day) to the right, $N = 150$.

Since the smoothing with a Gaussian kernel has given smaller spread of obtained values, only this procedure was used for smoothing the functions $g_\delta(t)$.

Recovery results: $\alpha_e = 3.07 \cdot 10^{-2}$ and $\beta_e = 5.22$, the relative error – 2.36 and 4.36 % respectively.

Fig. 3 shows the results of the recovery of values α_i and β_i . We see that an error of the recovery has decreased.

It should be noted that the calculations for each pair of $(t_{1,i}, t_{2,i})$ and $(t_{3,i}, t_{4,i})$ can be conducted in parallel.

4.3 Third numerical method of solving

The following method can be considered as a traditional one. We write a function of the discrepancy:

$$J(\alpha, \beta) = \sum_{i=1}^N n^2(t_i), \quad n(t_i) = g(t_i) - \tilde{g}_\delta(t_i). \quad (16)$$

To find the minimum we use Newton's method (see, for example, [40]):

$$\begin{bmatrix} \alpha^{k+1} \\ \beta^{k+1} \end{bmatrix} = \begin{bmatrix} \alpha^k \\ \beta^k \end{bmatrix} - H^{-1}(\alpha^k, \beta^k) \nabla J(\alpha^k, \beta^k).$$

In order to use the method, we need to know the expression for the gradient and the matrix of second derivatives of the function J , which may be obtained as follows:

$$\nabla J(\alpha, \beta) = \begin{bmatrix} J_\alpha \\ J_\beta \end{bmatrix}, \quad H(\alpha, \beta) = \begin{bmatrix} J_{\alpha\alpha} & J_{\alpha\beta} \\ J_{\alpha\beta} & J_{\beta\beta} \end{bmatrix},$$

where

$$\begin{aligned} J_\alpha &= \sum_{i=1}^N 2n(t_i)g_\alpha(t_i), & J_\beta &= \sum_{i=1}^N 2n(t_i)g_\beta(t_i), \\ g_\alpha(t) &= -\int_0^t g(s)e^{-\alpha(t-s)}ds, & g_\beta(t) &= -\int_0^t K(s)e^{-\alpha(t-s)}ds, \\ J_{\alpha\alpha} &= \sum_{i=1}^N 2(g_\alpha^2(t_i) + n(t_i)g_{\alpha\alpha}(t_i)), & J_{\beta\beta} &= \sum_{i=1}^N 2g_\alpha^2(t_i), \\ J_{\alpha\beta} &= \sum_{i=1}^N 2(g_\alpha(t_i)g_\beta(t_i) + n(t_i)g_{\alpha\beta}(t_i)), \\ g_{\alpha\alpha}(t) &= -2\int_0^t g_\alpha(s)e^{-\alpha(t-s)}ds, & g_{\alpha\beta}(t) &= -\int_0^t g_\beta(s)e^{-\alpha(t-s)}ds. \end{aligned}$$

It is easy to see that the functions introduced above are the solutions of the following problems:

$$\begin{aligned} g'_\alpha(t) + \alpha g_\alpha(t) &= -g(t), & g'_\beta(t) + \alpha g_\beta(t) &= K(t), \\ g_\alpha(0) &= 0, & g_\beta(0) &= 0, \\ g'_{\alpha\alpha}(t) + \alpha g_{\alpha\alpha}(t) &= -2g_\alpha(t), & g'_{\alpha\beta}(t) + \alpha g_{\alpha\beta}(t) &= -g_\beta(t), \\ g_{\alpha\alpha}(0) &= 0, & g_{\alpha\beta}(0) &= 0. \end{aligned}$$

The dependence of J of the arguments α and β is nonlinear. In general, this function may have local minima and maxima, thus the minimization process can lead to a local minimum. It is also known that Newton's method requires that the initial

