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Inverse algorithm for Streeter–Phelps equation in water pollution control problem

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Abstract

In this study, for the first time in the literature, we consider the inverse problem that arises in the problem of controlling water pollution in streams. The problem here is to determine the source's load of pollution based on the results of measuring water quality in places remote from the waste source. Based on the results of measuring the concentration of dissolved oxygen (DO), which characterizes the level of pollution of surface water in a stream, will determine the level of the pollutant load of the waste discharger. Using classical Streeter–Phelps model, showing the relationship between the source power and the water quality of river channels, the inverse algorithm is constructed to determine the load capacity of the waste source. The resulting algorithm in this study is for general case and refers to several sources of waste. The article also presents the numerical results of applying the algorithm obtained for specific examples. The results of this study contribute to the scientific and substantiated issue of environmental decision making.

Keywords: Streeter — Phelps equation; Inverse problem; BOD/DO model; Pollution control; Water pollution

1. Introduction

Water pollution from human activities and industry is an important issue in many countries. The stream is the most important source of water supply for urban, agricultural and industrial use but now a significant increase in wastewater directly into the river increases the pollution of this water. The actual problem of protecting the aquatic environment has become one of the most important tasks of science in general and mathematics in particular [6,8,10–12,18,22]. In early studies for Ganga and Yamuna rivers, India, [1,22] have presented models allow accurate prediction of polluted streams' BOD and DO sag parameters using classical Streeter–Phelps model. Research [3] noted that, the major processes for water quality modeling are expressed in mathematical terminology in the form of differential equations. The list of chemical reactions and biological processes described in [3] would explicitly simulate the important relationship between the source of waste and the receptor environment. In the study [8], a product named SIAQUA-IPH was developed to simulate water quality for the Brazil river basin. [11] presented results of building an integrated tool named EnvimQ2K, integrating waste source database, Qual2K and GIS

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assessing river water quality of Vietnam. Currently, there are several models developed for modeling water quality, often used to assess the impact of pollutant discharges on rivers, such as Qual2K, Mike11 [2,5,6,14,17,23–25].

Currently, quite a lot of mathematical models have been developed to study the distribution and transformation of pollutants, including the classical mathematical model of Streeter–Phelps, based on the mass balance, in 1925 [3,11,20,22] and also models describing the hydrodynamic process in combination with a biochemical transport model with an emphasis on biochemical changes [3,6]. Within these models, a “direct” problem based on characteristics of waste dischargers, such as flow, pollutant load, temperature of wastewater and hydrodynamics of water bodies, calculated the concentration of pollutants in surface water [7,8,13,18,22].

However, in fact, when studying the influence of discharge sources on surface water quality, in almost all cases it is very difficult to measure the load of the pollutant in the discharge of waste, even it was too dangerous to meet. Therefore, it is necessary to develop a mathematical model based on “indirect” data, which provides measured information to obtain the information we need. In this study, the inverse problem is understood as the task of determining some parameters of the model in accordance with the specific results of indirect measurements [16].

Strict in the mathematical sense terms — direct and inverse problems that can be solved within the framework of an already constructed model are introduced by russian academician A.N. Tikhonov [16,21]. Direct problems are the problem of finding the consequences of known or given causes, that is, problems solved “along” causal or causal relationships. Inverse problems — problems of finding the causes of known or given consequences. They arise when the characteristics of an object of interest to us are not available for direct observation. Investigation of the inverse problem using a modeling approach to detect suspicious sources in the case of air pollution is very modest [4,9,15]. From a review of the literature, it has been shown that the study of the problem, as opposed to a model approach for detecting sources of waste causing water pollution, has not yet been carried out. For the example, paper [19] using the regression method, the correlation is very cumbersome due to the need for a large amount of monitoring data that are difficult to implement in the absence of measurement data. In this study, the proposed approach, based on measuring the concentration of pollutants in a stream remotely from sources, reveals a discharge level of waste dischargers that exceeds the standard. It is also an important tool for controlling water pollution.

