Mathematical models for effluent bioremediation to improve environmental safety of wastewater infrastructure

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Abstract
The article is devoted to the mathematical modelling of bioremediation processes of wastewater contaminated with nutrients. The model of a consumer-resource water system in which the resource is harmful impurities and the consumer is Euglena gracilis was built. The proposed system of differential equations with predefined initial conditions in general describes the dynamics of changes in the concentrations of euglena and phosphorus impurities during their interaction quite qualitatively. In particular, the graphs of the functions of microalgae and impurities dependencies on time have a clearly expressed S-shape.

Keywords
mathematical modelling, microalgae, bioremediation, wastewater infrastructure, environmental safety

1. Introduction

Today, many technologies are used to clean up environmental pollution and bioremediation processes, as green technologies, are becoming one of the main environmental technologies that scientists use in their research. Key research findings show that some strains of microalgae can be successfully used for biological water treatment, providing fast and efficient removal of phosphorus and nitrogen, which contribute to eutrophication of water bodies [1, 2, 3]. This opens up the possibility of using them in wastewater treatment systems as an environmentally friendly and cost-effective alternative to chemical methods [4, 5, 6, 7]. Biological methods of wastewater treatment have recently attracted increasing attention, in particular those using unicellular and multicellular aquatic organisms. Among these organisms, microalgae are of particular interest, as they are the leading bioagents for biological treatment [8, 9, 10]. Interest in the use of microalgae in biological wastewater treatment is explained by their ability to actively influence the sanitary condition of water. Algae play an important role in natural ecosystems, as they are actively involved in the removal of pollutants and improvement of water quality [11, 12, 13, 14]. In the initial stages, microalgae effectively remove the bulk of nutrients and organic matter, reducing the overall level of pollutants in wastewater. In the final stages, their use allows for deeper treatment, ensuring the removal of residual elements such as ammonium, phosphates and nitrates that are difficult to treat chemically.

The effective management of natural resources and ecological systems has been a matter of concern in recent decades, as the problems of intense anthropogenic impact on the environment have put humanity in need of preserving natural systems and preventing their destruction. Achieving a reasonable and effective ecosystem management strategy is quite difficult, as there are many conflicting factors to consider, which must be balanced due to the complexity of the real-world problems. Moreover, various processes and activities are interconnected, leading to complex systems with interactive, dynamic,

CH&CMiGIN'25: Fourth International Conference on Cyber Hygiene & Conflict Management in Global Information Networks, June 20–22, 2025, Kyiv, Ukraine
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nonlinear, multi-purpose, multi-stage, multi-layered and uncertain features.

One of the prerequisites for this is the modelling and forecasting of anthropogenic processes in nature. The most important socio-environmental problems that need to be addressed through modelling are twofold. The first is the need to model the distribution of pollutants in the aquatic environment in order to localise their impact and prevent negative social consequences. The second area, which is of great social importance, is the preservation of water sources as an entire ecosystem, provided that its parameters are stable within certain limits. It is a systematic approach to the study of a water body that can ensure, on the basis of regulatory and search forecasting, compliance with environmental requirements [15, 16, 17]. Mathematical modelling of wastewater treatment processes has recently become increasingly popular.

2. Problem statement

The use of modelling and forecasting methods determines the understanding of everything that is happening and can happen in water systems, atmosphere, soils, flora, the consequences of human intervention in them, pragmatises assessments and conclusions, and helps to find optimal technical, technological, organisational and environmental solutions. Mathematical models are recognised as effective tools that can help investigate the economic, environmental and ecological impact of alternative pollution control and resource conservation measures, and thus assist in decision-making in the formulation of environmentally and economically efficient management policies.

Therefore, the development of mathematical models of the interaction of pollutants, including nutrients contained in wastewater, with microalgae is an urgent task. Our task was to build and study a model of a consumer-resource water system in which the resource is harmful impurities and the consumer is Euglena gracilis. We will limit ourselves to the case when there is a certain amount of impurities in the reservoir and no new impurities enter the system.