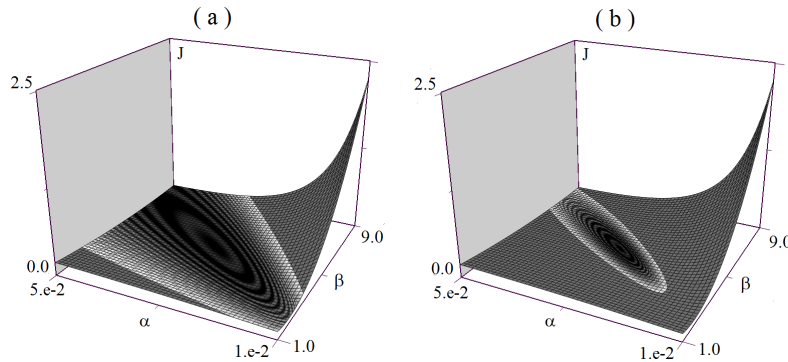


Figure 4: The shape of the function $J(\alpha, \beta)$. It reaches minimum at $(\alpha, \beta) = (3.0 \cdot 10^{-2}, 5)$. a) separately highlighted region $J(\alpha, \beta) < 0.1$, b) separately highlighted region $J(\alpha, \beta) < 0.01$

approximation is close enough to the minimum point. However, this problem could be resolved as follows (see., for example [40]): first, several steps are made using, for example, the Conjugate Gradient Method, and then, the Newton's method is applied. Since the approach is well known, we will not mention it onwards.

Fig. 4 shows the function $J(\alpha, \beta)$ which has a convex and ravine graph. Fig. 4a displays a mapped area where $J[\alpha, \beta] \leq 0.1$, while Fig. 4b – $J[\alpha, \beta] \leq 0.01$.

The figure shows that, on the one hand, the function has no local minima and maxima; on the other hand, it has a ravin (level lines extend in the same direction) and a sloping form (a region where the value of J is less than some ε , is sufficiently large). If there are errors in the data of the inverse problem then a region of the function values, where it is less than some ε , increases (see. [41, 42, 43]), which causes an error in searching for a global minimum. It follows from the foregoing that the result of the minimization of the function $J(\alpha, \beta)$ may depend on the location of an initial approximation.

In order to apply the Newton's method for the numerical solution of the inverse problem, we choose four different initial approximations. After minimization of function (16) we get the following recovery results:

- initial approximation – $\alpha^0 = 1.0 \cdot 10^{-2}$ and $\beta^0 = 1.0$; result of minimization – $\alpha^* = 2.91 \cdot 10^{-2}$ and $\beta^* = 4.72$; relative error – 3.0 and 5.6 % respectively;
- initial approximation – $\alpha^0 = 5.0 \cdot 10^{-2}$ and $\beta^0 = 9.0$; result of minimization – $\alpha^* = 3.34 \cdot 10^{-2}$ and $\beta^* = 5.48$; relative error – 6.8 and 9.6 % respectively;
- initial approximation – $\alpha^0 = 1.0 \cdot 10^{-2}$ and $\beta^0 = 9.0$; result of minimization – $\alpha^* = 3.07 \cdot 10^{-2}$ and $\beta^* = 5.18$; relative error – 2.33 and 3.6 % respectively;
- initial approximation – $\alpha^0 = 5.0 \cdot 10^{-2}$ and $\beta^0 = 1.0$; result of minimization – $\alpha^* = 3.08 \cdot 10^{-2}$ and $\beta^* = 4.81$; relative error – 2.67 and 3.8 % respectively.

4.4 Conclusions from numerical experiments

After trying three methods for solving inverse problem (1)-(5) we found that the first method is the least resistant to the presence of errors in the data. The reason for this is that the approach involves numerical differentiation, which is an ill-posed problem. The second and third methods with an appropriate choice of the initial approximation give results comparable in accuracy of recovery. However, in terms of ease of implementation, the speed of computation and possibilities for parallelization, the second approach to the numerical solution of the inverse problem is preferred.

4.5 Numerical solution of the inverse problem, the case of several 'humps'

All the above calculations were performed when data of the inverse problem had one 'hump', i.e. the contamination has taken place, and it was possible to allocate a time period when the given concentration $C(x_0, t)$ has taken the form as, for example, in Fig. 1. However, there could be a case when at $x = 0$, at some time intervals several facts of groundwater contamination occur. In this case, the curve $g(t)$ may have two or more 'humps', see Fig. 5.