Not every field has been studied in the inverse problem [16]. Moreover, the study of the inverse problems of controlling water pollution is rather modest. In addition, some studies on inverse problems that are not focused on the use of computer science, so its practical application is limited. This is the reason for this study. The structure of the article is following: Section 2 describes classical Streeter-Phelps model, which clarifies the relationship between the sources of discharges and water quality, and at the end of this section presents how to setup the inverse problem. Section 3 presents an algorithm for solving the inverse problem for case of one source and several sources. Finally, Section 4 presents a numerical solution that identifies the discharge load from “suspected” sources.

2. Direct problem description

Streams as river or channel are often used to dilute wastewater. The inclusion of substances with oxygen demand, including organic and inorganic substances in the stream leads to a decrease in dissolved oxygen in stream water [1,3,22]. To predict the deterioration of oxygen depletion, it is necessary to know what type of wastewater is discharged into the stream and how much oxygen is needed for the decomposition of the waste [22]. Oxygen is being loaded from the atmosphere or from photosynthesis of algae and aquatic plants, in addition, a certain amount of oxygen is consumed by organisms, therefore the oxygen concentration in surface water is always determined by the relative speed of competitive processes [3,22].

In 1914–1916, Streeter and Phelps [20] regularly monitored water quality in the Ohio river, USA and from a series of DO measurements along the stream, Streeter and Phelps developed a method to assess the impact of waste discharger on the water quality of the Ohio river. This model is called the BOD/DO model, because the BOD represents the level of wastewater pollution from the discharge point, DO represents the water quality from the river [1,11,20,22]. The model makes it possible to explain the DO change in accordance with the distance in the direction of the stream flow due to BOD decomposition, and this equation is named the Streeter–Phelps equation [1,3,11,20]. Assuming that the wastewater is continuously discharged into the stream from the discharge point, stream and wastewaters flow downstream and mix well in cross sections of the stream, there is no dispersion of wastewater in the direction of flow, this means that the flow is an advection process. In the classical paper [1], Streeter-Phelps considered oxygen deficiency as a function of the competition between oxygen use and reaeration from the atmosphere and obtained the equation [3]:

$$\frac{dL}{dx} = \frac{k_1}{U}L - \frac{k_2}{U}D$$

where x is the distance along the reach moving downstream, L is the amount of oxidizable organic material as oxygen equivalents (i.e. the BOD) by the waste discharger, k_1 - oxidation rate constant in the stream (day^{-1}), k_2 – reaeration rate constant in the stream (day^{-1}), D is the DO (dissolved oxygen) deficit (the difference between the DO concentration if saturated and the actual concentration). If $L = L_0$ and $D = D_0$ at time zero then these equations can be solved for [11]:

$$\left[\begin{array}{l} D(x) = D_0 e^{(-k_2/U)x} + \dfrac{k_1 L_0}{k_2 - k_1}\left(e^{(-k_1/U)x} - e^{(-k_2/U)x}\right), \quad k_1 \neq k_2 \\ D(x) = \left(k_1 * \dfrac{x}{U} * L_0 + D_0\right) * e^{k_1 * \frac{x}{U}}, k_1 = k_2 \end{array}\right. \tag{1}$$

where U is average stream velocity. In [3] this model incorporates the two primary mechanisms governing the fate of DO in streams receiving sewage, the decomposition of organic matter and atmospheric reaeration. According to [3,20,22] biochemical oxidation is the only sink and atmospheric reaeration is the only source of oxygen (i.e. photosynthesis and respiration are ignored). The simplest manifestation of the Streeter–Phelps model is for a reach in steady-state (i.e. time invariant) characterized by plug flow with constant hydrology and geometry.

