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Research Article

Comparison of Methods for Assessing the Assimilation Capacity of the Kazakhstani Sector of the Ili River

A. T. Nurseitova,[1] **J. K. Jamalov**,[2] **A. A. Azimov**,[2] **D. B. Nurseitov**,[3] **and E. A. Tursunov**[4]

[1]*International Information Technology University, Almaty, Kazakhstan*
[2]*Satbayev University, Almaty, Kazakhstan*
[3]*KazMunayGas Engeneering LLP, Nur-Sultan, Kazakhstan*
[4]*Institute of Geography and Water Security JSC, Almaty, Kazakhstan*

Correspondence should be addressed to J. K. Jamalov; j.jamalov@norlist.kz

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A mixed inverse problem for determining the biochemical oxygen demand of water (L_0) and the rate of biochemical oxygen consumption (k_0), which are important indicators of water quality, has been formulated and numerically solved based on real experimental data. The inverse problem is reduced to the optimization problem consisting in minimization of the deviation of the calculated values from the experimental data, which is solved numerically using the Nelder–Mead method (zero order) and the gradient method (first order). A number of examples of processing both model experimental data and field experimental data provided by hydrological stations monitoring pollutants in the Kazakhstani part of the Ili River basin are presented. A mathematical model that adequately describes the processes in the river system has been constructed.

1. Introduction

Many models describing the processes of pollution and purification of water resources are based on the work of Streeter and Phelps published in 1925 [1], where a simple model (considered classical in our time) was proposed, which for many years satisfied the needs of engineers and other practitioners in the field of monitoring of water pollution in many countries. In the course of the development of this direction, it became clear that there are many rather important factors that have a great influence on the studied processes but are not taken into account by the classical Streeter-Phelps model. A reasonably good analysis of the models proposed over 40 years, taking into account new input data, was made in [2], but, as the author himself noted, all these models are semiempirical and require a lot of input data that are not always available for measurements. At first glance, the classical Streeter-Phelps model is simple to implement, and even its more complicated versions allow an analytical solution, which is undoubtedly an advantage for engineers, i.e., for practical use. Indeed, even with the advent of computers until the end of the 20th century, the issue of economical use of computer time in calculations had a priority position in the choice of models and methods of their implementation. Therefore, there are many works that consider different factors of oxygen consumption and recovery in water (dispersion, photosynthesis, reaeration, etc.), but all of them are based either on a large amount of input data, or on assumptions that are inconvenient in practice, but this is not the main weakness of these studies. For example, in [3], to calculate the missing (inaccessible for measurement) input data, where reaeration is taken into account, the original Streeter-Phelps model is synthesized with the shallow water equation, and here, the scientists already face the problem of cumbersome calculations. As shown in the work of Gotovtsev [4], the classical Streeter-Phelps model does not guarantee physically correct solutions for any input data, i.e., a rather difficult process of data calibration leads to a separately posed problem that requires separate consideration [2]. In [4], a modification of the classical Streeter-Phelps model (a closed Streeter-Phelps system) is proposed, which does not require additional hydrochemical analyzes; moreover, it is shown that it is physically correct. To obtain an analytical solution of the Streeter-Phelps closed-loop system, certain conditions are again set on the input data, for example, the frequency of incubation times [5], which is not applicable in practice. Thus, a positive aspect of these models is the explicit form of the desired value, which greatly facilitates the work of practitioners, but the models are complicated by introduction of additional factors imposing new conditions and restrictions on the input data, which creates a number of new problems; the solution of which already requires other resources. With development of more powerful computers, the capabilities of calculators have increased significantly and works have appeared where application of the modified Streeter-Phelps models is considered solutions to some inverse problems, for example [6]. That is, the general tendency to consider some problems as inverse to direct ones, which appeared in the 20th century [7, 8], was also reflected in the implementations of models describing the processes of pollution and purification of water resources.