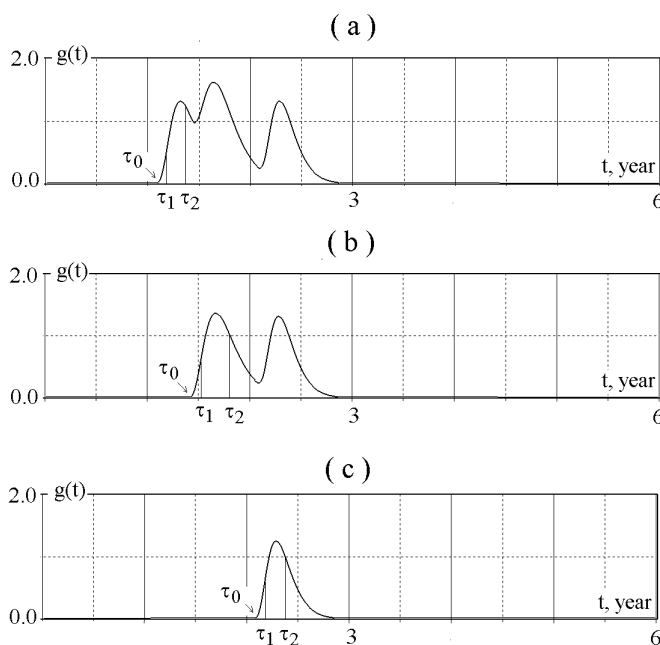


Figure 5: An example of long-term observations of the concentration of a contaminant in groundwater. a)-c) – stages of the recovery of parameters associated with each 'hump'.

Using the linearity of the inverse problem we determine the parameters α_k and β_k ($k = 1, 2, 3$) responsible for each 'hump' according to the following algorithm:

- smooth data of long-term records;
- define a time τ_0 (see Fig. 5a), which will be considered as the initial one;
- allocate a time interval $[\tau_1, \tau_2]$, which will be used for the recovery of the parameters α_1 and β_1 for the first 'hump';
- after solving direct problem (12) with the help of found α and β , obtain the function $g(t)$ and subtract it from the long-term records data (see. Fig. 5a);
- define a new initial time τ_0 (see Fig. 5d), which will be considered as the new starting point of countdown;
- select a new time interval $[\tau_1, \tau_2]$ which will be used for the recovery of the parameters α_2 and β_2 for the second 'hump';
- after solving direct problem (12) with the help of found α and β , obtain the function $g(t)$ and subtract it from the long-term records data (see Fig. 5c);
- re-define the initial time τ_0 (see Fig. 5c), which will be taken as the new starting countdown;
- select a new time interval $[\tau_1, \tau_2]$ which will be used for the recovery of the parameters α_3 and β_3 for the third 'hump';

For solving of inverse problems of determining the parameters α_k and β_k we used the second method. Recovery results are below:

- exact values – $\alpha_1 = 3.0 \cdot 10^{-2}$ and $\beta_1 = 5.0$; recovered values – $\alpha_{1e} = 2.93 \cdot 10^{-2}$ and $\beta_{1e} = 5.28$; relative error – 2.33 and 5.6 % respectively;
- exact values – $\alpha_2 = 2.0 \cdot 10^{-2}$ and $\beta_2 = 4.0$; recovered values – $\alpha_{2e} = 2.09 \cdot 10^{-2}$ and $\beta_{2e} = 4.28$; relative error – 4.5 and 7.0 % respectively;
- exact values – $\alpha_3 = 5.0 \cdot 10^{-2}$ and $\beta_3 = 7.0$; recovered values – $\alpha_{3e} = 5.15 \cdot 10^{-2}$ and $\beta_{3e} = 7.31$; relative error – 3.0 and 4.43 % respectively.

Thus, we have quite satisfactory recovery results. However, in the example above, you can clearly see the presence of three 'humps', i.e. there were three facts of groundwater contamination spaced over time. The second contamination took place 120 days after the first, and the third – a year later.