In (1), the coefficients k_1 and k_2 depend on the temperature as follows:

$$k_1(T) = k_1(20\ ^\circ\mathrm{C}).1,05^{T-20},\ \ k_2(T) = k_2(20\ ^\circ\mathrm{C}).1,0241^{T-20} \tag{2}$$

The symbol T_r and T_w are the temperature (°C) of the stream and the waste discharger respectively, Q_r and Q_w are the flow (m^3/s) of the stream and discharger. Then the temperature (T_mix) and total BOD at time zero (L_mix) after the wastewater mixed with stream water is calculated according to the formula [3,11]

$$T_{mix} = \frac{T_r.Q_{r+}T_w.Q_w}{Q_r + Q_w}, L_{mix} = \frac{L_r Q_r + L_w Q_w}{Q_r + Q_w} \tag{3}$$

On practice, parameter total BOD, L, is calculated according to the measure of BOD$_5$, so in the actual calculation, the following formula is used: $L_0 = \frac{BOD_5}{1-e^{-5k_1(T)}}$. The coefficient $k_1(20\ ^\circ\mathrm{C})$ depends on the type of wastewater [1,11,22]. The coefficient $k_2(20\ ^\circ\mathrm{C})$ depends on the stream velocity and average depth of the stream and is the subject of research in many papers [1,3,11]. In this study, the formula O'Connor-Dobbins [11] is used:

$$k_2^{20} = 3,93\frac{v^{0,5}}{H^{1,5}} \tag{4}$$

where U - is the average velocity of the flow, H - is the average depth of the stream.

The classical Streeter–Phelps equation (1) and the formulas (2)–(4) show the relationship between the "Waste discharger–Receptor", in which the "dirty" level of the waste discharger is expressed through parameter L_0 - total BOD quantity from the waste discharger and D(x) - dissolved oxygen deficiency (mg/l) at position x (km) from the source is representing the quality of the river water that affected by waste discharger. From the formula

$$\mathrm{DO} = \mathrm{DO}_{\mathrm{saturated}} - \mathrm{D(x)} \tag{5}$$

will determine the dissolved oxygen concentration at position x, that mean, determine the extent of the influence of the river due to the impact of the waste discharger. The DO$_\mathrm{saturated}$ parameter is calculated based on the table of DO values at integer temperatures and is interpolated at other temperature values.

In this study, the direct problem is understood as based on the source parameters and stream parameters, assessing the level of pollution of the stream, affected by waste dischargers. The relevant parameters for solving the direct problem are shown in Table 1.

3. Inverse algorithm for determining the discharger load

In fact, it is difficult to determine the load pollutant of the waste discharger due to the lack of cooperation from the owner of the waste dischargers, while measuring dissolved oxygen below the flow source is quite simple. Thus, the reverse problem posed in this study. Based on the results of measuring the level of dissolved oxygen, determine

Table 1
Parameters related to flow, waste discharger and coefficients are used in the direct problem.

Stream parameters	Source parameters	Coefficients
Q_r - river discharge at upstream of the first waste discharger (m^3/h)	Q_w - waste discharger discharge (m^3/day)	k_1(20 °C) - rate constant for the nonsettleable organic matter (day^{-1})
$BOD_{5,r}$ (20 °C) - river BOD_5 at upstream of the first waste discharger (mg/l)	$BOD_{5,w}$ (20 °C) – BOD5 of waste discharger (mg/l)	k_2 (20 °C) - reaeration rate constant (day^{-1})
DO_r – dissolved oxygen at upstream of the first waste discharger (mg/l)	DO_w - dissolved oxygen of waste discharger (mg/l)	
T_r - river temperature (°C)	T_w – temperature of waste water (°C)	
v - river flow velocity (m/s)		
H - averaged depth of river (m)		

the "dirty" level of wastewater from discharger, in other words, find out the cause of pollution. In this study, the concentration of $BOD_{5,w}$ (characterizing the level of wastewater pollution) was selected for the determination of the inverse algorithm.