In this paper, the sought BOD (L_0) and k_0 are considered solutions to an inverse problem for which additional information is given at a fixed moment of time $T > 0$. More exactly, a closed Streeter-Phelps model is considered, for which there are no data restrictions (taken from real sources), which is achieved by using iterative methods instead of searching for an analytical solution. It is shown that the inverse problem is ill-posed [7]; therefore, two optimization methods for its solution are considered: the semiheuristic Nelder–Mead [9] and the gradient (also known as regularizing [10]). The Nelder–Mead method is an unconstrained zero-order optimization method, i.e., the method that does not require computation of either the first or the second derivatives of the objective function, which is an undoubted advantage in the implementation of this iterative algorithm, especially in the case of many variables. However, the convergence of this method was investigated only for strictly convex functions in the one-dimensional case; for multidimensional objective functions, the convergence has not been proven (although for the two-dimensional case weak convergence was established under certain restrictions on the algorithm) [11]. The use of gradient methods (of the first order) in the case of a multidimensional objective function is complicated by the calculation of the gradient, but the convergence of these iterative algorithms has been sufficiently well studied [12]. This paper presents a comparative analysis of the numerical results of realization of the considered modified Streeter-Phelps model by the Nelder–Mead method and the steepest descent method for synthesized data. More exactly, two aspects of the methods are compared: the complexity of realization and investigation of convergence. The fact that for the Nelder–Mead method the relative "efficiency at the best case" outweighs the absence of a theory of convergence, noticed in [11], was also confirmed by the results of our comparative analysis. As this method is still a favorite among other zero-order optimization methods, it was used for testing the model under consideration based on real experimental data (provided by hydrological stations monitoring pollutants in the Kazakhstani part of the Ili River basin). The analysis of the obtained numerical results was carried out on the basis of the report on the research work of the *JSC Institute of Geography and Water Security* [13].

2. Materials and Methods

2.1. Statement of the Inverse Problem. In [4] and in the previous studies, the correctness of the physical formulation of the Streeter-Phelps closed system, describing the process of biochemical oxygen consumption, was shown:

$$\begin{aligned} \frac{dL}{dt} &= -\frac{k_0}{C_s}\bullet C(t)\bullet L(t), \\ \frac{dC}{dt} &= -\frac{k_0}{C_s}\bullet C(t)\bullet L(t) + k_2(C_s - C(t)), \end{aligned} \tag{1}$$

Here, t is the time, $L(t)$ is the concentration of dissolved organic substance, $C(t)$ is the concentration of dissolved oxygen, k_0 is the rate of biochemical oxygen consumption, C_s is the concentration of oxygen saturation, and k_2 is the rate of reaeration.

In this work, it is assumed that $k_2 = 0$, i.e., the process of decomposition of organic matter, which occurs in a water sample, is placed in a sealed flask or in the ice-covered river channels and reservoirs. For a given $T > 0$ in the space $L_2[0, T]$, we have the following *direct problem*:

$$\begin{aligned} \frac{dL}{dt} &= -\frac{k_0}{C_s}\bullet C(t)\bullet L(t), \quad t \in (0, T), \\ \frac{dC}{dt} &= -\frac{k_0}{C_s}\bullet C(t)\bullet L(t), \quad t \in (0, T), \end{aligned} \tag{2}$$

$$\begin{aligned} L(0) &= L_0, \\ C(0) &= C_0, \end{aligned} \tag{3}$$

where using the given values of constants $k_0, L_0, C_0, C_s \in \mathbb{R}_+$, it is necessary to determine functions $L, C \in L_2[0, T]$ satisfying system (2) and (3).

Definition 1. For some $T > 0$, a pair of functions $L, C \in L_2[0, T]$ will be called *a solution of direct problems* (2) and (3) if for any functions $\omega \in H^1[0, T]$ such that $\omega(T) = 0$, the following equalities hold:

$$\begin{aligned} L_0\bullet\omega(0) + \int_0^T L(t)\bullet\omega'(t)dt &= \frac{k_0}{C_s}\int_0^T C(t)\bullet L(t)\bullet\omega(t)dt, \\ C_0\bullet\omega(0) + \int_0^T C(t)\bullet\omega'(t)dt &= \frac{k_0}{C_s}\int_0^T C(t)\bullet L(t)\bullet\omega(t)dt. \end{aligned} \tag{4}$$

Note 1. Direct problems (2) and (3) are correct in the sense of Hadamard in the space $L_2[0, T]$ for $T > 0$.