3. Mathematical modeling

3.1. Development of mathematical models for the interaction of microalgae with phosphates

Consider the equation of the interaction of impurities in water with Euglena gracilis. Denote by C_m and C_i according to the concentration of algae and impurities. Let the concentrations of microalgae and impurities be equal, respectively, at the moment of time $t = 0$:

$$C_m(0) = C_{m0} > 0, C_i(0) = C_i > 0. \tag{1}$$

The dynamics of changes in the concentration of impurities and microalgae, assuming that the trophic function is directly proportional to the amount of resource, i.e. the concentration of impurities, can be described by a system of differential equations of the form:

$$\begin{cases} \frac{dC_m}{dt} = \alpha_1 C_m C_i - \gamma C_m, \\ \frac{dC_i}{dt} = -\beta_1 C_m C_i, \end{cases} \tag{2}$$

where α is the parameter, characterizes the process of increasing the concentration of algae with time consumption of impurities; γ is the parameter, characterizes the rate of decrease in the concentration of algae by account of natural processes (specific mortality); β is the parameter, characterizes the process of reducing the concentration of impurities in water environment due to interaction with algae.

This system is a special case of the mathematical model of Lotka and Volterra, which they proposed to describe the interaction of two species - a population of predators and a population of prey. In our case, the microalgae Euglena gracilis act as predators, and impurities in water act as prey [18, 19].

System (2) takes into account the following assumptions:

- in the absence of microalgae, the concentration of impurities does not change according to the equation $\frac{dC_i}{dt}$;
- in the absence of impurities in the water, microalgae die off according to the equation $\frac{dC_m}{dt} = -\gamma\, C_m$, so $C_m = C_{m0}e^{-\gamma t}$;
- the expression $C_m C_i$, taken with a certain coefficient, describes the effect of the microalgae population on the change in the amount of impurities in the water, i.e. the result of 'eating' impurities by microalgae leads to a decrease in the rate $\frac{dC_i}{dt}$ of change in the concentration of impurities by the value $C_m C_i$, proportional to the concentration of microalgae.

In the following, we introduce the notation: $\alpha_1 = \frac{\alpha}{C_{m0}C_{i0}}, \beta_1 = \frac{\beta}{C_{m0}C_{i0}}$. Then the system (2) will take the form:

$$\begin{cases} \frac{dC_m}{dt} = \alpha \frac{C_m}{C_{m0}} \cdot \frac{C_i}{C_{i0}} - \gamma C_m, \\ \frac{dC_i}{dt} = -\beta \frac{C_m}{C_{m0}} \cdot \frac{C_i}{C_{i0}}. \end{cases} \tag{3}$$

Thus, it is necessary to solve the Cauchy problem - to find a solution to the system (3) that satisfies the initial conditions (1). For given values of the parameters, this Cauchy problem has a unique solution, and it is convenient to search for it approximately, using, for example, the fourth-order Runge-Kutta method.

Let's find out the meaning of the parameters α and β in system (3) and propose an algorithm for determining their values depending on the initial concentrations C_{m0} and C_{i0}.

About parameter values α and β Note that $\alpha > 0, \beta > 0, \gamma \geq 0$. In addition, the following equations hold

$$\frac{dC_m(0)}{dt} = \alpha \frac{C_{m0}}{C_{m0}} \cdot \frac{C_{i0}}{C_{i0}} - \gamma\, C_{m0} = \alpha - \gamma\, C_{m0}, \tag{4}$$

where we get it from

$$\alpha = \frac{dC_m(0)}{dt} + \gamma\, C_{m0}, \frac{dC_i(0)}{dt} = -\beta \frac{C_{m0}}{C_{m0}} \cdot \frac{C_{i0}}{C_{i0}} = -\beta. \tag{5}$$

