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Semi-empirical method for calculating diffuse runoff of conservative pollutants in small rivers: 1. Method for reconstructing the total mass flow rate

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ABSTRACT

Relevance. The quality of river water is the most important factor in ensuring environmental safety and rational use of natural resources. Diffuse runoff of pollutants into watercourses is the most dangerous because it is uncontrolled and unregulated. The impossibility of direct estimation of the pollutants flow rate during diffuse pollution requires fundamental research and the development of adequate mathematical models based on methods for solving inverse problems. The presented work proposes a method for calculating the total mass flow rate of conservative pollutants entering a watercourse from a catchment area. **Methods.** Based on the integral representation of the stationary one-dimensional equation of pollutant transport, a method for calculating the spatial distribution of the total mass flow rate of conservative pollutants in a catchment area is proposed. To determine the unknown distribution parameters, the global nonlinear optimization method and the Monte Carlo method were used. **Results.** The use of the nonlinear global optimization method allowed us to determine both the value of the total mass flow rate of the pollutant in the study area and the value of the Peclet number included in the advection-diffusion equation. Using the Monte Carlo method, the stability of the obtained results with respect to random deviations in concentration values is demonstrated when a thousand possible deviations are realized in a given interval.

KEYWORDS: catchment area, diffuse pollution, inverse problem, global optimization, Monte-Carlo method.

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INTRODUCTION

Chemical pollution of watercourses is now assuming enormous proportions worldwide. In case of surface water pollution, of the greatest danger is the diffuse runoff (or non-point runoff) of pollutants flowing to riverbeds from urbanized areas, unequipped landfills, agricultural fields and livestock farms located within the catchment area [1]. Unlike point sources, the diffuse runoff is not controlled or regulated, its negative impact on water quality being more significant for small rivers than for large ones.

The quality of river water is characterized by the presence of dissolved substances in it, determined by analyzing samples taken in the watercourse section under study. However, this indicator does not provide any information on the localization and spatial distribution of pollution sources, as well as characteristics of the mass flow of the pollutant [2, 3]. One of the ways to solve this problem is mathematical modeling of the catchment area [1]. Relevant methods, considered in the study [4], make it possible to calculate the quantity of pollutants in certain areas and simulate the runoff on the basis of digital relief models and soil maps. However, this approach requires an extremely large amount of detailed information on the characteristics of catchment areas and represents a kind of "effective" runoff model, which is realized with a certain probability and is not universal. An alternative method is to calculate the diffuse runoff of pollutants directly on the basis of the measured distribution of pollutant concentration in the riverbed, i.e. to solve the inverse problem for the advection-diffusion equation. In this case, no information on the characteristics of the catchment area is required. As a result, for practical needs, it is necessary to develop a simple method of determining the runoff of pollutants, which does not require a large amount of empirical data and is easily implemented with a relatively small number of chemical sample analysis results.

The existing inverse problem-solving methods used to determine the flow rate of conservative pollutants are based on the advection-diffusion equation, test functions of the spatial distribution of the specific mass flow rate of a pollutant being pre-set. When solving the inverse problem, the original functions are reconstructed with subsequent verification of results [5–13]. However, identifying the source of pollution on the basis of a finite number of measured concentrations of pollutants is an ill-posed problem, even if its spatial distribution is assumed to be known. In the cited works [5–13], the aim of the study is to reconstruct distribution of the specific mass flow rate of a pollutant, i.e. the amount of a pollutant flowing to the watercourse per unit time, per unit length of riverbed (linear density of the pollution source). There are no restrictions on this dependence, and the researcher has no a priori information about the behavior of this function. The distribution of the specific mass flow rate is reproduced only based on the pollutant concentration distribution data.

It should be noted that along with the specific mass flow rate, an important feature of diffuse pollution is the total mass flow rate, showing the total amount of a pollutant getting into the watercourse per unit of time in the area under study. This value is an integral flow characteristic and, in fact, determines the final goal of solving the inverse problem. Unlike the specific mass flow rate of pollutant, the total mass flow rate increases monotonically in the riverbed section which makes the problem of determining it more predictable and narrows the class of functions under study. It should be noted that no works devoted to the direct comparison of data of real field measurements measurements and the ones on the diffuse runoff calculation have been found in the literature available.

This is due to the fact that in order to solve the inverse problem correctly, a large number of field measurements measurements of the pollutant concentration in the watercourse section under study (hundreds of calculation points) are necessary. Actually, this number is insignificant and amounts (at best) to dozens of calculation points. The purpose of this study is to develop a method for reconstruction of the distribution of the total mass flow of conservative pollutants based on the available data on the distribution of their concentration.

SOLUTION METHODS

Problem Statement

When analyzing the processes of diffuse pollution of small lowland rivers, one can assume that during the low-water season, flow velocities and discharges along the riverbed change insignificantly. Then the stationary advection-diffusion equation can be given in the dimensionless form:

$$\frac{d\theta}{dz} - \frac{1}{\alpha}\frac{d^2\theta}{dz^2} = \tilde{\varphi}(z). \qquad (1)$$

The following dimensionless values are given below:

$$z = x/L,\ \theta = (c - c_A)/c_A,\ \alpha = VL/E,\ \tilde{\varphi}(z) = L\varphi(z)/Qc_A, \qquad (2)$$

where x is the coordinate;

L – length of the watercourse section under study;

c – pollutant concentration at point x;

c_A – pollutant concentration in the upper section;

V – flow velocity;

E – longitudinal dispersion coefficient;

Q – water discharge;

φ – specific mass flow rate of a pollutant.

In addition, it is important to consider the total mass flow rate of the pollutant at the point z:

$$\widetilde{\Phi}(z) = \int_0^z \widetilde{\varphi}(z)dz. \quad (3)$$

It should be noted that this dependence is monotonically increasing, as by definition. Next, it is important to analyze the hydrological aspect of the problem and substantiate problem statement (1). In order to describe runoff processes of a pollutant adequately, it is important to know its basic component (base runoff) unrelated to precipitation, floods, snowmelt processes, etc. (the reasons for this flow runoff are listed in the introduction). As a rule, this component is determined by transporting pollutants through soil filtration and groundwater [14]. To estimate it, we should analyze steady-state flows, i.e. to solve the stationary problem (1).