Fig. 6a displays an example of the function $g(t)$, when the second contamination took place 10 days after the first, and the third – 25 days. We can see that all the 'humps' have merged. We apply the recovery method to the data in Fig. 6 assuming that only one fact of pollution took place, i.e. the contamination is under conditions of model (11). It is reasonable to assume that, in this case, the recovered parameter α would be close to the lowest of three α_k , while β – to the sum of the three β_k , but slightly less since the facts of contamination are separated in time.

The result of recovery is $\alpha_e = 2.48 \cdot 10^{-2}$ and $\beta_e = 14.11$. Fig. 6a and b presents the results of calculation of α_i and β_i , where data of the inverse problem were taken either without noise or with noise $P = 3\%$. The fact that the 'hump' shown in Fig. 6a is the sum of several 'humps' is confirmed by the presence of a curved trend component in Fig. 6a and b (compare with Fig. 2b,c,e and f, and Fig. 3). The presence of the trend component tells us that the adopted model of contamination (11) does not work properly and should be replaced by another one.

If we apply the third method for the recovery of the parameters α and β (the method of minimizing of the target functional), we get the curve $g(t)$ that is very close to the curve in Fig. 6a and some values α^* and β^* , which will be taken as a solution of the inverse problem (in the numerical simulations, we obtained: $\alpha^* = 2.38 \cdot 10^{-2}$ and $\beta^* = 14.03$). However, we will not have any information that the adopted model of contamination (11) is not suitable for the interpretation.

5 The recovery in the case of merging several 'humps'

As we have already noted, the theorem of existence of solutions of the Volterra integral equation of the first kind (10), which can not be reduced to the Volterra integral equation of the second kind, in general, is not proved. However, in a particular case, it is possible to formulate conditions for the existence of a solution of integral equation (10) in the form of (11). The proof was constructive suggesting a method of finding of a solution of integral equation (10). Nevertheless, the results of the numerical calculations have shown that the model of a single source of contamination (11) could be inapplicable because there could be several sources of type (11) little spaced over time. The responses from them at a distance $x = x_0$ could merge and the result would be similar to the response from a single pollution source. The presence of the trend

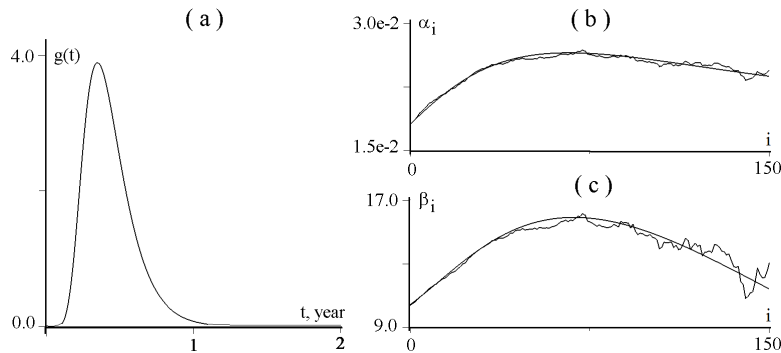


Figure 6: a) An example of observations of the concentration of a contaminant in groundwater, when the 'humps' of three different facts of contamination have merged; b,c) the results of the recovery values α_i and β_i , the solid line – the recovery is based on the accurate data, the dotted line – the recovery is based on data with noise.

component will indicate the inapplicability of the single pollution source model (see. Fig. 6 a and b).

The material below helps to solve the Volterra integral equation of the first kind in a more general case.

5.1 Existence of a solution of the Volterra integral equation

Let us consider the Volterra integral equation of the 1st kind of convolution type (10) assuming that the right part of $g(t)$ satisfies the condition $g(0) = 0$.

We do not assume that any of the conditions allowing to reduce the integral equation (10) to the Volterra integral equation of the second kind are met. On the contrary, for example, a case is possible when $K^{(n)}(0) = 0$ ($n = 0, 1, 2, \dots$) that does not allow such reducing.