It is obvious that problems (2) and (3) are reduced to an equivalent system of Volterra integral equations of the second kind, which are known to be correct.

To determine the most important indicators of water quality L_0 and k_0, the *problem inverse to ((2)) and ((3)) is considered*: for some $T \geq 5$ determine the values $L_0, k_0 \in \mathbb{R}_+$, where the functions $L, C \in L_2[0, T]$ are a solution to direct problems (2) and (3), using the given values of $C_0, C_s \in \mathbb{R}_+$ and the additional information:

$$\begin{aligned} L(T) &= L_T, \\ C(5) &= C_5. \end{aligned} \tag{5}$$

Note 2. Inverse problems (2) and (5) are incorrect.

Indeed, inverse problems (2) and (5) are incorrect, since direct problems (2) and (3) are correct [10].

Note 3. Let for some $T \geq 5$ functions $L, C \in L_2[0, T]$ be a solution to direct problems (2) and (3), then, there are traces of $L(T), C(5) \in \mathbb{R}$ and the following estimates:

$$\begin{aligned} L(T) &\leq L_0 + \frac{k_0}{C_s} \|C\|_{L_2(0,T)} \bullet \|L\|_{L_2(0,T)}, \\ C(5) &\leq C_0 + \frac{k_0}{C_s} \|C\|_{L_2(0,T)} \bullet \|L\|_{L_2(0,T),} \end{aligned} \tag{6}$$

are correct.

2.2. Statement of the Optimization Problem and Methods for Its Solution. In view of Note 3, formulated inverse problems (2) and (5) naturally reduce to an equivalent optimization problem associated with minimization of the following objective functional:

$$I(L_0, k_0) = (L(T) - L_T)^2 + (C(5) - C_5)^2. \tag{7}$$

Here, L_T and C_5 are given values and $L(t)$ and $C(t)$ are solutions of direct problems (2) and (3), which correspond to parameters L_0 and k_0.

Thus, parameters $L_0, k_0 \in \mathbb{R}_+$ must be determined from the condition of minimum of functional (7).

A convenient way to solve the optimization problems is the Nelder–Mead method [9], which is an unconditional optimization of the functional in several variables without using its gradient. Since the convergence of the Nelder–Mead method has not been established for the two-dimensional case, for comparison, we also consider the regularizing gradient method, which gives us conditional convergence [10]. The gradient of functional (7) is equal to

$$I' = \left(I'_{L_0}, I'_{k_0}\right), \tag{8}$$

Table 1: Results of calculations with exact values of C_5 and L_T.

	Nelder–Mead method		Gradient method	
	L_0	k_0	L_0	k_0
Reconstructed value	20.000036	0.230001	19.9985	0.229947
Absolute error	0.000036	0.000001	0.001414	0.000053
Relative error	0.00018%	0.00043%	0.00707%	0.02304%
Functional value	$6.3 \cdot 10^{-10}$		$1.0 \cdot 10^{-6}$	

where

$$\begin{aligned} I'_{L_0} &= p_1(0), \\ I'_{k_0} &= -\frac{1}{C_s} \int_0^T C(t) L(t) (p_1(t) + p_2(t))\, dt, \end{aligned} \tag{9}$$

functions $p_1(t), p_2(t)$ are solutions for adjoint system

$$\begin{aligned} \frac{dp_1}{dt} &= \frac{k_0}{C_s} C(t)(p_1(t) + p_2(t)) - 2(L(t) - L_T)\delta(t - T), t \in (0, T), \\ \frac{dp_2}{dt} &= \frac{k_0}{C_s} L(t)(p_1(t) + p_2(t)) - 2(C(t) - C_5)\delta(t - 5), t \in (0, T), \\ p_1(T) &= 0, \\ p_2(T) &= 0. \end{aligned} \tag{10}$$

3. Results and Discussions

3.1. Comparison of Numerical Results for Synthetic Data. To carry out computational experiments, as sought values, we take $L_0 = 20$, $k_0 = 0.23$. Let also $C_0 = C_s = 9$, $T = 5$.