3.1. Case for one waste discharger

Applying the Streeter–Phelps formula calculates the oxygen deficiency at any point of the source of discharge x (m).

$$D\,(x) = \frac{k_1(T).L_0}{k_2(T)-k_1(T)}\left(e^{-k_1(T)x/v}-e^{-k_2(T)x/v}\right)+D_0.e^{-k_2(T).x/v} \tag{6}$$

from here, it follows

$$D_0.e^{-k_2(T).x/v} = D\,(x) - \frac{k_1(T).L_0}{k_2(T)-k_1(T)}\left(e^{-k_1(T)x/v}-e^{-k_2(T)x/v}\right) \tag{7}$$

wherein

$$L_0 = \frac{Q_r.BOD_{5,r}+Q_w.BOD_{5,w}}{(Q_r+Q_w).(1-e^{-5k_1(T)})},\ T=\frac{T_r.Q_{r+}T_w.Q_w}{Q_r+Q_w}, DO=\frac{DO_r.Q_r+DO_w.Q_w}{Q_{mix}}, D=DO_{bh}-DO \tag{8}$$

From (3), (8) we deduce

$$k_1\,(T)=k_1(20\text{ °C}).1,05^{\frac{T_r.Q_r+T_w.Q_w}{Q_r+Q_w}-20},\ k_2\,(T)=k_2(20\text{ °C}).1,0241^{\frac{T_r.Q_r+T_w.Q_w}{Q_r+Q_w}-20} \tag{9}$$

Substituting (8) in (7) we get the following equation

$$\left(DO_{bh}-\frac{DO_r.Q_r+DO_w.Q_w}{Q_r+Q_w}\right)e^{-k_2(T).x/v} = D\,(x) - \frac{k_1(T)}{k_2(T)-k_1(T)}\left(e^{-k_1(T)x/v}-e^{-k_2(T)x/v}\right) \times\left(\frac{Q_r.BOD_{5,r}+Q_w.BOD_{5,w}}{(Q_r+Q_w)(1-e^{-5k_1(T)})}\right) \tag{10}$$

To determine $BOD_{5,w}$ we perform the following steps: from Eq. (10), it follows:

$$\begin{aligned}&[DO_{bh}(Q_r+Q_w)-DO_r.Q_r-DO_w.Q_w]\,e^{-k_2(T)\frac{x}{v}}.\,(k_2(T)-k_1(T))\,.\left(1-e^{-5k_1(T)}\right)\\&=D\,(x)\,.\,(k_2(T)-k_1(T))\,(Q_r+Q_w)\left(1-e^{-5k_1(T)}\right)-k_1\,(T)\left(e^{-k_1(T)\frac{x}{v}}-e^{-k_2(T)\frac{x}{v}}\right)\\&\times\left(Q_r.BOD_{5,r}+Q_w.BOD_{5,w}\right)\end{aligned} \tag{11}$$

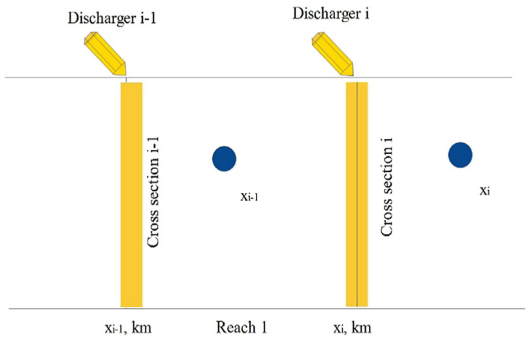

Fig. 1. The case of multi waste source dischargers.

It follows

$$k_1(T)\left(e^{-k_1(T)\frac{x}{v}}-e^{-k_2(T)\frac{x}{v}}\right)Q_w.BOD_{5,w}=D\left(x\right).\left(k_2(T)-k_1(T)\right)\left(Q_r+Q_w\right)\left(1-e^{-5k_1(T)}\right)$$
$$-\left[DO_{bh}(Q_r+Q_w)-DO_r.Q_r-DO_w.Q_w\right]e^{-k_2(T)\frac{x}{v}}.\left(k_2(T)-k_1(T)\right).\left(1-e^{-5k_1(T)}\right)-k_1(T)$$
$$\times\left(e^{-k_1(T)\frac{x}{v}}-e^{-k_2(T)\frac{x}{v}}\right).Q_r.BOD_{5,r} \tag{12}$$