According to the results of numerous studies (in particular [15-22]), analyses of water samples (taken during the low-water season) show the presence of areas of accelerated growth in the solute concentration, which is associated with its continuous runoff from the catchment area. For example, in study [16], concentration of dissolved arsenic is increasing by 3.5 times in an area of about 80 km in the Buerhatong River basin (China); copper concentration in the Erren River (China) shows a fivefold growth in a 10 km long area [17]. According to the results of [15], concentration of manganese in the Barnaulka River (Russia) is monotonously increasing by three times over a section of 4.5 km. Such areas are potentially dangerous and require a detailed theoretical and practical study as sources of increased anthropogenic load.

Exact Solution

Direct problem. The purpose of solving the direct problem (1) is to determine the distribution of pollutant concentration in a watercourse using the known given function $\widetilde{\varphi}(z)$. If we consider the problem as a semi-empirical one, then the Dirichlet conditions should be accepted as boundary ones, assuming that concentration in the lower section is known from field measurements:

$$\theta(0) = 0, \theta(1) = \theta_1. \quad (4)$$

For further analysis, the following test functions were introduced:

$$\widetilde{\varphi}(z) = 0{,}2 + 0{,}3z - 0{,}25z^2, \quad (5)$$

$$\widetilde{\varphi}(z) = 0{,}2e^z + 0{,}2z^4, \quad (6)$$

$$\widetilde{\varphi}(z) = 0{,}2 + 0{,}2e^{-\left(\frac{z-0{,}3}{0{,}1}\right)^2} + 0{,}45e^{-\left(\frac{z-0{,}7}{0{,}3}\right)^2}. \quad (7)$$

The test functions were selected based on the following considerations. Distribution (5) is close to uniform and defines a section of uniform distribution of specific mass flow rate of pollutant. This may correspond to runoff from a hydrochemically homogeneous section of the catchment. Distribution (6) characterizes a section of increasing anthropogenic load. Distribution (7) defines a section that is non-homogeneous in terms of hydrochemical conditions. Thus, distributions (5) – (7) correspond to the most typical situations associated with the entry of pollutants from the studied areas of watersheds [1, 22].

Fig. 1*a* shows dependences (5) – (7). The corresponding dependences for the total mass flow rate (3) are shown in Fig. 1*b*. The integration step is $\Delta z = 0.02$. The relevant number of points is 50 (hereinafter, the numbering of dependences is according to Fig. 1). It should be noted that this number of points reflects the possibilities of a real field experiment. The direct problem (1) is considered for the parameter values $\alpha = 10$, $\theta_1 = 1.5$. The results of solving the -direct problem are presented in Fig. 1*c*.

To analyze the inverse problem, one should solve equation (1) with boundary conditions (4), which is expressed via unknown dependence $\widetilde{\Phi}(z)$. This solution looks like this:

$$\theta(z,\alpha) = \frac{e^{\alpha z} - 1}{e^{\alpha} - 1}\left(\theta_1 + \alpha e^{\alpha}\int_0^1 \widetilde{\Phi}(\xi)e^{-\alpha\xi}\,d\xi\right) - \alpha e^{\alpha z}\int_0^z \widetilde{\Phi}(\xi)e^{-\alpha\xi}\,d\xi. \tag{8}$$

If we represent the unknown function as a polynomial:

$$\widetilde{\Phi}(\xi) = \sum_{n=1}^{m} a_n \xi^n. \tag{9}$$

Then, solution (8) may be represented as an expansion over a set of functions $H_n(z, \alpha)$:

$$\theta(z) = H_0(z, \alpha) + \sum_{n=1} a_n H_n(z, \alpha), \tag{10}$$

where:

$$H_0 = \theta_1 \frac{e^{\alpha z} - 1}{e^{\alpha} - 1},$$

$$H_1(z, \alpha) = z - \frac{e^{\alpha z} - 1}{e^{\alpha} - 1},$$

$$H_2(z, \alpha) = \left[z^2 + \frac{2}{\alpha} z - \left(1 + \frac{2}{\alpha}\right)\frac{e^{\alpha z} - 1}{e^{\alpha} - 1}\right], \tag{11}$$

$$H_3(z, \alpha) = \left[z^3 + \frac{3z^2}{\alpha} + \frac{6z}{\alpha^2} - \left(1 + \frac{3}{\alpha} + \frac{6}{\alpha^2}\right)\frac{e^{\alpha z} - 1}{e^{\alpha} - 1}\right].$$

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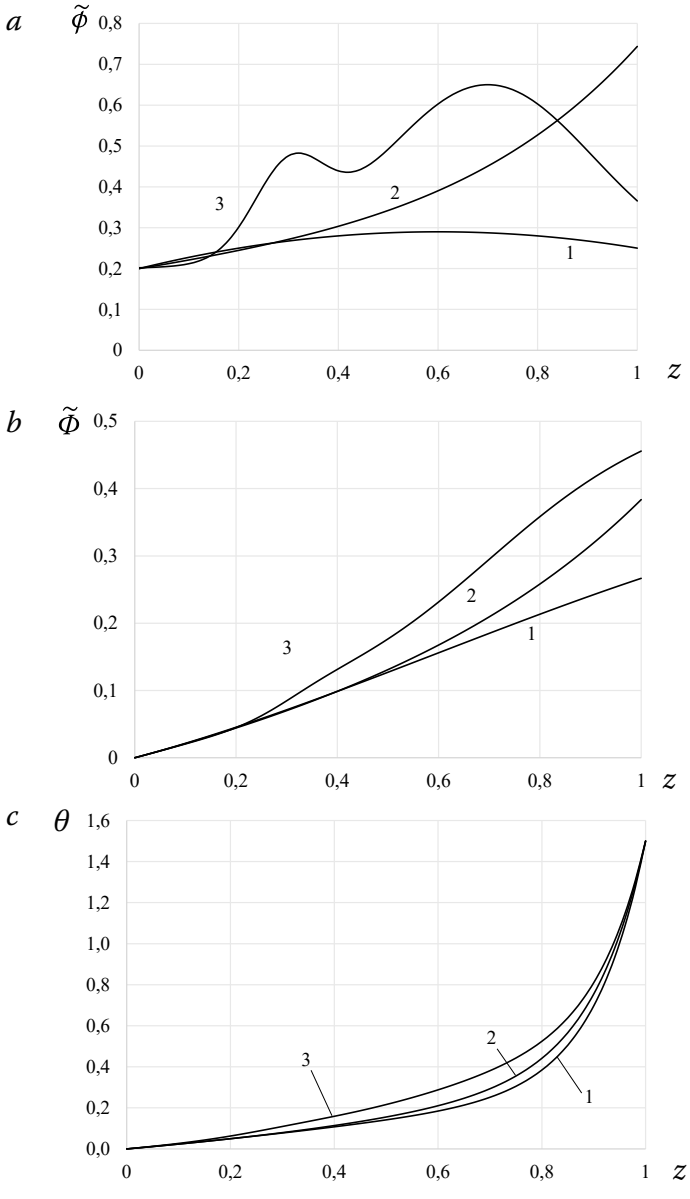