Solving direct problems (2) and (3), we find functions $L(t), C(t)$, from which we obtain the values $C_5 = C(5)$, $L_T = L(T)$, which we take as additional information (5). And, using these data, we will reconstruct the parameters L_0, k_0 from the condition of functional minimum (7). Using the Nelder–Mead (NM) and gradient (GM) methods, the results presented in Table 1 were obtained. Here, the exact values of C_5 and L_T are taken as additional information. Figure 1 shows the graphs of the functions $L(t), C(t)$, corresponding to the values of parameters L_0, k_0 obtained by the NM and GM methods.

As can be seen from Table 1, in the case when the exact values of L_T and C_5 are known, the values of L_0 and k_0 are reconstructed quite accurately. In particular, the relative NM error was less than a hundredth of a percent.

Let us consider the case when the additional information (5) is given with some error α; that is, the values of L_T and C_5 can randomly deviate from their true value by less than α. After performing a number of computational experiments, it is possible to estimate the range of variation of the sought parameters and the corresponding functions $L(t), C(t)$. Tables 2–5 show the corresponding calculation results for different α. Note that these tables present the maximum error values.

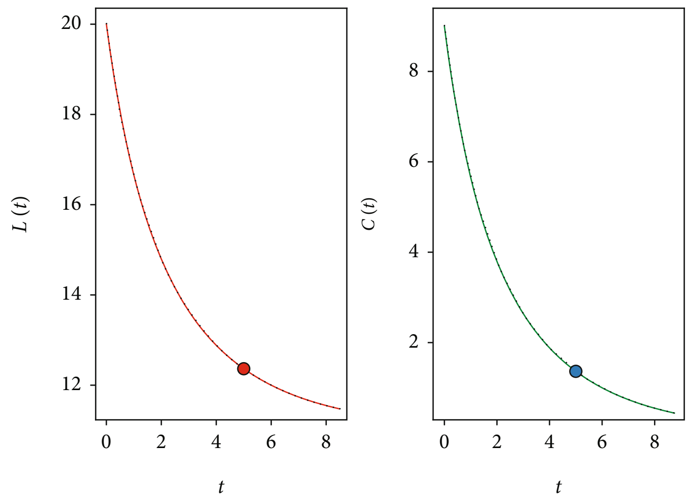

Figure 1: Functions $L(t)$ and $C(t)$ calculated with exact values of L_T and C_5.

Table 2: Results of calculations with an error $\alpha = 5\%$.

	Nelder–Mead method		Gradient method	
	L_0	k_0	L_0	k_0
Maximum absolute error	0.55	0.02	0.55	0.02
Maximum relative error	2.75%	7.35217%	2.76%	7.33%

Table 3: Results of calculations with an error $\alpha = 10\%$.

	Nelder–Mead method		Gradient method	
	L_0	k_0	L_0	k_0
Maximum absolute error	1.10	0.03	1.10	0.03
Maximum relative error	5.50%	15.58%	5.51%	15.55%

Table 4: Results of calculations with an error $\alpha = 15\%$.

	Nelder–Mead method		Gradient method	
	L_0	k_0	L_0	k_0
Maximum absolute error	1.65	0.05	1.65	0.05
Maximum relative error	8.25%	24.85%	8.25%	24.82%

Table 5: Results of calculations with an error $\alpha = 20\%$.

	Nelder–Mead method		Gradient method	
	L_0	k_0	L_0	k_0
Maximum absolute error	2.20	0.08	2.20	0.08
Maximum relative error	11.00%	35.36%	11.00%	35.32%

Figure 2 shows the graphs of the functions $L(t)$, $C(t)$, corresponding to the values of parameters L_0, k_0 obtained by the NM and GM methods. The solid lines show the functions constructed by the results of solving the inverse problem with exact data for L_T and C_5. Dashed lines indicate maximum deviations when additional information (5) is specified with 5% error. As can be seen from Table 2 and Figure 2, the numerical results obtained by the NM and GM methods almost coincide.