Consider a space $F^\beta[0, T]$ ($\beta > 1$) of continuous functions $f(t)$ on the interval $[0, T]$ decomposable in a Fourier series

$$f(t) = \hat{b}_0 + \sum_{k=1}^{\infty} \left(\hat{a}_k \sin(\omega_k t) + \hat{b}_k \cos(\omega_k t) \right), \quad \omega_k = 2\pi k/T, \quad (17)$$

and $|\hat{a}_k| \leq Ak^{-\beta}$ and $|\hat{b}_k| \leq Bk^{-\beta}$ ($b_0, A > 0$ and $B > 0$ are some constants).

Denote $\mathcal{O}_0^\varepsilon$ to be a punctured ε -neighborhood of the point $t = 0$.

Theorem 1. *Suppose that $K(t) \not\equiv 0$ is a piecewise continuous function on the interval $[0, T]$ and $|K(t)| \leq m_0$. A solution $f(t) \in F^\beta[0, T]$ ($\beta = 1 + \alpha$, $\alpha > 0$) of the integral equation (1) exists if and only if, on the interval $[0, T]$, the function $g(t)$, can be represented as*

$$g(t) = b_0 g'_0(t) + \sum_{k=1}^{\infty} \left(a_k g_k(t) + b_k g'_k(t) \right), \quad (18)$$

where

1. functions $g_k(t)$ ($k = 0, 1, \dots$) are the solutions of problems

$$\begin{aligned} g_k''(t) + \omega_k^2 g_k(t) &= K(t), \\ g_k(0) &= 0, \quad g'_k(0) = 0; \end{aligned} \quad (19)$$

2. $|a_k| \leq Ak^{-\alpha}$ and $|b_k| \leq Bk^{-(1+\alpha)}$, and $A > 0$, $B > 0$ and b_0 are some constants.

The solution takes the form

$$f(t) = b_0 + \sum_{k=1}^{\infty} \left(\frac{a_k}{\omega_k} \sin(\omega_k t) + b_k \cos(\omega_k t) \right). \quad (20)$$

□ *Necessity.* Let the solution of the integral equation (10) $f(t) \in F^{1+\alpha}[0, T]$, where $\alpha > 0$, then due to the uniform convergence of the series (17) the function $g(t)$ is

representable in the form

$$g(t) = \tilde{b}_0 g'_0(t) + \sum_{k=1}^{\infty} \left(\tilde{a}_k \int_0^t K(s) \sin(\omega_k(t-s)) ds + \tilde{b}_k \int_0^t K(s) \cos(\omega_k(t-s)) ds \right).$$

It is obvious that the functions

$$g_0(t) = \int_0^t (t-s)K(s)ds, \quad g_k(t) = \frac{1}{\omega_k} \int_0^t K(s) \sin(\omega_k(t-s))ds \quad (21)$$

are solutions of the problem (19), and $g_k(t) \in C^1[0, T]$. Thus, the function $g(t)$ could be written in the form (18) and $b_0 = \tilde{b}_0$, $a_k = \tilde{a}_k \omega_k$ and $b_k = \tilde{b}_k$ ($k = 1, 2, \dots$). Since $|K(t)| \leq m_0$, the series converges uniformly. Hence, it converges to a continuous function. Due to the boundary conditions (19) $g(0) = 0$.

Sufficiency. Let the function $g(t)$ can be represented in the form (18). A solution of problem (19) could be represented in the form (21). It is easy to see that the following equality takes place:

$$\int_0^t K(s) \left[b_0 + \sum_{k=1}^{\infty} \left(\frac{a_k}{\omega_k} \sin(\omega_k(t-s)) + b_k \cos(\omega_k(t-s)) \right) \right] ds = g(t).$$

We have $|\tilde{a}_k| = |a_k/\omega_k| \leq 2\pi T^{-1} A k^{-(1+\alpha)}$ and $|\tilde{b}_k| = |b_k| \leq B k^{-(1+\alpha)}$, then the series in brackets converges uniformly, therefore it converges to a continuous function $f(t)$, and $f(t) \in F^{1+\alpha}[0, T]$. ■

If we assume that there exists such $\varepsilon > 0$ that $K(t) \neq 0$ when $t \in \mathcal{O}_0^\varepsilon$, then the uniqueness of the solution of integral equation (10) follows from the Titchmarsh Theorem [35] (see also [36, стр. 49]).