Fig. 1. Distribution of characteristic values along the riverbed: *a* – distributions of specific mass flow rate for functions (5) – (7): 1 – function (5), 2 – function (6), 3 – function (7); *b* – corresponding distributions for total flow rate (3); *c* – distribution of pollutant concentrations as a result of solving primal problem (1).

Here $H_0(z, \alpha)$ is the solution of homogeneous equation (1). The set of functions (11) has common properties:

$$H_n(0, \alpha) = H_n(1, \alpha) = 0; H_n(z, \alpha) \geq 0; H_n(z, \alpha) \leq M_n(\alpha), \quad (12)$$

where $M_n > 0$ is the upper limit of the range of values of functions H_n.

Representation (9) was chosen for reasons of the possibility of obtaining analytical dependencies, which determines the clarity and simplicity of the considered expansions (11). In addition, such a polynomial simplifies significantly practical application of the above method.

As follows from (11), the function under study is characterized by a strong dependence on the Peclet number, which, in turn, depends on the longitudinal dispersion coefficient. Consequently, using any inaccurate value of the longitudinal dispersion coefficient (found from indirect, a priori considerations or calculations [24–29]) can lead to incorrect results of solving the inverse problem when analyzing the data on a real full-scale experiment. The latter once again emphasizes the need to determine the Peclet number directly from the available data (field measurements). When solving inverse problems of this class (e.g., [5–13]), the Peclet number is considered to be given.

Inverse problem. The purpose of solving the inverse problem is to determine the unknown parameter α and coefficients a_n of the polynomial (9) for calculating dependence $\widetilde{\Phi}(z)$. It should be noted here that existence, uniqueness, and stability of solving the inverse problem for the stationary equation (1) are proven in [31]. Model parameters a_n (n = 1, 2, ... , m), included in (10) are determined from the condition of minimizing the functional:

$$S = \sum_{i=1}^{k} (\theta(z_i, \omega) - \theta_i)^2 \underset{\omega}{\rightarrow} min, \qquad (13)$$

where $\theta(z_i, \omega)$ – is the calculated value of concentration based on formula (10);

θ_i – is the known (measured) value of concentration

ω – is the vector of parameters (α, a_1 ... a_m), minimizing functional S.

Summing up in (13) is carried out on the number of calculated points, the latter being equal to k. The unknown parameters of model (10), (11) were determined using the global optimization method [32–34]. For these purposes, the MatLab software package (MathWorks Inc.) with the Global Optimization Toolbox extension [34] was used. The global minimum was selected from the local minima achieved on a set of 100 random starting points generated by the MultiStart function [34]. The Levenberg-Marquardt nonlinear optimization algorithm without constraints [35] was used to determine the local minima. Figure 2 illustrates the method used for function 1 (Fig. 1*a*).

Figure 2 shows the results of using the above method for function 1 (fig. 1*a*). The figure shows the isolines of the surface section $S(\alpha, \widetilde{\Phi}(1))$, where: $\widetilde{\Phi}$ (1) is the sum of the coefficients an (14) for m = 1.

Fig. 3 shows the distributions of pollutant mass flow rate $\widetilde{\Phi}(z)$ reconstructed by this method for different degrees m of polynomial (9).

As shown in Fig. 3, with the degree of the polynomial increasing, convergence of reconstructed functions to the dependence determined by the exact solution

is observed. Table 1 gives the values of the required parameters for the test functions used. According to the data in Table 1, the main parameters of the problem under study – α, $\tilde{\Phi}(1)$ (1) converge to the exact value with the degree of the polynomial increasing. Thus, it can be stated that the representation (9) is applicable to solving the inverse problem and gives quite correct results.

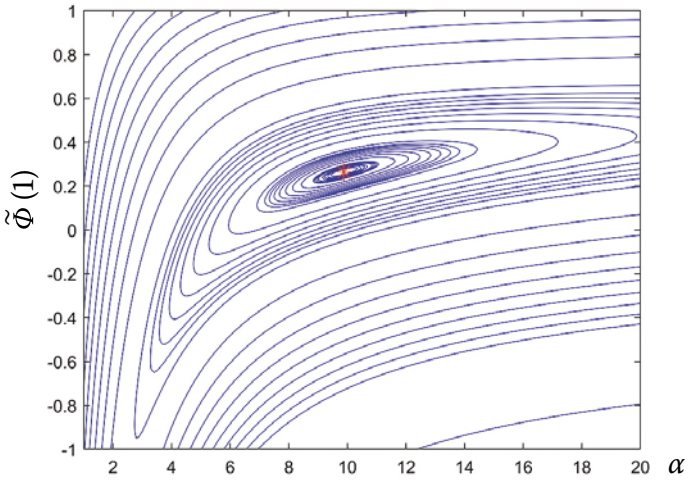


Fig. 2. Isolines (contours) of functional (13) in the space α, $\tilde{\Phi}(1)$, where $\tilde{\Phi}(1)$ is the sum of coefficients a_n(9) for function 1 at m = 1. The point indicates the global minimum.