Similar results for $\alpha = 10\%$, $\alpha = 15\%$, and $\alpha = 20\%$ are presented in Tables 3–5 and in Figures 3–5, respectively.

The results of Tables 2–5 show that an increase in the input error causes an increase in the error of the results. Moreover, it can be noted that the relative error for k_0 is about 3 times greater than that for L_0, while the value of the objective functional always remains sufficiently small. It is also easy to see that the function $C(t)$ as a whole is reconstructed much more accurately: in the case when the additional information (5) is given with some error, the deviation of the graph of function $C(t)$ from the true one is insignificant. This is likely to be explained by the fact that the initial condition C_0 for $C(t)$ in the studied problem is known, whereas the initial condition for $L(t)$ is not known.

Thus, the optimization problem, equivalent to inverse problems (2) and (5), associated with minimization of functional (7), was solved by the Nelder–Mead method and by the gradient method, and the sought parameters L_0, k_0 were reconstructed quite accurately with the same maximum deviations for data errors. A series of calculations were carried out using field experimental data provided by the Institute of Geography. Oil products were considered pollutants, as they are included in the list of parameters, which must be obligatory determined according to the mandatory program of monitoring the quality of surface waters by hydrochemical and hydrological indicators.

3.2. Numerical Results for Experimental Data. Kazakhstani part of the Ili River, which is the main tributary of lake Balkhash basin, was chosen as the object of modeling. In the system of the economy of Kazakhstan, the basin is a diversified economic complex, which has environmentally hazardous enterprises of the extractive industry and nonferrous metallurgy. About 30% of the water resources of the Ili

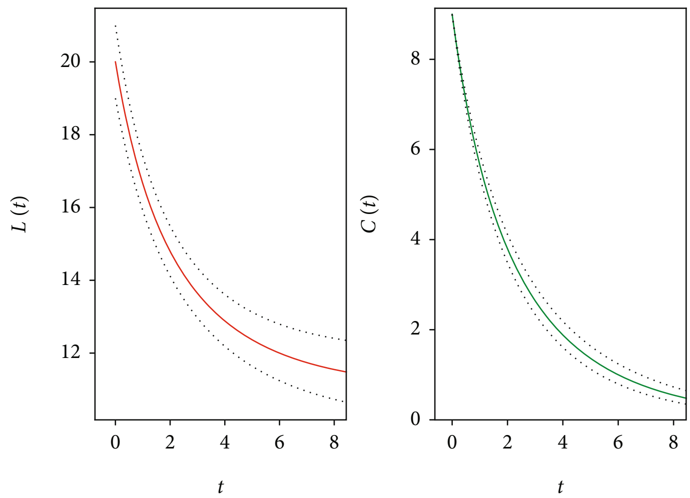

Figure 2: Functions $L(t)$ and $C(t)$, $\alpha = 5\%$.

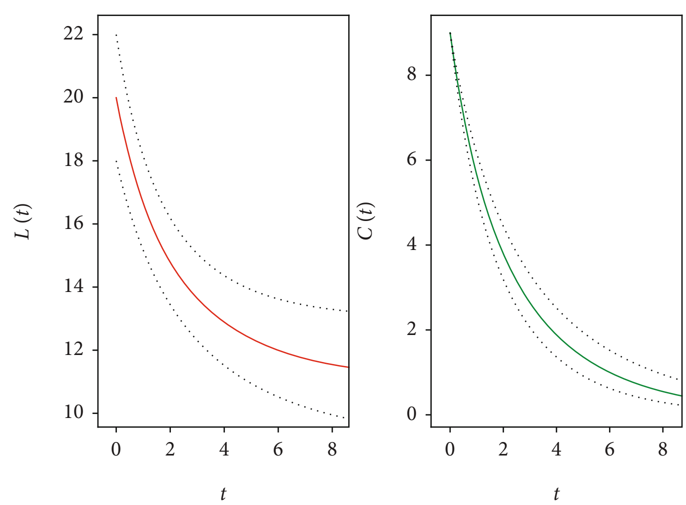

Figure 3: Functions $L(t)$ and $C(t)$, $\alpha = 10\%$.