Theorem 2. *Let there exist two functions, $g^1(t)$ and $g^2(t)$, for which following representations are valid*

$$g^i(t) = b_0^i g'_0(t) + \sum_{k=1}^{\infty} \left(a_k^i g_k(t) + b_k^i g'_k(t) \right), \quad i = 1, 2,$$

where b_0^i , a_k^i and b_k^i ($k = \overline{1, k}$, $i = 1, 2$) satisfy condition 2 from Theorem 1. If $K(t) \neq 0$, $|b_0^1 - b_0^2| \leq \delta$, $|a_k^1 - a_k^2| \leq \delta k^{-\alpha}$, $|b_k^1 - b_k^2| \leq \delta k^{-(1+\alpha)}$ ($k = 1, 2, \dots$) then the solutions $f^1(t)$ and $f^2(t)$ of integral equation (1) satisfy the following inequality:

$$|f^1(t) - f^2(t)| \leq C\delta,$$

where $C = C(T, \alpha)$.

□ First of all, it is obvious that the difference $g(t) = g^1(t) - g^2(t)$ could be represented in form (18). Hence, the solution $f(t) = f^1(t) - f^2(t)$ of equation (1), which

could be represented in form (20), corresponds to it. Let us estimate the difference

$$\begin{aligned} |f^1(t) - f^2(t)| &= \left| b_0^1 - b_0^2 + \sum_{k=1}^{\infty} \left(\frac{a_k^1 - a_k^2}{\omega_k} \sin(\omega_k t) + (b_k^1 - b_k^2) \cos(\omega_k t) \right) \right| \\ &\leq \left[1 + (T/2\pi + 1) \sum_{k=1}^{\infty} \frac{1}{k^{1+\alpha}} \right] \delta \\ &= \left[1 + (T/2\pi + 1) \zeta(1 + \alpha) \right] \delta \equiv C(T, \alpha) \delta, \end{aligned}$$

where $\zeta(\cdot)$ is Riemann function. ■

Note that Theorem 2 implies the uniqueness and continuous dependence on the input data of the solution of integral equation (10) in $F^\beta[0, T]$ without the assumption that $K(t) \neq 0$ at $t \in \mathcal{O}_0^\varepsilon$.

5.2 Reconstruction method

Based on the results of the previous section, we search the function $f(t)$ approximating the function $g(t)$ by the sum

$$b_0 g_0'(t) + \sum_{k=1}^N \left(a_k g_k(t) + b_k g_k'(t) \right)$$

by means of minimization of the residual functional

$$J[b_0, \dots, a_k, \dots, b_k, \dots] = \sum_{j=0}^N \left[g(t_j) - b_0 g_0'(t_j) - \sum_{k=1}^N \left(a_k g_k(t_j) + b_k g_k'(t_j) \right) \right]^2. \quad (22)$$

The number N in both sums is selected based on the following considerations. If, for example, observations are being made during one year, while the concentration of pollution data are taken once a day, then $N = 365$.

Residual functional (22) is quadratic and for its minimization the Conjugate Gradient Method is applicable (see, for example, [40]).

We consider the example from Section 4.4 with 'humps' merged, i.e. the function $g(t)$ has the form shown in Fig. 6a. We minimize residual functional (22) using the Method of Conjugate Gradients (due to its evidence, we do not provide the expression for the gradient of the residual functional). The results of calculations are presented in Fig. 7 and data error $g(t)$ is 3%.