Thus, the value of the parameter α is equal to the sum of the initial growth rate of the microalgae concentration and the specific mortality rate γ multiplied by the initial value of the microalgae concentration,

$$\alpha = \frac{dC_m(0)}{dt} + \gamma\, C_{m0}, \tag{6}$$

and the value of the parameter β is equal to the absolute value of the rate of decrease in the concentration of impurities at the initial time $t = 0$:

$$\beta = -\frac{dC_i(0)}{dt}. \tag{7}$$

If we assume that $\gamma = 0$, then $\alpha = \frac{dC_m(0)}{dt}$. In the following, we will assign a certain value to the parameter γ, assuming that this value does not exceed 0.05, for example, 0.02.

The values of the parameters α and β are also not subject to precise determination. However, using the concept of the first-order differential of the functions $C_i(t)$ and $C_m(t)$, we can estimate these values.

3.2. Improvement of mathematical models of microalgae-phosphate interaction on the example of euglena gracilis strain

Let us formulate the basic requirements for a mathematical model of the interaction of impurities with microalgae. The concentrations of impurities and microalgae, respectively, and the curves describing the dynamics of their changes, must meet certain requirements:

1) the function $C_i = C_i(t)$ must be decreasing, taking values from $C_{i0} = C_i(0)$ to $C_i(T)$, T – the number of days during which microalgae interact with impurities. Most of the time, the concentration of $C_i(T)$ is close to zero, and as a rule, $T \in [4; 7]$;

2) the graph of the function $C_i = C_i(t)$ must have a pronounced S-shape. In particular, the function $C_i = C_i(t)$ at the initial point in time$t = 0$ should decrease at a rate $C_i{}'(0)$, determined by formula (3), so that the value of $C_i(1)$ is approximately equal to the calculated value $(C_i(1))^*$, determined by formula (3). The fastest decay of the function $C_i(t)$ should be reached at the point$t = t^*$ and the ordinate of the point $(t^*; C_i(t^*))$ – the curve inflection point $C_i = C_i(t)$, should satisfy the inequality $C_i(t^*) > \frac{C_{i0}}{2}$. The steepest function graph $C_i = C_i(t)$ should be mostly in the interval $t \in (1; 3)$ (during the second or third day). In the interval $(0; t^*)$ the curve $C_i(t)$ must be convex and concave in the interval $(t^*; T)$;

3) the function $C_m = C_m(t)$ should increase in the interval $t \in [0; T_1]$, where $T_1 \leq T$. If $T_1 = T$, then the function $C_m = C_m(t)$ should increase during all days of interaction between microalgae and impurities; if $T_1 < T$, then the function would increase in the interval $t \in [0; T_1]$, acquire values from $C_{m0} = C_m(0)$ to $(C_m)_{max}$, and decrease in the interval $t \in [T_1; T]$. The rate of growth of the function $C_m(t)$ should initially increase from $C_m{}'(0)$ to $(C_m{}')\, m'^{**}{}_{max}$ and then the rate should monotonically decrease to a certain small value or be equal to zero at the point $t = T_1$. The graph of the function $C_m = C_m(t)$ on the interval $[0; T_1]$ should also have a pronounced S-shape. In the interval $(0; t^{**})$, the curve $C_m(t)$ must be concave, and in the interval $(t^{**}; T)$ – convex. The point $(t^{**}; C_m(t^{**}))$ of the curve $C_m(t)$ must be an inflection point, and the following conditions must be met: $t^{**} > \frac{T}{2}$, approximately $C_m(t^{**}) > \frac{2}{3}(C_m)_{max}$, i.e. the curve $C_m(t)$ should change from concavity to convexity essentially at the final stage (in the last one or several days, depending on the initial values of the concentrations of impurities and microalgae) of the interaction of microalgae with impurities.

The achievement of the corresponding effect depends on the perfection of the choice of trophic functions that determine the qualitative properties of the mathematical model of the systems 'predator-prey', 'consumer-resource', etc. Many works [20, 21] have been devoted to the problem of adequacy of the choice of trophic functions, which consider the theoretical aspects of their choice, mostly trophic functions are chosen based on the results of experimental studies.

