MATHEMATICAL MODELLING
МАТЕМАТИЧЕСКОЕ МОДЕЛИРОВАНИЕ

UDC 519.6
https://doi.org/10.23947/2587-8999-2023-7-4-47-53

Original article

Pollutions Spreading Process Modelling in an Aquatic Ecosystem

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Abstract
Introduction. Pollution of shallow waters is becoming an increasingly serious problem. It is important to study the mechanisms of pollution distribution in them to protect and restore such vulnerable ecosystems, it is necessary to develop strategies for the development of sustainable and environmentally friendly use of natural resources, minimizing the negative impact on the environment. Part of this work is the construction of a mathematical model for the spread of pollutants (in particular, phosphates) in shallow reservoirs. The aim of the work is to construct scenarios for changes in the concentration of phosphates at various parameters of the model.
Materials and Methods. The phosphate transport mathematical model in a shallow reservoir is described, implemented using a modified alternating triangular iterative method to solving grid equations.
Results. The developed mathematical model is numerically implemented in the form of a software module. This model is an important tool for assessing and predicting the various pollution sources impact to the water quality of ecosystems such as lakes and reservoirs.
Discussion and Conclusion. The resulting model can be used to analyze various pollution scenarios, for example, to determine optimal waste management strategies and prevent pollution of water resources. In addition, the software module developed by the authors allows you to simulate the process of the phosphates concentration changing and can be useful for conducting scientific and engineering research in the aquatic ecology field and developing effective methods for adapting hydrobiocenosis to changes in the aquatic ecosystem.

Keywords: mathematical model, pollutants, shallow water body, phosphates, algorithm, software module

Funding information. The study was supported by the Russian Science Foundation grant no. 22-11-00295. https://rscf.ru/en/project/22-11-00295/

For citation. Lyashchenko T.V., Chistyakov A.E., Nikitina A.V. Pollutions spreading process modelling in an aquatic ecosystem. *Computational Mathematics and Information Technologies*. 2023;7(4):47–53. https://doi.org/10.23947/2587-8999-2023-7-4-47-53

Научная статья

Моделирование процесса распространения загрязнения водной экосистемы фосфатами

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Аннотация
Введение. Загрязнение мелководных водоемов является очень серьезной проблемой. Для защиты и восстановления таких уязвимых экосистем крайне важно изучить механизмы распространения в них загрязнений, разработать стратегии по развитию устойчивого и экологически чистого использования природных ресурсов, минимизации

негативного влияния на окружающую среду. Частью этой работы является построение математической модели распространения загрязнений (в частности, фосфатов) в мелких водоемах. Целью работы является построение сценариев изменения концентрации фосфатов при различных параметрах модели.

Материалы и методы. С помощью модифицированного попеременно-треугольного итерационного метода решения сеточных уравнений (МПТМ) создается математическая модель транспорта фосфатов в мелководном водоеме.

Результаты исследования. Разработанная математическая модель численно реализована в виде программного модуля. Эта модель представляет собой важный инструмент для оценки и прогнозирования воздействия различных источников загрязнения на качество вод экосистем, таких как море, озеро и водохранилище.

Обсуждение и заключение. Полученная модель может быть использована для анализа различных сценариев загрязнения, например, для определения оптимальных стратегий управления отходами и предотвращения загрязнения водных ресурсов. Кроме того, разработанный авторами программный модуль позволяет моделировать процесс изменения концентрации фосфатов и может быть полезен для проведения научных и инженерных исследований в области водной экологии и разработки эффективных методов адаптации гидробиоценоза к изменениям водной экосистемы.