Table 1. Exact solution. Inverse problem parameters

Functions	Function 1 Polynomial Degree			Function 2 Polynomial Degree				Function 3 Polynomial Degree		
Coefficients	1	2	3	1	2	3	4	1	3	6
α	9,88	10,17	10,00	8,75	9,62	9,87	9,97	8,7	10,64	10,12
a_1	0,26	0,23	0,20	0,28	0,17	0,21	0,20	0,41	0,15	0,14
a_2		0,06	0,15		0,17	0,05	0,12		0,46	0,6
a_3			-0,08			0,11	-0,03		-0,103	-0,48
a_4							0,09			0,17
a_5										0,47
a_6										-0,44
$\tilde{\Phi}(1)$ estimated	0,26	0,28	0,27	0,28	0,34	0,37	0,38	0,41	0,51	0,46
$\tilde{\Phi}(1)$ exact	0,267			0,384				0,456		

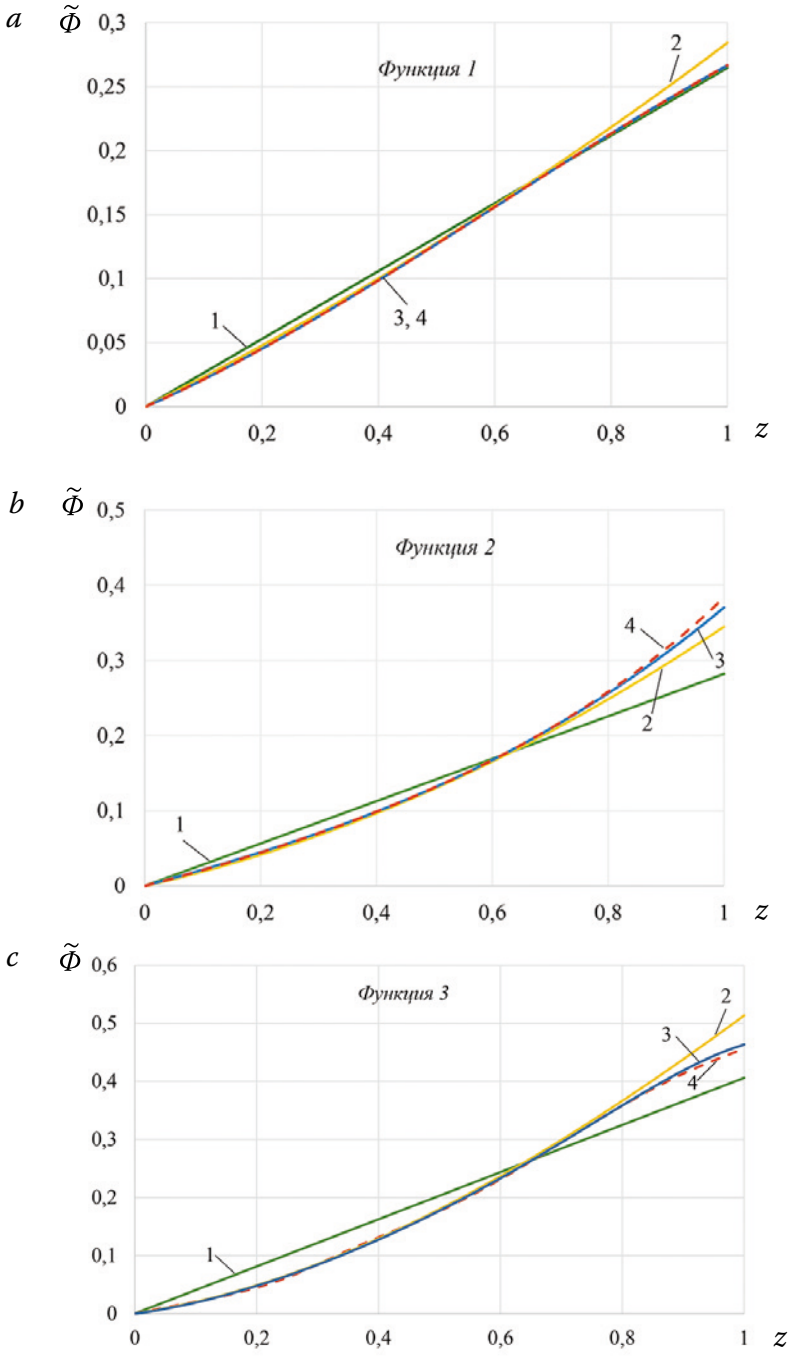


Fig. 3. Distributions of pollutant flow rate reconstructed with the optimization method at various degrees of the polynomial m (9): *a* – function 1: 1–m =1, 2–m =2, 3–m =3, 4 – exact solution (Fig. 1*b*); *b* – function 2: 1–m =1, 2–m= 2, 3–m= 3, 4 – exact solution; *c* – function 3: 1–m=1, 2–m=2, 3–m=3, 4 – exact solution.

However, when solving the inverse problem, the main difficulties are due to random deviations from the values simulating real measurements. As a rule, randomization is performed with the use of the normal law of distribution, the variance of the distribution determining the magnitude of the deviation [10]. Here, one should remember that using a single generated realization of random values of the variable under study may lead to incorrect values of the parameters to be determined.

In this study, a more general approach based on the Monte Carlo method is proposed.

Randomization. Monte Carlo Method

Randomization was carried out as follows. For each point θ_i (z_i) of the exact solution for the concentration distribution (Fig. 1*c*) in the interval $\Delta\theta_i = \pm\delta$, a concentration value was set with the help of a random number generator. The application of the Monte Carlo method was based on examining N different realizations of the random spread of points in the given interval and calculating the average values of the corresponding parameters α, α_n [35]. When solving the problem, it was found that polynomials higher than a cubic give unstable and physically unrealizable values of required parameters. It is known that in the case of expansion like (10), during randomization, there are an optimal number of terms above which the representation of the function becomes incorrect [36]. The latter is due to the fact that the reconstructed dependence begins to reproduce random deviations and the calculation results cease to be stable.