Putting

$$\alpha_1=k_1(T)\left(e^{-k_1(T)\frac{x}{v}}-e^{-k_2(T)\frac{x}{v}}\right)Q_w$$
$$\beta_1=D\left(x\right).\left(k_2(T)-k_1(T)\right)\left(Q_w+Q_r\right)\left(1-e^{-5k_1(T)}\right)-\left[DO_{bh}(Q_r+Q_w)-DO_r.Q_r-DO_w.Q_w\right]$$
$$\times e^{-k_2(T)\frac{x}{v}}.\left(k_2(T)-k_1(T)\right)$$
$$\times\left(1-e^{-5k_1(T)}\right)-k_1(T)\left(e^{-k_1(T)\frac{x}{v}}-e^{-k_2(T)\frac{x}{v}}\right).Q_r.BOD_{5,r} \tag{13}$$

Denote by x_{m} is the position for measuring the concentration of dissolved oxygen, then $D(x_m)$, α_1, β_1 are determined and from formulas (8), (9), (13) we get

$$BOD_{5,w}=\frac{\beta_1}{\alpha_1} \tag{14}$$

Formula (14) means that in accordance with the measurement of the concentration of dissolved oxygen in the x_{m} position from the waste discharger, the concentration of BOD_5 of the waste discharger may be exceeded than the permission standard.

3.2. Case of many waste dischargers

Number waste dischargers in order $1, 2, \ldots, \mathrm{n}$. Calling the locations for measuring the dischargers respectively $x_1, x_2, \ldots, x_n$. It is assumed that the value of DO concentration in the river is determined through field measurements of DO_{w1}, DO_{w2}, …, DO_{wn}. From these measured values, $D_1 = D(x_1), D_2 = D(x_2), \ldots, D_{\mathrm{n}} = D(x_{\mathrm{n}})$ are determined. With source i ($i = 1, \ldots, \mathrm{n}$) we implement the following algorithm (see Fig. 1):

$$\alpha_i=k_1(T_i)\left(e^{-k_1(T_i)\frac{x_i}{v}}-e^{-k_2(T_i)\frac{x_i}{v}}\right)Q_{wi}$$
$$\beta_i=D\left(x_i\right).\left(k_2(T_i)-k_1(T_i)\right)\left(Q_{w_i}+Q_{i-1}\right)\left(1-e^{-5k_1(T_i)}\right)$$
$$-\left[DO_{bh}(Q_{wi}+Q_{i-1})-DO_{i-1}.Q_{i-1}-DO_{wi}.Q_{wi}\right]e^{-k_2(T_i)\frac{x_i}{v}}$$
$$\times\left(k_2(T_i)-k_1(T_i)\right)\times\left(1-e^{-5k_1(T_i)}\right)-k_1(T_i)\left(e^{-k_1(T_i)\frac{x_i}{v}}-e^{-k_2(T_i)\frac{x_i}{v}}\right).Q_i.BOD_{5,\mathrm{i}} \tag{15}$$

The following intermediate results are made:

$$T_i=\frac{T_{i-1}.Q_{i-1}+T_{w_i}.Q_{w_i}}{Q_{i-1}+Q_{w_i}},\ Q_i=Q_{i-1}+Q_{wi} \tag{16}$$