It should be noted that today, most scientists who study these issues do not have a unanimous opinion on how to solve the problem of choosing trophic functions [22, 23, 24].

The above requirements for a mathematical model of the interaction of impurities with microalgae are generally satisfied by the system of differential equations:

$$\begin{cases} \frac{dC_m}{dt} = \alpha \cdot q \cdot \frac{C_m}{C_{m0}} \cdot \left(1 - \frac{1-\left(\frac{C_i}{C_{i0}}\right)^{n_1}}{1+\delta_1\left(\frac{C_i}{C_{i0}}\right)^{n_1}} \cdot \frac{1}{1+\delta_2\left(\frac{C_m}{C_{m0}}\right)^{n_2}}\right) - \gamma C_m, \\ \frac{dC_i}{dt} = -\beta \cdot q \cdot \frac{C_i}{C_{i0}} \cdot \frac{C_m}{C_{m0}} \cdot \frac{1}{1+\delta_3\left(\frac{C_i}{C_{i0}}\right)^{n_3}} \cdot \frac{1}{1+\delta_4\left(\frac{C_m}{C_{m0}}\right)^{n_4}} \end{cases} \tag{8}$$

with initial conditions (1). Compared to the form of system (2), the equations of system (8) contain two trophic functions:

$$T_1(C_i, C_m) = \frac{1}{C_{m0}} \cdot \frac{1 - \left(1 - \frac{C_i}{C_{i0}}\right)^n}{\left(1 + \delta_1\left(\frac{C_i}{C_{i0}}\right)^{n_1}\right)\left(1 + \delta_2\left(\frac{C_m}{C_{m0}}\right)^{n_2}\right)}. \tag{9}$$

$$T_2(C_i, C_m) = \frac{1}{C_{m0}} \cdot \frac{\frac{C_i}{C_{i0}}}{\left(1 + \delta_1\left(\frac{C_i}{C_{i0}}\right)^{n_3}\right)\left(1 + \delta_2\left(\frac{C_m}{C_{m0}}\right)^{n_4}\right)}. \tag{10}$$

The main difference between them is the presence in the numerator of the function $T_1(C_i, C_m)$ of the multiplier $(C_i) = 1 - \left(1 - \frac{C_i}{C_{i0}}\right)^n$, where the indicator n takes on a certain value, mostly greater than 20. The multiplier $R(C_i)$ has the following properties:

1) at the initial time $t = 0 : R(C_{i0}) = 1$;

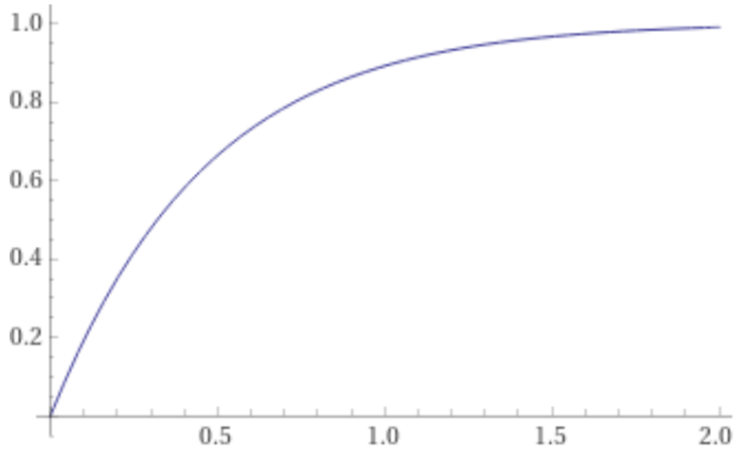

Figure 1: Graph of the function $R\left(C_i\right) = 1 - \left(1 - \frac{C_i}{14}\right)^{30}$ on the interval [0;2].