Distributions of the total mass flow rate of the pollutant for $\delta = 0.05$, $N = 1\,000$ are presented in Fig. 4 *a-c*. Table 2 shows the values of the required parameters for non-randomized and randomized concentration distributions.

Table 2. Parameters of the inverse problem for non-randomized ($\delta = 0$), and randomized $\delta = 0{,}05$ distributions at $N = 1\,000$

Calculation	Function 1		Function 2		Function 3	
	α	$\tilde{\Phi}(1)$	α	$\tilde{\Phi}(1)$	α	$\tilde{\Phi}(1)$
Exact value	10	0,267	10	0,384	10	0,456
$\delta = 0$	10,0001	0,267	9,868	0,370	10,642	0,513
$\delta = 0{,}05$	10,108	0,250	10,009	0,340	10,720	0,495

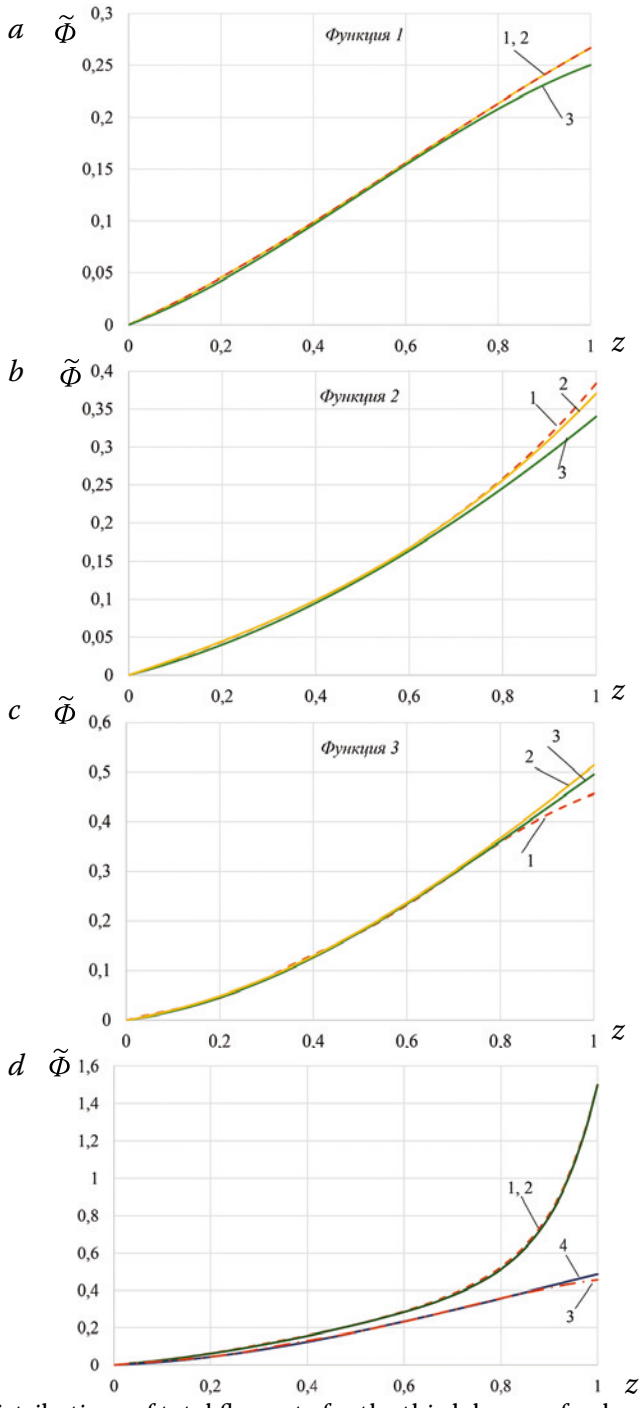


Fig. 4. Distributions of total flow rate for the third degree of polynomials (*a*–*c*): 1 – exact solution, 2 – cubic at $\delta = 0$, 3 – cubic at $\delta = 0{,}05$, $N = 1\,000$ (numbers are given in the figures). Final calculation results for function 3 (*d*): 1 – exact calculation for concentration distribution, 2 – reconstructed concentration distribution adjusted for randomization, 3 – exact calculation for total mass flow rate distribution, 4 – reconstructed distribution of total mass flow rate adjusted for randomization.

As follows from the data in Table 2, deviations of the parameters calculated on randomized values from their exact values do not exceed 8 % for function 3. For functions 1 and 2, deviations are about 1 %, and deviations for parameter $\widetilde{\Phi}(1)$ are about 4 %. Deviations from non-randomized values ($\delta = 0$) do not exceed 2 %. Thus, the obtained results can be considered stable with respect to randomization in the specified interval. Fig. 4*d* presents the calculation results for function 3 adjusted to randomization. The analysis of the obtained distributions allows us to conclude that the deviations of the calculated values from the exact values are quite insignificant.

It should be kept in mind that value θ_1 was chosen arbitrarily, so it is necessary to check whether this value affects the parameters of the inverse problem. In addition, one should check whether the method used is applicable to any values of parameter α. Fig. 5 shows the distributions of the total mass flow rate of the pollutant for different values of parameter θ_1 =1.5. Tables 3*a* and 3*b* give relevant parameter values.