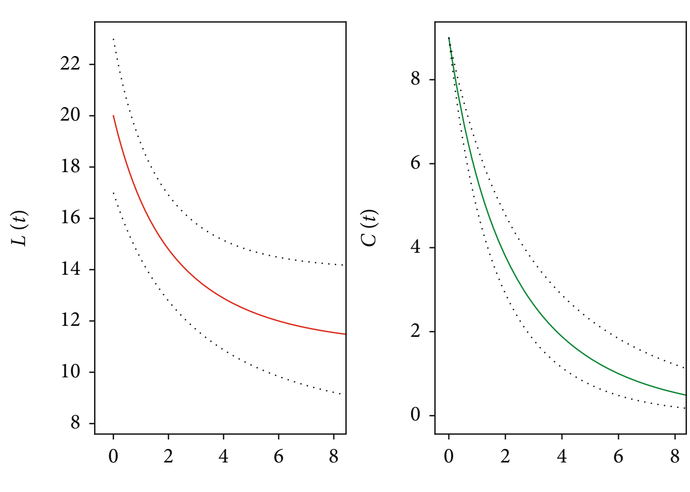

Figure 4: Functions $L(t)$ and $C(t)$, $\alpha = 15\%$.

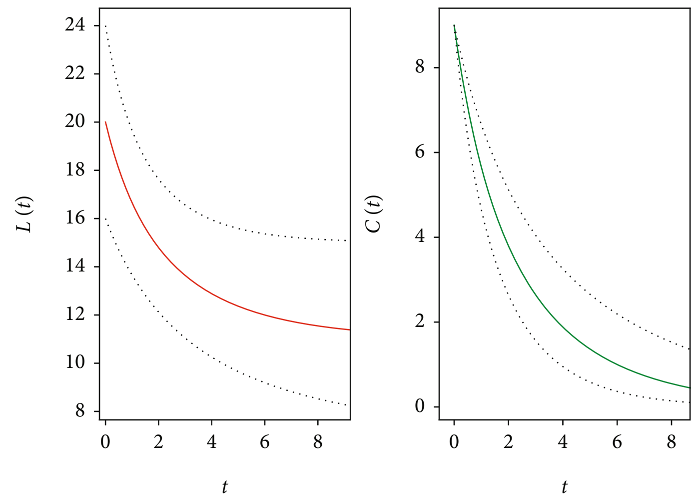

FIGURE 5: Functions $L(t)$ and $C(t)$, $\alpha = 20\%$.

TABLE 6: The main points of quality control of surface waters in the Ili River basin.

Waterbody code	Location	Post code	Distance from the outfall (km)	Catchment area (square km)
113200001	Pier Dobyn	14003	723	64388
113200001	164 km above the Kapshagai hydroelectric station	14004	607	85400
113200001	37 km below the Kapshagai hydroelectric station	14011	434	111000
113200001	Ushzharma village	14014	264	129000