2) $R\left(C_i\right)$ is an increasing function, which, when the argument C_i is continuously changing from C_{i0} to 0, takes continuous values from 1 to 0, and in the interval $[C_i; C_{i0}]$, where $C_i = 0.15C_{i0}$, the double inequality $0.99 < R\left(C_i\right) \leq 1$ is satisfied. A significant change in the value of the function $R\left(C_i\right)$ from 0 to 0.99 is observed in the interval $[0; C_i]$. For example, if we take $[C_{i0} = 14, n = 30, C_i = 2$, then on the interval $[[0; C_i]$ the graph of the function $[R\left(C_i\right) = 1 - \left(1 - \frac{C_i}{14}\right)^{30}$ has the form shown in Figure 1;

3) at small values of $[C_i$ concentration, the approximate equality $[R\left(C_i\right) = 1 - \left(1 - \frac{C_i}{C_{i0}}\right)^n \approx \frac{nC_i}{C_{i0}}$ is true, i.e., this function approaches the linear one.

From the above properties of the function $R\left(C_i\right)$, its role in the trophic function $T_1\left(C_i, C_m\right)$ follows, namely, this function is intended primarily to prevent a rapid increase in the concentration of $C_m\left(t\right)$ of microalgae during the first few days of their interaction with impurities.

In order to reproduce the dynamics close to the results of the experiments, regulating factors that appear in the denominators of trophic functions are introduced into the mathematical model. In particular, based on the results of the research, the following values of the indicators are proposed $n_1 - n_4$:

$$n_1 = 4.5, n_2 = 0.89, n_3 = 5, n_4 = 2.2.$$

To determine the values of the coefficients $\delta_1 - \delta_4$, the parameter q is introduced, which has a certain relationship with these coefficients. Let us illustrate it. To do this, consider the system (8) at the initial time $t = 0$:

$$\begin{cases} \frac{dC_m(0)}{dt} = \alpha \cdot q \cdot \frac{1}{(1+\delta_1)(1+\delta_2)} - \gamma C_{m0}, \\ \frac{dC_i(0)}{dt} = -\beta \cdot q \cdot \frac{1}{(1+\delta_3)(1+\delta_4)} \end{cases} \quad (11)$$

To preserve the meaning of the parameters α and β we require that at the initial time $t = 0$ the following equations are satisfied:

$$\begin{cases} \alpha = \alpha \cdot q \cdot \frac{1}{1+\delta_1} \cdot \frac{1}{1+\delta_2}, \\ -\beta = -\beta \cdot q \cdot \frac{1}{1+\delta_3} \cdot \frac{1}{1+\delta_4} \end{cases} \quad (12)$$

which means that $(1 + \delta_1)(1 + \delta_2) = q$ and $(1 + \delta_3)(1 + \delta_4) = q$. Given that the coefficients $\delta_1 - \delta_4$ take on positive values, let us assume, for example, that $q = 4$, then $\delta_1 \in (0; 3)$ - a certain constant, respectively $\delta_2 = \frac{q}{(1+\delta_1)} - 1$. Similarly, $\delta_3 \in (0; 3), \delta_4 = \frac{q}{(1+\delta_3)} - 1$. Based on the results of the research, we propose calculation formulas for determining the values of the coefficients δ_1 and δ_3 :

Table 1
Results of Calculation

	0	1	2	3	4	5	6	7
C_m	120	170.111	308.908	566.283	787.259	830.443	821.828	806.675
C_i	14	11.202	5.532	1.342	0.195	0.023	0.003	0