Table 3*a*. Values of calculated parameters for function 3 at $\theta_1 = 1{,}5$, $\delta = 0{,}05$ (exact value: $\widetilde{\Phi}(1) = 0{,}456$)

α exact values	α calculated Values	$\widetilde{\Phi}(1)$
10	10,788	0,495
20	20,866	0,4801
50	51,724	0,471

Table 3*b*. Values of calculated parameters at various values of θ_1 at $\alpha = 20$, $\delta = 0{,}05$

θ_1 exact values	α calculated values	$\widetilde{\Phi}(1)$
1,5	20,866	0,486
1,2	21,210	0,4856
1	21,679	0,485
0,8	22,769	0,485

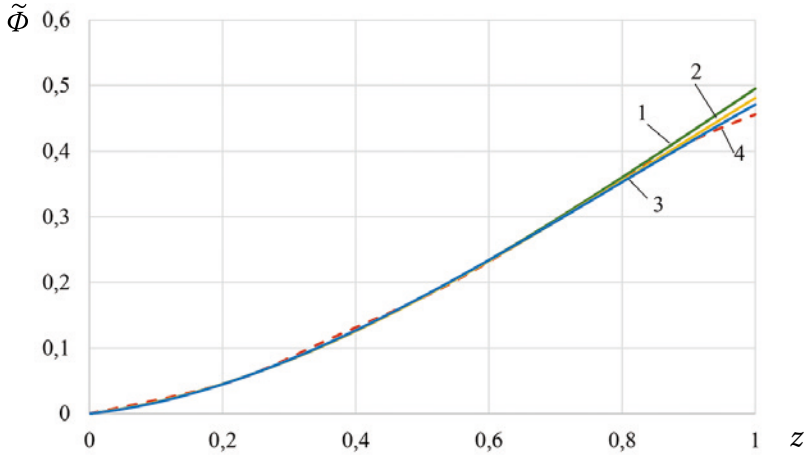


Fig. 5. Distributions of total mass flow rate for various values of parameter α at θ_1 = 1,5 for function 3 under randomization: 1–α=10; 2–α=20; 3–α=50; 4 – exact solution.

As follows from the obtained results, changing parameter α does not lead to a noticeable change in dependence $\tilde{\Phi}(z)$, also the above method quite correctly determines the values of parameter α.

Field measurements

To apply the proposed method to the results of field measurements measurements, the data of [22] were used. In this work, the distribution of pollutant concentration in the catchment area of the Hawkesbury-Nepean River (Eastern Australia) was investigated. It is an urbanized area, which leads to the discharge of significant amounts of pollutants from large territories. As can be seen from the measurement results, river water contains significant amounts of heavy metals. Runoff from agricultural lands also contributes significantly to river water pollution.

Fig. 6 shows values of measured dissolved cobalt (*Co*) concentrations in the 80 km long river section and calculation results. *Co* concentration at the upper section corresponds to the value of 0.16 mg/L. The dependence is characterized by an accelerated monotonic growth of *Co* concentration, which indicates the presence of a continuously operating source of pollution. Optimization of functional *S* (13) determines the global minimum for the polynomial of the first degree, achieved at the parameter values: α = 7.3, α_1 = 0.228 (Fig. 6*b*).

The obtained calculation results can be considered as estimates of parameters to be determined. However, a number of questions arise, primarily related to the number of measurements. Namely: how can the number of measurements affect the accuracy of calculation according to the proposed methodology? How many measurements are necessary to obtain correct results? The above questions require additional research.

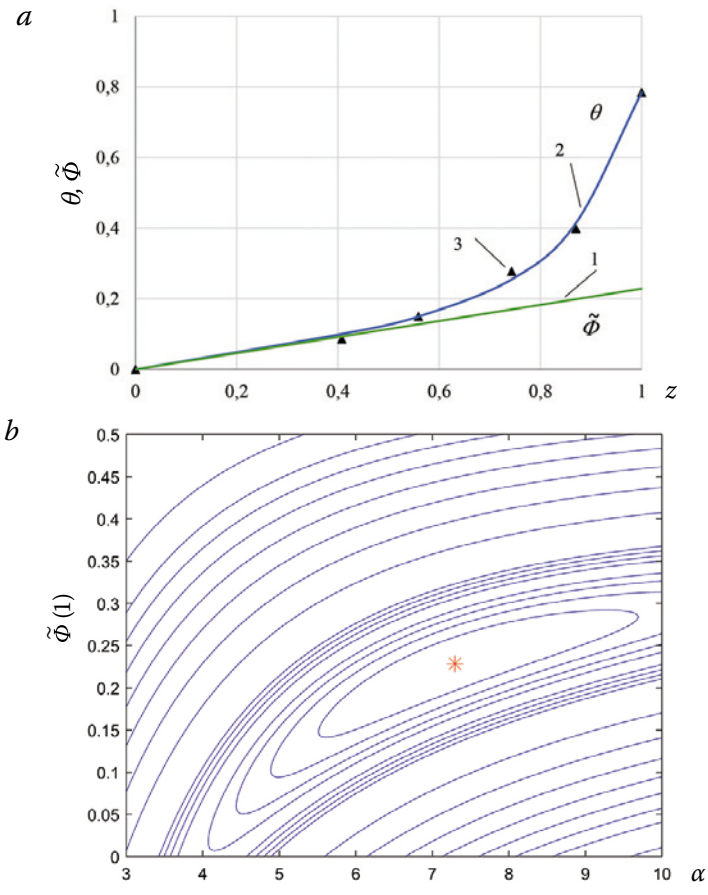


Fig. 6. Distribution of Cobalt concentration for data obtained as a result of a field experiment [22]: *a*) – 1 concentration distribution reconstructed with the global optimization method, 2 – distribution of the total mass flow rate; b) – corresponding contours of functional S(13) in the space α, $\tilde{\Phi}(1)$ at m = 1. The point indicates the global minimum.

RESULTS AND DISCUSSION

The vast majority of studies considering the solution of inverse problems for the advection-diffusion equation are devoted to reconstructing the distribution of the specific mass flow rate of pollutants entering a watercourse from various sources. Mathematically, the problem is solved for a given value of the Peclet number based on a quasi-experiment, where a given distribution of the specific mass flow rate of a pollutant is reconstructed. However, there are some problems arising from the instability of the obtained solutions, which are leveled with the known regularization methods [15]. However, many questions arise here as well. Indeed, as follows from Fig. 1, the peculiarities of behavior of test functions for the specific mass flow rate are poorly reflected in the corresponding concentration

distribution obtained when solving the direct problem. A large number of points are needed to simulate these features in the test experiment. The complexity of the calculation increases significantly when random deviations from the considered distributions are specified.

Meanwhile, from the practical point of view, there is a need to estimate the total amount of pollutants entering the watercourse per unit time in the section under study. This value is an integral characteristic determining the basic diffuse runoff of pollutants. Unlike the specific mass flow rate, the total mass flow rate is a monotonically increasing function of the coordinate, which facilitates the solution of the inverse problem.