Ключевые слова: математическая модель, загрязняющие вещества, фосфаты, мелководный водоем, алгоритм, программный модуль

Финансирование. Исследование выполнено за счет гранта Российского научного фонда № 22-11-00295. https://rscf.ru/project/22-11-00295/

Для цитирования. Лященко Т.В., Чистяков А.Е., Никитина А.В. Моделирование процесса распространения загрязнения фосфатами в водной экосистеме. *Computational Mathematics and Information Technologies*. 2023;7(4):47–53. https://doi.org/10.23947/2587-8999-2023-7-4-47-53

Introduction. Shallow waters are vulnerable ecosystems exposed to various sources of pollution. This is becoming an increasingly serious problem, especially for systems such as the Azov Sea, Tsimlyansk and Rybinsk reservoirs, small lakes, etc. Pollution of shallow waters occurs due to emissions of various harmful, toxic and insufficiently purified substances that can have a negative impact on living organisms and ecosystems of reservoirs. Waste from agricultural production, industry, and transport become permanent sources of pollution of water systems. Mathematical modelling makes it possible to better understand the mechanisms of pollution transfer, changes in their concentrations and the impact on the environment. This, in turn, will help to develop effective measures to prevent and reduce pollution of reservoirs, as well as to assess the effectiveness of actions already taken.

Various pollutants have a wide range of properties characteristic of them, and the methods of their transportation in water systems also differ. Some substances may be soluble in water and evenly distributed in it, while others may accumulate in the form of particles or settle to the bottom of a reservoir. This can cause an uneven distribution of pollutants in the aquatic environment and have a negative impact on living organisms. It is also important to take into account factors related to the biological activity of pollutants. Some substances can undergo biochemical decomposition, which affects their concentration and degree of toxicity. In addition, pollutants can accumulate in living organisms, causing significant harm to them. For example, heavy metals accumulate in the tissues of fish and other aquatic organisms, which can lead to violations of their vital functions and even threaten human health when eating such fish and other aquatic organisms. For effective control and prevention of pollution of reservoirs, it is important to investigate not only the physico-chemical properties of pollutants, but also the parameters of the surrounding aquatic environment, the activity of biological processes and ecological interactions of aquatic organisms.

Phosphates are chemical compounds that affect water quality by stimulating excessive growth of blue-green algae. Although all plants need phosphates for normal growth, the concentration of phosphorus in surface waters should be only 0.02 parts per million. The presence of a high concentration of phosphates makes the water cloudy, it turns green, and has a low oxygen content. The excess amount of phosphates in the water feeds algae, which grow uncontrollably in aquatic ecosystems, produce harmful toxins during decomposition and create an imbalance that leads to the destruction of other forms of life. During flowering, and then the death of microalgae, anaerobic decomposition products are formed, hydrogen sulfide appears and fish starvation occurs. Fig. 1 a demonstrates a dangerous phenomenon — the “blooming of waters” of the Taganrog Bay in the summer, caused by the ingress of biogenic substances (nitrogen, phosphorus, silicon compounds) into the reservoir with the drains of the Don, Kuban, etc. rivers, as well as by settling on the surface of the reservoir from the air. Fig. 1 b demonstrates the same phenomenon in the Tsimlyansk reservoir, Fig. 1 c shows that even at the Rybinsk reservoir located much to the north, at low air temperature, the water turns green. The problem of “blooming” water and interruptions in the water supply of cities cannot be completely solved only by such methods as the introduction of chlorella or silver carp [1, 2]. It is necessary to know where the largest amount of these algae will accumulate (including in order to reduce the cost of methods to combat them). This problem can be solved on the basis of mathematical modelling of the process of spreading pollutants, including the main types of biogens. These include phosphorus, sodium and silicon compounds. The model is based on the assumption that a decrease in the concentration of phosphates occurs, among other things, due to its consumption for the growth of phytoplankton cells.

a) *b)* *c)*

Fig. 1. Aquatic ecosystems exposed to the dangerous phenomenon of "blooming waters":
a — Taganrog Bay of the Azov Sea; *b* — Tsimlyansk reservoir;
c — Rybinsk reservoir

Mathematical modelling of the transport of pollutants in reservoirs is an effective method used in environmental research. This approach makes it possible to study pollution propagation processes more deeply and systematically, predict their potential consequences, and contribute to the development of effective strategies for the management and protection of water resources [3, 4].