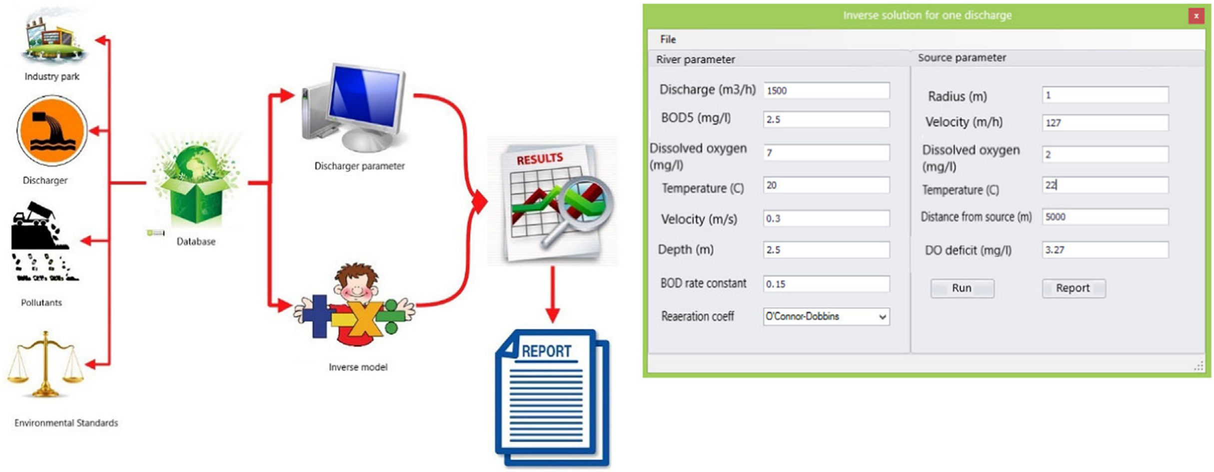

Fig. 2. Data flow and interface of module for automatic processing for inverse problem.

$$k_1(T_i) = k_1(20\ ^\circ\mathrm{C}).1,05^{T_i-20} = k_1(20\ ^\circ\mathrm{C}).1,05^{\frac{T_{i-1}.Q_{i-1}+Tw_i.Qw_i}{Q_{i-1}+Qw_i}-20}$$
$$k_2(T_i) = k_2(20\ ^\circ\mathrm{C}).1,0241^{T_i-20} = k_2(20\ ^\circ\mathrm{C}).1,0241^{\frac{T_{i-1}.Q_{i-1}+Tw_i.Qw_i}{Q_{i-1}+Qw_i}-20} \tag{17}$$

where Q_{i-1} - is the discharge before the join of the ith source, Q_i - is the discharge after the join of the ith waste discharger; T_{i-1} is the stream temperature before the join of discharger i; T_i - is the temperature after the join of discharger i; T_{w_i}- wastewater temperature of discharger i, $BOD_{5,ri}$ is BOD_5 concentration in the reach i of the stream; $BOD_{5,wi}$ is BOD_5 concentration in wastewater of discharger i, DO_i is the dissolved oxygen concentration at the first section after the mixing of the source i with flow, where $i = 2, \ldots,$ n. Based on the Streeter–Phelps equation, it follows:

$$\begin{aligned}
&k_1(T_i)\left(e^{-k_1(T_i)\frac{x_i}{v}} - e^{-k_2(T_i)\frac{x_i}{v}}\right) Q_{wi}.BOD_{5,wi} = D\left(x_i\right).\left(k_2(T_i) - k_1(T_i)\right)\left(Q_{i-1} + Q_{wi}\right)\left(1 - e^{-5k_1(T_i)}\right)\\
&-\left[DO_{bh}(Q_{i-1} + Q_{wi}) - DO_{i-1}.Q_{i-1} - DO_{wi}.Q_{wi}\right] e^{-k_2(T_i)\frac{x_i}{v}}.\left(k_2(T_i) - k_1(T_i)\right).\left(1 - e^{-5k_1(T_i)}\right)\\
&-k_1(T_i)\left(e^{-k_1(T_i)\frac{x_i}{v}} - e^{-k_2(T_i)\frac{x_i}{v}}\right).Q_i.BOD_{5,\mathrm{r}_{i-1}}
\end{aligned} \tag{18}$$