As already mentioned, we model the pollution by a decaying exponential because its coefficients and index have physical meaning. A practitioner needs them for the interpretation of the results. Looking at the form of the restored curve $g(t)$ in Fig. 7 we search the function $f(t)$ as follows

$$f(t) = \sum_{m=1}^3 \beta_m e^{-\alpha_m(t-t_m)} \theta(t - t_m), \quad (23)$$

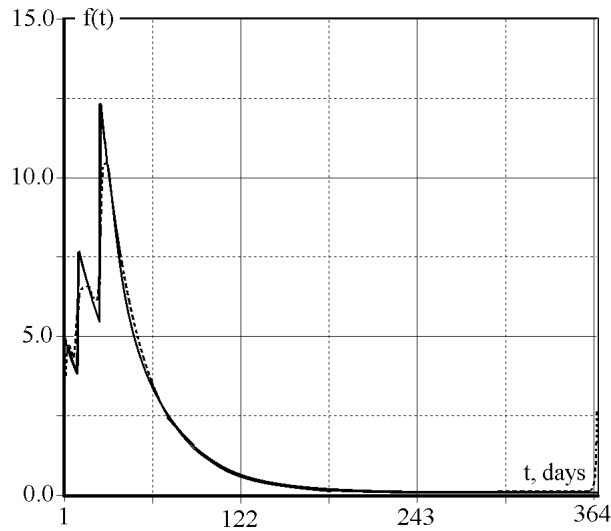


Figure 7: The results of restoring of the function $f(t)$. The exact value is highlighted by the solid line, the restored one - by the dotted line.

where $\theta(t)$ is Heaviside function. In this case, the number of contamination cases is equal to three and we can roughly estimate values $\alpha_m, \beta_m, t_m, t = \overline{1, 3}, t_1 = 0$. For the more accurate values we minimize the residual functional:

$$J[\dots, \alpha_m, \dots, \beta_m, \dots, t_m, \dots] = \sum_{j=0}^N \left[g(t_j) - \int_0^{t_j} K(t_j - s) f(s) ds \right]^2. \quad (24)$$

Recovery results:

- exact values – $\alpha_1 = 3.0 \cdot 10^{-2}$ and $\beta_1 = 5.0$; recovered values – $\alpha_{1e} = 2.94 \cdot 10^{-2}$ and $\beta_{1e} = 5.11$;
- exact values – $\alpha_2 = 2.0 \cdot 10^{-2}$, $\beta_2 = 4.0$, and $t_2 = 10$; recovered values – $\alpha_{2e} = 2.10 \cdot 10^{-2}$, $\beta_{2e} = 4.23$, and $t_2 = 10$;
- exact values – $\alpha_3 = 5.0 \cdot 10^{-2}$, $\beta_3 = 7.0$, and $t_2 = 25$; recovered values – $\alpha_{3e} = 5.17 \cdot 10^{-2}$, $\beta_{3e} = 7.29$, and $t_2 = 26$.

It should be noted that if we skip the first step - the minimization of the residual functional (22) - and immediately seek a solution as sum (23), it is not clear how many terms of the sum to take. In addition, after the minimization of the residual functional (22), approximate values of the unknown parameters can be obtained. It is also worth mentioning that the proposed method of finding a solution of integral equation (10) used at the first step of determining the parameters of the source of groundwater pollution could be applied in general case of the solution of the Volterra integral equation of the 1st kind of the convolution type. To the best of our knowledge, this method is not mentioned in the reference literature [33, 44, 45].

6 Conclusions

The paper considered the inverse problem of determining the parameters of a source of groundwater contamination. We proposed and tested on simulated data three methods of solution. It is shown that, in the presence of noise in the data of the inverse problem, the first method gives unsatisfactory results of recovery, while the second and third ones are comparable in terms of accuracy of recovery of desired parameters. It is proposed to solve the inverse problem using the second method due to the ease of implementation, computing speed and a potential for parallelization.

Where the facts of contamination were sufficiently separated in time from each other and appeared in the observed function $g(t)$ in the form of a separate 'hump' the proposed algorithm allowed to determine the parameters of the source of contamination rather well. However, when the facts of contamination were separated in time insufficiently and merged into one 'hump' of function $g(t)$, the proposed method produced some integral characteristics of the pollution parameters and an indication that the chosen model of contamination is not suitable. In the case where the 'humps' of the function $g(t)$ were merged into one, a method based on the minimization of a residual functional have been also proposed allowing to calculate the parameters of a pollution source in this general case.

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