Materials and Methods. The mathematical model of transport of pollutants (PS), which makes it possible to assess and predict the impact of various sources of pollution on water quality in a shallow reservoir, has the form:

$$\frac{\partial S_i}{\partial t}+u\frac{\partial S_i}{\partial x}+v\frac{\partial S_i}{\partial y}+(w-w_{gi})\frac{\partial S_i}{\partial z}=\mu_i\Delta S_i+\frac{\partial}{\partial z}\left(\nu_i\frac{\partial S_i}{\partial z}\right)-(k_i+d_i)S_i+\psi_i(x,y,z,t), \quad (1)$$

where S_i is the concentration of the *i*-th impurity, $i=\overline{1,6}$, and 1 is total organic nitrogen (N); 2 is phosphates (PO_4); 3 is phytoplankton; 4 is zooplankton; 5 is dissolved oxygen (O_2); 6 is hydrogen sulfide (H_2S); $\mathbf{U}=(u, v, w)^{\tau}$ is the velocity vector of the water flow; w_{gi} is sedimentation rate; μ_i ,ν_i are the coefficients of turbulent exchange, respectively, in horizontal and vertical directions; k_i is the solubility coefficient for PS, loss — for oxygen and hydrogen sulfide, mortality — for hydrobiont; d_i is the coefficient of reduction of PS due to the eating of blue-green algae (cyanoprokaryotes), reduction due to respiration (for oxygen) and chemical reactions (for oxygen and carbon dioxide), the coefficient of eating away of hydrobionts by representatives of higher trophic levels; ψ_i is the chemical and biological source (drain) [5].

Initial and boundary conditions are added to the system (1), taking into account the type and concentration of PS deposited on the surface of the reservoir from the air environment.

The solution area G of the problem is an enclosed basin bounded by the undisturbed surface of the sea $z = 0$, the bottom $H_0 = H_0(x, y)$ is the depth to the solid surface of the reservoir (excluding sediments). Boundary conditions:

– on the sea surface: $z = -\xi(x, y, t)$: $S_i = \varphi_i(S_i)$, φ_i where are the known functions;

– on the ocean bottom $z = H(x, y)$ for the velocity of flow and adhesion:

$$u = 0,\ v = 0,\ w = 0,\ S_i = 0, \text{ если } \mathbf{U}_\mathbf{n} > 0;\quad \frac{\partial S_i}{\partial \mathbf{n}}=0, \text{ если } \mathbf{U}_\mathbf{n} < 0;\quad \frac{\partial S_i}{\partial z}=-\varepsilon_i S_i,$$

where $\mathbf{n}$ is the vector of the external normal to the surface, ε_i is the absorption coefficient of the *i*-th component by bottom sediments.

In the formulation of the initial boundary value problem for the system , it is sufficient to set the initial conditions for the functions u, v, w, S_i:

$$u(x, y, z, 0) = u_0(x ,y, z);\ v(x, y, z, 0) = v_0(x, y, z);\ w(x, y, z, 0) = w_0(x, y, z);\ S_i = S_{i,0},\ i=\overline{1,6}.$$

The initial model of hydrophysics is solved by the pressure correction method, while the system is divided into two subtasks: the first includes the equations of diffusion, the second of convection and continuity.

The results of the study. Let us consider discrete analogues of the convective (uS'_x) and diffusion transfer $(\mu S'_x)'_x$ operators for the concentration of phosphates S_2, which can be written as follows:

$$(q_0)_{i,j} uS'_x = (q_1)_{i,j} u_{i+1/2,j} \frac{S_{i+1,j} - S_{i,j}}{2h_x} + (q_2)_{i,j} u_{i-1/2,j} \frac{S_{i,j} - S_{i-1,j}}{2h_x}, \tag{2}$$

$$(q_0)_{i,j} (\mu S'_x)'_x = (q_1)_{i,j} \mu_{i+1/2,j} \frac{S_{i+1,j} - S_{i,j}}{h_x^2} - (q_2)_{i,j} \mu_{i-1/2,j} \frac{S_{i,j} - S_{i-1,j}}{h_x^2} - \tag{3}$$

$$- \left| (q_1)_{i,j} - (q_2)_{i,j} \right| \mu_{i,j} \frac{\alpha_x S_{i,j} + \beta_x}{h_x},$$

where q_0, q_1, q_2 are the occupancy coefficients of control areas; α, β are the coefficients in boundary conditions [6].