Finally we get

$$BOD_{5,w_i} = \frac{\beta_i}{\alpha_i} \tag{19}$$

4. Software database and numerical simulation

To automate the calculation, in this study assumed software that consists of a database of three groups of parameters: first, the group of data on the hydraulics of the stream: flow discharge, BOD_5 concentration, the concentration of dissolved oxygen, temperature, velocity, average depth of the stream; secondly, the second group of data on the wastewater discharger: wastewater discharge, BOD5, oxygen concentration, temperature in wastewater, deficiency of oxygen at the location from the discharge source, thirdly, a group of coefficients in Streeter – Phelps model: $k_1(20\ ^\circ\mathrm{C})$ - rate constant for the nonsettleable organic matter (day^{-1}) k_2 (20 °C) - reaeration rate constant (day^{-1}) (see Fig. 2)

To apply the above software, in this section consider two numerical examples:

Example 1. A plant that discharges water into the receiving object is the stream, the dissolved oxygen concentration in the wastewater is 2.0 mg/l, the wastewater flow temperature is 22 °C. The discharge culvert has a flow discharge of 399 m^3/h. The stream has a discharge of 1500 (m^3/h), BOD_5 at 20 °C is 2.5 mg/l, dissolved oxygen concentration is 7.0 mg/l. Stream temperature is 20 °C. The stream has an average velocity of 0.3 m/s, an average depth of 2.5 m.

Taking the rate constant for the nonsettleable organic matter (day^{-1}) k_1 (20 °C) = 0.15, the reaeration rate constant (day^{-1}) used is the O'Connor-Dobbins formula (4)

It is known that in order to control pollution, oxygen deficiency is measured 5 km from the source of discharge, the result of measuring oxygen deficiency is 3.27 mg/l. Determine the level of the source exceeds the prescribed level?

Based on formulas (4), (8), (12), (13) we get:

$$\alpha_1 = 17.202, \beta_1 = 417, BOD_{5,w} = \frac{\beta_1}{\alpha_1} \approx 24,241 \text{ mg/l}$$

Example 2. To assess the level of pollution from two sewers discharging into a stream. The first sewer has a dissolved oxygen concentration of 2.5 mg/l, the wastewater temperature is 22 °C, the wastewater discharge is: 600 m^3/h. The discharge of the stream is 1400 m^3/h, BOD_5 at 20 °C is 4.5 mg/l, dissolved oxygen concentration is 6.0 mg/l. The stream temperature is 20 °C. The stream has an average velocity is 0.1 m/s, an average depth is 2.5 m. At a distance of 10 km from the above discharge source, there is a second sewer with a dissolved oxygen concentration of 2.0 mg/l, a wastewater is 23 °C, a discharge is 500 (m^3/h). The rate constant for the nonsettleable organic matter is used the k_1 (20 °C) = 0.25 (day^{-1}), the reaeration rate constant is used the Owens–Gibbs formula [11]:

$$k_2^{20} = 9,4.\frac{u^{0,67}}{H^{1,85}} \text{ (day}^{-1}\text{)}$$

In order to control water pollution, it is measured at 2 locations as follows: the first position is 10 km from discharge source 1 (right before sewer 2), the oxygen deficiency measurement result is 6633 mg/l. The second measurement point is 5 km from the discharge source 2. Measurement result is 6.5 mg/l. Determine the pollution level of the two discharge sources by using BOD_5 parameter.

Based on the algorithm presented in (16)–(19), we get:

$$\alpha_1 = 14,4241, \beta_1 = 516, BOD_{5,w1} = \frac{\beta_1}{\alpha_1} = \frac{516}{14,4241} = 35.77 \text{ (mg/l)}$$

$$\alpha_2 = 5,34, \beta_2 = 126,97, BOD_{5,w2} = \frac{\beta_2}{\alpha_2} = \frac{216,97}{5,34} = 23,77 \text{ (mg/l)}$$

5. Conclusion

In this paper we study the inverse problem in environmental modeling. Based on the classical Streeter–Phelps model, we have made an estimate to determine the capacity of pollution dischargers based on the results of measuring the water quality parameter of stream channels. This result helps managers to make decisions to punish polluters. The methods used in this paper can be extended to similar problems with other pollutants.

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Appendix A. Supplementary data

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.matcom.2019.12.005.

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