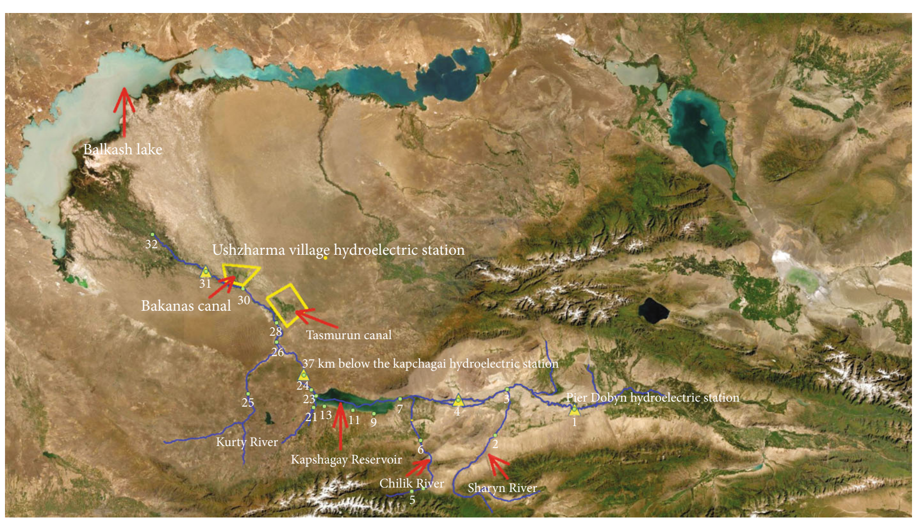

FIGURE 6: Location of hydrological posts on the map (yellow triangles denote hydrological posts),

River are formed on the territory of Kazakhstan [14–16]. The Ili River is a transboundary river, and in the recent decades, Kazakhstan has faced the growing water deficit, and one of the reasons for this is the policy of China to increase unilaterally the water intake from transboundary rivers Irtysh and Ili ignoring herewith the interests of the Kazakh side. The chemical composition of the Ili River on the territory of the Kazakhstan to the Kapshagai water reservoir is formed under the influence of pollutants coming from the territory of China as well as contaminated surface runoff and washout from the farmland adjacent to the basin. [17] The data of chemical analysis of water from 4 hydrological stations for the period from 2000 to 2014 were obtained. Table 6 presents the data for these hydrological stations. Figure 6 shows their location on the map.

To study the transfer of pollution, as well as to assess the assimilation capacity of the Kazakhstani part of the Ili River, epy data from two hydrological stations were considered:

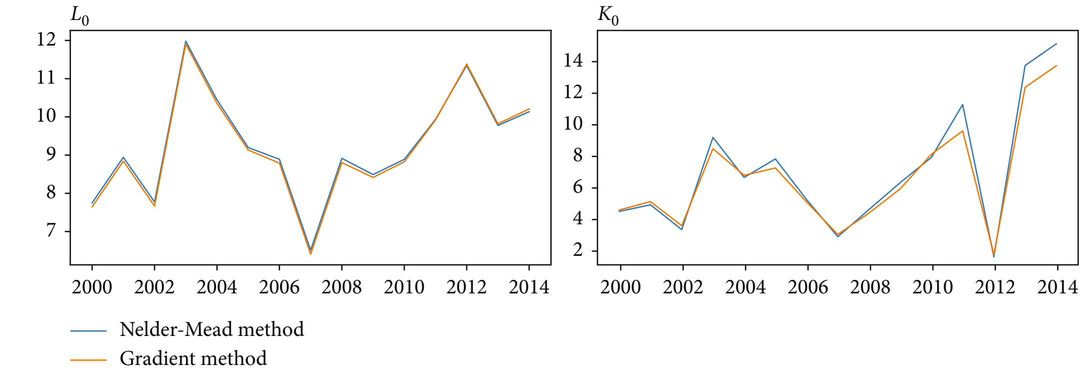

Figure 7: Initial concentration L_0 and biochemical oxidation rate k_0 of oil products at the hydrological station the Dobyn pier