To determine the approximation error of expressions (2), (3), we define the calculated area. Expression (2) can be considered in the case $(q_1)_{i,j} = (q_2)_{i,j} = 0$, while we will assert that the error of approximation of the resulting expression is equal to the error of the original expression. To determine the approximation error of expression (3), two cases need to be considered: the first case does not take into account the influence of the boundary $(q_1)_{i,j} = (q_2)_{i,j} = 1$, the second one takes into account the influence of the boundary $(q_1)_{i,j} = 1$; $(q_2)_{i,j} = 0$, because the approximation (3) can be written through a linear combination of approximations obtained in the two cases described earlier. Thus, to determine the errors, it is sufficient to investigate the accuracy of the following approximations:

– the discrete analogue of the convective transfer operator in the absence of the influence of the boundary of the region

$$uS'_x = u_{i+1/2,j} \frac{S_{i+1,j} - S_{i,j}}{2h_x} + u_{i-1/2,j} \frac{S_{i,j} - S_{i-1,j}}{2h_x}, \tag{4}$$

– the discrete analog of the diffusion transfer operator in the absence of the influence of the boundary of the domain

$$(\mu S_x)'_x = \mu_{i+1/2,j} \frac{S_{i+1,j} - S_{i,j}}{h_x^2} - \mu_{i-1/2,j} \frac{S_{i,j} - S_{i-1,j}}{h_x^2}. \tag{5}$$

To find the approximation error of expression (4), it is necessary to use the Taylor series expansion relative to the node (i, j) of the values of the functions in the nodes $(i + 1, j)$ and $(i - 1, j)$:

$$S_{i+1,j} = S_{i,j} + (S_{i,j})' h_x + (S_{i,j})'' \frac{h_x^2}{2} + O(h_x^3),$$

$$S_{i-1,j} = S_{i,j} - (S_{i,j})' h_x + (S_{i,j})'' \frac{h_x^2}{2} + O(h_x^3).$$

Taking into account the approximation (4), we write as

$$u\overline{S'_x} = \frac{u_{i+1/2,j} + u_{i-1/2,j}}{2} (S_{i,j})' + \frac{u_{i+1/2,j} - u_{i-1/2,j}}{4} (S_{i,j})'' h_x + O(h_x^2).$$

Taking into account the expression

$$u_{i+1/2,j} + u_{i-1/2,j} = 2u_{i,j} + O(h_x^2), \quad u_{i+1/2,j} - u_{i-1/2,j} = O(h_x),$$

we establish that the discrete analogue of the convective transfer operator will take the form

$$u_{i+1/2,j} \frac{S_{i+1,j} - S_{i,j}}{2h_x} + u_{i-1/2,j} \frac{S_{i,j} - S_{i-1,j}}{2h_x} = u_{i,j} (S_{i,j})' + O(h_x^2).$$

To find the approximation error of expression (5), we use the Taylor series expansion at the node (i, j) of the calculation function S at the nodes $(i + 1, j)$ and $(i - 1, j)$ [7, 8]:

$$S_{i+1,j} = S_{i,j} + (S_{i,j})' h_x + (S_{i,j})'' \frac{h_x^2}{2} + O(h_x^3),$$

$$S_{i-1,j} = S_{i,j} - (S_{i,j})' h_x + (S_{i,j})'' \frac{h_x^2}{2} + O(h_x^3).$$

Taking into account the approximation (5), it will be written as:

$$\left(\mu S'_x\right)'_x = \frac{\mu_{i+1/2,j}-\mu_{i-1/2,j}}{h_x}\left(S_{i,j}\right)' + \frac{\mu_{i+1/2,j}+\mu_{i-1/2,j}}{2}\left(S_{i,j}\right)'' + \left(\mu_{i+1/2,j}-\mu_{i-1/2,j}\right)\left(S_{i,j}\right)''' \frac{h_x}{6} + O\left(h_x^2\right).$$