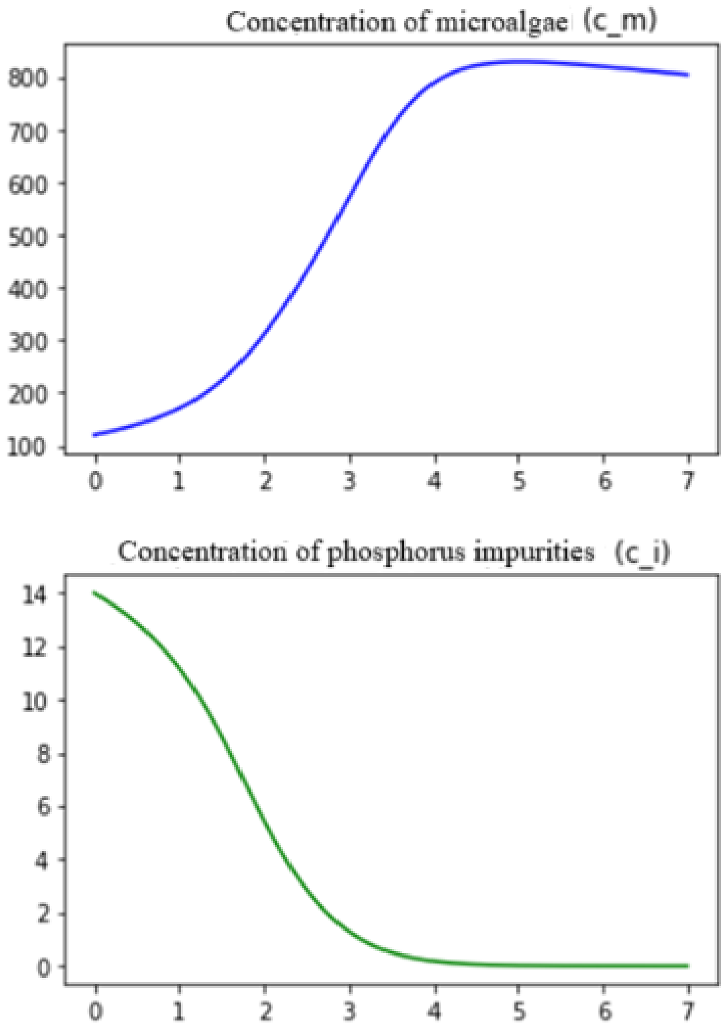

Figure 2: Testing the mathematical model with predetermined initial concentrations.

$$\delta_1 = ln(1 + 4.928(C_{m0}C_{i0})^{0.058}), \delta_3 = ln(1 + 19.96(C_{m0}C_{i0})^{-0.037}).$$

For the case of $C_{m0} = 120, C_{i0} = 14$, the values of the coefficients $\delta_1 - \delta_4$ to the nearest thousandth are as follows: $\delta_1 = 2.150, \delta_2 = 0.270, \delta_3 = 2.780, \delta_4 = 0.058$.

3.3. Testing of mathematical models and results of modelling the interaction of microalgae with phosphates

Consider the example when $C_{m0} = 120, C_{i0} = 14$. The results of calculation are shown in Table 1 and Figure 2.

4. Conclusions

The proposed system of differential equations (8) with initial conditions (1) in general describes the dynamics of changes in the concentrations of euglena and phosphorus impurities during their interaction quite qualitatively. In particular, the graphs of the functions $C_m = C_m(t)$ and $C_i = C_i(t)$ have a clearly expressed S-shape. The curve $C_i = C_i(t)$ adequately reflects the dynamics of changes in the concentration of phosphorus impurities during all days of interaction, except, perhaps, the second day. Thus, during the second day, the calculated concentration of phosphorus impurities in Examples 1-3 decreased by 50.6-53.2 %, while according to experimental data, it decreased by 62.8-92.9 %. During the third day, according to the calculations, a faster decrease in the concentration of phosphorus impurities was observed (more than 4 times compared to the previous day).

According to the calculations on the first two days of interaction, the obtained concentration of $C_m(t)$ of microalgae practically coincided with the experimental concentrations. On the third day, the calculated results slightly exceeded the experimental results - by 15.9%, 9.9%, 12.3%, respectively. On the fourth day, the difference between the calculated and experimental concentrations of microalgae was almost levelled.

Declaration on Generative AI

The authors have not employed any Generative AI tools.

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