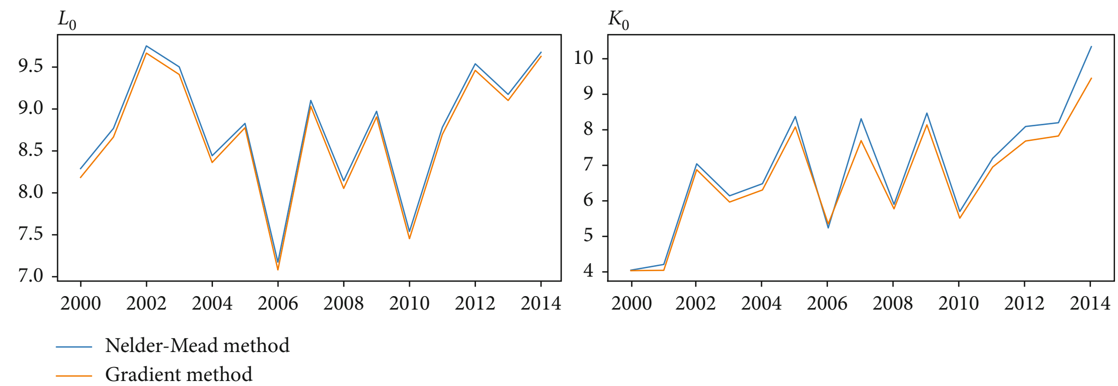

Figure 8: Initial concentration L_0 and biochemical oxidation rate k_0 of oil products at the hydrological station in the village of Ushzharma

Dobyn pier (the first hydrological station on the Kazakhstani part of the Ili River) and the village of Ushzharma (the last hydrological station before the Ili delta). Figures 7 and 8 show the results of usage of two methods for numerical calculations of the sought parameters L_0 and k_0 at hydrological stations for the period from 2000 to 2014.

Figures 7 and 8 show that the solutions of the inverse problem by the Nelder–Mead method and the gradient method give very close results. It can be argued that the constructed mathematical model adequately describes the processes in the Ili River system, as evidenced by the results of a series of numerical experiments. Intra-annual hydrochemical regime of pollution of the Ili River in the section of the Dobyn pier is, in general, consistent with the theoretical description of its natural flow. There is a decrease in pollution in the March, an increase in the July low-water period with an improvement in quality during the period of precipitation in August. Further, during the period of rains, an improvement in quality should be observed, but its quality is deteriorated, which can be explained by the washout of pollutants from the adjacent territories. The increased water content in 2001 and 2008 led to an increase in the oxygen content in the water due to a more rapid flow of water in the river, and as a result of increased aeration. High concentrations of both mineral substances and pollutants, some of which are characterized by high chemical activity, led to more active oxidative reactions, as a result of which, in Figures 7 and 8, extremely high values of L_0 and k_0 are observed oil products in these years. These data are confirmed by the high values of CIWP (a complex index of water pollution, obtained by averaging all substances that exceed the maximum permissible concentration) in these years. Figure 7 shows that in 2006 the minimum value of the concentration of the pollutant after that the value increases. According to the space images [18], the area of irrigated land in China's Xinjiang Uygur Autonomous Region (XUAR) had grown to 465,500 hectares. The increase in water consumption affects the river inflow into the territory of Kazakhstan which is one of the factors that affect the increase of concentration of pollutants [16, 18].

4. Conclusions

On the basis of the closed Streeter-Phelps system, an inverse problem that determines the power of point sources of pollutants, at which the concentration of pollutants at hydrological posts is equal to the maximum permissible, has been formulated. A comparative analysis of optimization methods (NM and GM) for solving the formulated inverse problem was carried out, which showed the effectiveness of application of the Nelder–Mead method and the gradient method. The results of numerical experiments made it possible to assess the assimilation capacity of the Kazakhstani part of the Ili River basin. The resulting estimate determines the upper limit of the assimilation capacity of the basin (the highest seasonal value of the maximum permissible load), since the calculations for the BOD were carried out at $k = 0.23\ \mathrm{day}^{-1}$. This value corresponds to a water temperature of 20°C, which is usually observed during the summer low-water period. It is obvious that in winter, when the rate of decomposition of pollutants is significantly lower, the calculated value of the maximum permissible load will decrease. Also, the obtained results can be used to predict changes in the concentration of pollutants in case a decrease in the river inflow into the territory of Kazakhstan.

Data Availability

The natural hydrological data used to support the findings of this study were supplied by E.A. Tursunov under license and so cannot be made freely available. Requests for access to these data should be made to JSC (Institute of Geography and Water Security, website: https://ingeo.kz/?page_id=2813~~~~~~~~~^~^~^~^~~~~~~~~~~~amp;lang=en).

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Acknowledgments

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