Taking into account the expressions:

$$\mu_{i+1/2,j}+\mu_{i-1/2,j} = 2\mu_{i,j} + O\left(h_x^2\right),$$

$$\mu_{i+1/2,j}-\mu_{i-1/2,j} = \left(\mu_{i,j}\right)' h_x + O\left(h_x^2\right),$$

we obtain that the discrete analog of the diffusion transfer operator, in the absence of the influence of the boundary of the domain, will take the form [5]:

$$\mu_{i+1/2,j}\frac{S_{i+1,j}-S_{i,j}}{h_x^2} - \mu_{i-1/2,j}\frac{S_{i+1,j,}-S_{i-1,j}}{h_x^2} = \left(\mu_{i,j}\left(S_{i,j}\right)'\right)' + O\left(h_x^3\right).$$

To calculate the relative error of the solution, the formula was used [8]:

$$\delta S = \frac{\Delta S}{|S|} = \frac{\sum_1^N \left|\frac{\partial S(x_1,x_2,...,x_N)}{\partial x_i}\right| \Delta x_i}{\left|S(x_1,x_2,...,x_N)\right|} = \sum_1^N \left|\frac{\partial\left(\ln S(x_1,x_2,...,x_N)\right)}{\partial x_i} x_i\right| \delta x_i .$$