The purpose of this study was to solve the problem of determining the total mass flow rate of a pollutant and the Peclet number, which plays a determining role in the calculation. To solve the problem, we considered the stationary advection-diffusion equation expressed via the total mass flow rate in the form of (8). The dependence of the total mass flow rate on the coordinate was represented as a polynomial (9). The global optimization method (13) allowed us to determine both the unknown coefficients of the polynomial and the Peclet number, which is extremely important from the practical point of view. For the exact solution, the convergence of required parameters α, $\widetilde{\Phi}(1)$, to their predetermined values with the increasing degree of the polynomial was established, which testifies the correctness of the applied method.

The Monte Carlo method was used to analyze randomized values of pollutant concentrations, the concentration values being set randomly within a certain interval. The analysis of 1 000 simulations of random deviations allowed us to find out the average values of the specified parameters, which differed insignificantly from their exact values.

The proposed method was applied to the measurement data [22]. The optimization method made it possible to determine the global minimum of functional S (13) for the available data on the concentration distribution based on six measurements and further evaluate values of requied parameters. It should be noted that the results of solving the inverse problem depend significantly on the dimensionality of the data set used. This issue is still poorly studied. However, the latter is crucial when applying the described method to the results of field measurements.

CONCLUSION

The presented article proposes the method for calculating of the conservative pollutants total mass flow rate distribution on the catchment territory under study. The method is based on analysis of data of spatial distribution of conservative pollutants obtained by the field measurements results.

We have made the calculation with the use of three test functions of the pollutant specific mass flow rate distribution. To solve the inverse problem, we presented the total mass flow rate distribution as a polynomial. The use of the

global non-linear optimization has enabled to calculate both total mass flow rate for the territories under study and unknown value of Peclet number.

To study the impact of random diversions of the pollutants' concentration upon the determined parameters' values we have use Monte Carlo method. The essence of the method is in the parameters determination with a multitude of accidental realizations (values of concentration randomly distributed over the preset interval) and calculation of medium values.

The application of the method made it possible to determine the degree of the polynomial above which the calculation yields unstable results. Based on the analysis results, it was established that the method gives stable results with insignificant deviation of the parameters from their exact values determined by solving the direct problem. The application of the method to the results of field measurements is considered.

CONFLICT OF INTERESTS

The authors declare no relevant conflict of interests.

REFERENCES

1. Lintern A., Webb J.A., Ryu D., Liu S., Bende-Michl U., Waters D., Leahy P., Wilson P., Western A.W. Key factors influencing differences in stream water quality across space. *Wiley Interdisciplinary Reviews: Water.* 2018. Vol. 5 (1), e1260. https://doi.org/ 10.1002/wat2.1260.
2. Chen Y., Lin L.S., Viadero R.C., Gang D.D. Nonpoint Source Pollution. *Water Environment Research.* 2007. Vol. 79 (10). P. 2032–2048. https://doi.org/10.2175/106143007X218656.
3. Narendran N.A. A review on environmental problem due to water pollution. *International Journal of Scientific Engineering and Research.* 2015. Vol. 3 (4). P. 2014–2016.
4. Fashchevskaya T.B., Polyanin V.O., Kirpichnikova N.V., Motovilov Yu.G., Algushaeva A.V. Modern problems of hydrochemistry. IWP, Moscow, 2020. 105 p. (In Russ.).
5. Shen J., Jia J.J., Sisson G. Inverse estimation of nonpoint sources of fecal coliform for establishing allowable load for Wye River Maryland. *Water research*. 2006. Vol. 40 (18). P. 3333–3342. https://doi.org/10.1016/j.watres.2006.07.035.
6. Boano F., Revelli R., Ridolfi L. Source identification in river pollution problems: A geostatistical approach. *Water Resources Research*. 2005. Vol. 41 (7). P. 1–13. https://doi.org/10.1029/2004wr003754.
7. Permanoon E., Mazaheri M., Amiri S. An analytical solution for the advection-dispersion equation inversely in time for pollution source identification. *Physics and Chemistry of the Earth*. 2022. Vol. 128 (2). 103255. https://doi.org/10.1016/j.pce.2022.103255.
8. Rashedi K. A numerical solution of an inverse diffusion problem based on operational matrices of orthonormal polynomials. *Mathematical Methods in the Applied Sciences*. 2021. Vol. 44 (17). P. 12980–12997. https://doi.org/10.1002/mma.7601.
9. De Sousa D.M., Roberty N.C. An inverse source problem for the stationary diffusion-advection decay equation. *Inverse Problems in Science and Engineering.* 2012. Vol. 20 (7). P. 891–915. https://doi.org/10.1080/17415977.2011.609466

10. Kulbay M., Mukanova B., Sebu C. Identification of separable sources for advection diffusion equations with variable diffusion coefficient from boundary measured data. *Inverse Problems in Science and Engineering*. 2017. Vol. 25 (2). P. 279–308. https://doi.org/10.1080/17415977.2016.1160396.
11. Jun K.S., Kang J.W., Lee K.S. Simultaneous estimation of model parameters and diffuse pollution sources for river water quality modeling. *Water Science and Technology*. 2007. Vol. 56 (1). P. 155–162. https://doi.org/10.2166/wst.2007.447.
12. Chaikovskii D., Zhang Y. Convergence analysis for forward and inverse problems in singularly perturbed time-dependent reaction-advection-diffusion equations. *Journal of Computational Physics*. 2002. Vol. 470. 111609. https://doi.org/10.1016/j.jcp.2022.111609.
13. Lukyanenko D.V., Shishlenin M.A., Volkov V.T., Solving of the coefficient inverse problems for a nonlinear singularly perturbed reaction-diffusion-advection equation with the final time data. *Communications in Nonlinear Science and Numerical Simulation*. 2018. Vol. 54. P. 233–247. https://doi.org/10.1016/j.cnsns.2017.06.002.
14. Yasinskii S.V., Vishnevskaya I.A., Venitsianov E.V. Diffuse pollution of water bodies and estimation of export of biogenic elements under different scenarios of water use in the watershed. 2019. *Water Resources*. 2019. Vol. 46 (2). P. 266–277. https://doi.org/10.31857/S0321-0596462232-244.
15. Filimonov V.Y., Lovtskaya O.V. Zinoviev A.T. Diffuse pollution on small rivers. Features of distribution of dissolved pollutant concentrations. *Eurasian journal of mathematical and computer applications*. 2021. Vol. 9 (3). P. 39–52. https://doi.org/10.32523/2306-6172-2021-9-3-39-52.
16. Liu Q., Cheng Y., Fan C. Pollution characteristics and health exposure risks of heavy metals in river water affected by human activities. *Sustainability*. 2023. Vol. 15 (10). 8389. https://doi.org/10.3390/su15108389.
17. ChuehY.-Y., Fan C., Huang Y.-Z. Copper concentration simulation in a river by SWATWASP integration and its application to assessing the impacts of climate change and various remediation strategies. *Journal of Environmental Management*. 2021. Vol. 279. 111613. https://doi.org/10.1016/j.jenvman.2020.111613.
18. Byrne P., Onnis P., Runkel R.L., Frau I., Lynch S.F.L., Edwards P. Critical shifts in trace metal transport and remediation performance under future low river flows. *Environmental Science & Technology*. 2020. Vol. 54 (24). P. 15742–15750. https://doi.org/10.1021/acs.est.0c04016
19. Ren J, Hao J, Tao L. Concentrations, spatial distribution, and pollution assessment of heavy metals in surficial sediments from upstream of Yellow River, China. *Environmental science and pollution research*. 2021. Vol. 28. P. 2904–2913. https://doi.org/10.1007/s11356-020-10349-3.
20. Hoang H.G., Lin C., Tran H., Chiang C.F., Bui X.T., Cheruiyot N.K., Shern C.C., Lee C.W., Heavy metal contamination trends in surface water and sediments of a river in a highly-industrialized region. *Environmental Technology & Innovation*. 2020. Vol. 20. 101043. https://doi.org/10.1016/j.eti.2020.101043.
21. Lu Q., Bian Z., Tsuchiya N. Assessment of heavy metal pollution and ecological risk in river water and sediments in a historically metal mined watershed, Northeast

Japan. *Environmental monitoring and assessment.* 2021. Vol. 193 (12). 814. https://doi.org/10.1007/s10661-021-09601-1.
22. Markich S.J., Brown P.L. Relative importance of natural and anthropogenic influences on the fresh surface water chemistry of the Hawkesbury Nepean River, south-eastern Australia. *Science of the* total environment. 1998. Vol 217 (3). P. 201–230. https://doi.org/10.1016/s0048-9697(98)00188-0.
23. Miller P.D. Applied asymptotic analysis, Providence, Rhode Island. *American Mathematical Society.* 2006. Vol. 75. https://doi.org/10.1090/gsm/075.
24. Kashefipoura S.M., Falconer R.A. Longitudinal dispersion coefficients in natural channels. *Water Research*. 2002. Vol. 36 (6). P. 1596–1608. https://doi.org/10.1016/s0043-1354(01)00351-7.
25. Tayfur G., Singh V.P., Predicting longitudinal dispersion coefficient in natural streams by artificial neural network. *Journal of Hydraulic Engineering.* 2005. Vol. 131 (11). P. 991–1000. https://doi.org/10.1061/(asce)0733-9429(2005)131:11(991)
26. Pannone M., Mirauda D., Vincenzo A.D., Molino B. Longitudinal dispersion in straight open channels: Anomalous breakthrough curves and first-order analytical solution for the depth/averaged concentration. *Water.* 2018. Vol. 10 (4). 478. https://doi.org/10.3390/w10040478.
27. Pannone M. Longitudinal Dispersion in River Flows Characterized by Random Large-Scale Bed Irregularities: First-Order Analytical Solution. *Journal of Hydraulic Engineering.* 2012. Vol. 138 (5). P. 400–411. https://doi.org/10.1061/(asce)hy.1943-7900.0000537.
28. Goliatt L., Sulaiman S.O., Khedher K.M., Farooqueean A.A., Yaseen Z.M. Estimation of natural streams longitudinal dispersion coefficient using hybrid evolutionary machine learning model. *Engineering Applications of Computational Fluid Mechanics*. 2021. Vol. 15 (1). P. 1298–1320. https://doi.org/10.1080/19942060.2021.1972043.
29. Gualtieri C., Ciaravino G., Doria G.P. Analysis of longitudinal dispersion equations in streams and rivers. *Proceedings of the 7th International Conference on HydroScience and Engineering Philadelphia*, USA September 10–13, 2006 (ICHE 2006), Philadelphia, USA.
30. Filimonov V.Yu., Lovtskaya O.V., Zinoviev A.T. Calculation of dissolved pollutants mass flow according to the data of their concentration spatial distribution in the sites of small plaint rivers. *Eurasian journal of mathematical and computer applications.* 2023. Vol. 11 (4). P. 14–28. https://doi.org/10.32523/2306-6172-2023-11-4-14-28.
31. Alekseev G.V., Vakhitov I.S., Soboleva O.V., Stability estimates in identification problems for the convection-diffusion-reaction equation. *Computational Mathematics and Mathematical Physics*. 2012. Vol. 52 (12). P. 1635–1649. https://doi.org/10.1134/S0965542512120032 (In Russ.).
32. Nocedal J., Wright S.J., *Numerical Optimization*. Springer, New York, 2006. 651 p.
33. Dennis J.E., Jr., Schnabel R.B., Numerical methods for unconstrained optimization and nonlinear equations. SIAM Publ., New York, 1987. 395 p.
34. Global Optimization Toolbox. User's Guide. The MathWorks, Inc., 2020. 877 p.
35. Strijov V., Weber G.W., Nonlinear regression model generation using hyperparameter optimization. Computers & Mathematics with Applications. 2010. Vol. 60 (4). P. 981–988. https://doi.org/10.1016/j.camwa.2010.03.021.
36. Draper N.R., Smith H. *Applied Regression Analysis.* Wiley, New York, 1998. 736 p.

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