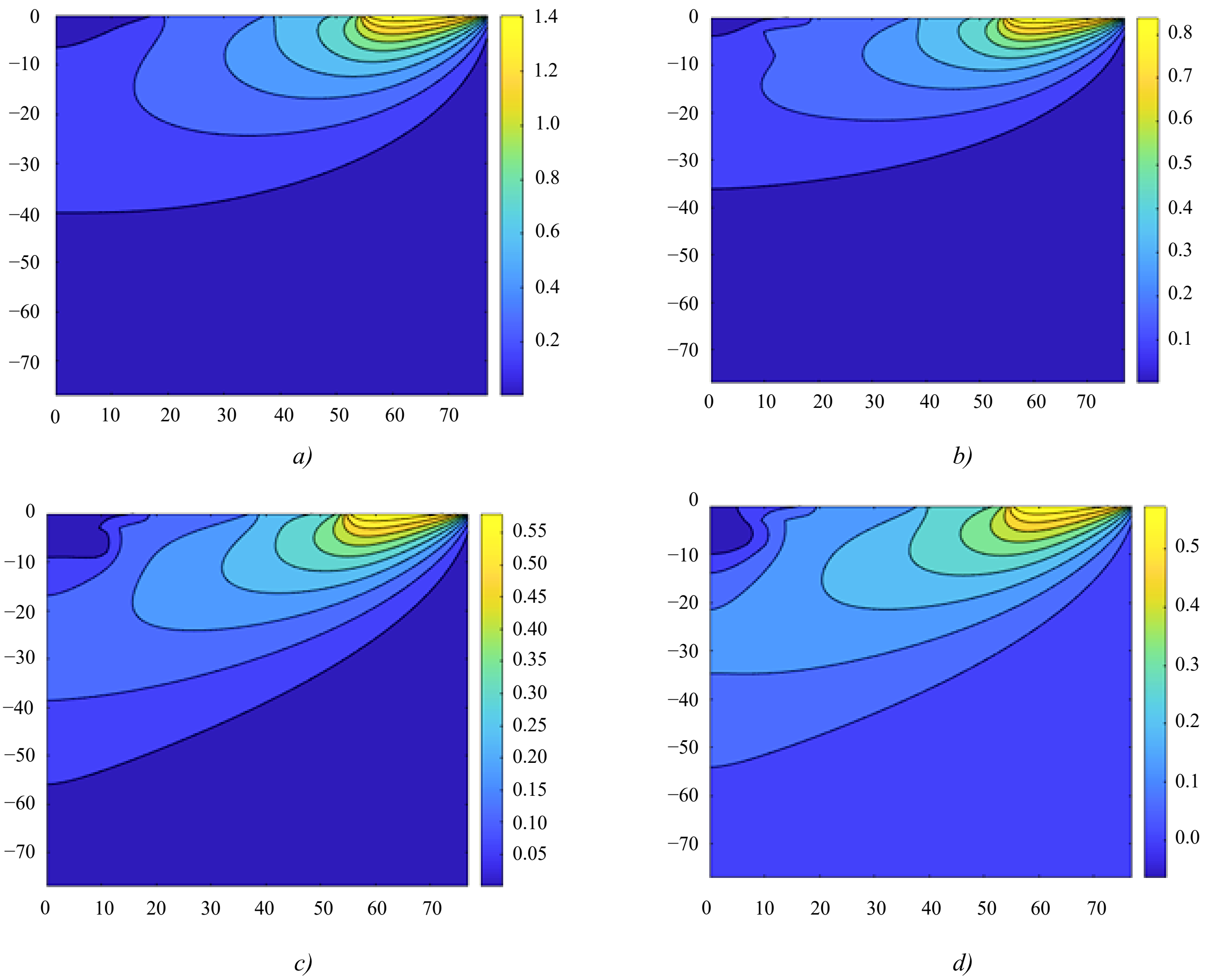

Fig. 2. Distribution of the PS concentration *a* — $t = 5$, $\mu = 0{,}005$, $v = 0{,}1$, $d = 1$; *b* — $t = 20$, $\mu = 0{,}01$, $v = 0{,}1$, $d = 1$; *c* — $t = 60$, $\mu = 0{,}005$, $v = 0{,}1$, $d = 1$; *d* — $t = 100$, $\mu = 0{,}01$, $v = 0{,}1$, $d = 1$

The minimum relative error takes the value 0.002 with an optimal time step of 0.001. During the study, various estimates of the error of the scheme for solving the PS propagation equation were considered, and the time step was optimized. Consider the following scenario: convective transport is practically nonexistent. A constant uniform function of the pollution source on the surface of the area. Type of impurity: heavy uniform; source of contamination $f = 10$. Fig. 2 shows the change in phosphate concentration with a decreasing coefficient of $d = 1$ in a vertical section based on a numerical experiment with the developed software module.

The proposed model makes it possible to study the processes of propagation of various types of pollutants from the surface of the reservoir, taking into account their dissolution and subsidence to the bottom. The results of calculations of the spread of pollutants with different flow rates, diffusion coefficients, intensity of polluting effluents and solubility coefficients of various phosphates are presented. A comparative analysis of the obtained results was carried out, which showed that the developed model adequately reflects the process of transport for. The numerical experiments used a developed software module that implements an algorithm for a mathematical model of the spreading and dissolution of phosphates with different solubility coefficients. This module allows you to predict and visualize the process of transport of pollutants in aquatic ecosystems.

Discussion and Conclusion. An adaptive modified alternately triangular iterative method was used to solve the problem of PS transport in a shallow reservoir obtained during the discretization process. To improve the accuracy of calculations, schemes of increased order of accuracy have been developed, which provide a better approximation of the boundaries of the sections of the medium. The developed model can be used to analyze various scenarios of pollution of aquatic ecosystems and determine the optimal measures to prevent or reduce their pollution. For example, it can help determine the optimal locations for sewage treatment plants or evaluate the effectiveness of measures to reduce pollutant emissions. In addition, the developed algorithm of the software module allows monitoring water pollution in real time, which allows you to quickly respond to possible threats to the environment and take the necessary measures to protect water resources.

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Received 20.10.2023
Revised 27.11.2023
Accepted 04.12.2023

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Claimed contributor-ship:
All authors have made an equivalent contribution to the preparation of the publication.

Conflict of interest statement
The authors do not have any conflict of interest.

All authors have read and approved the final manuscript.

Поступила в редакцию 20.10.2023
Поступила после рецензирования 27.11.2023
Принята к публикации 04.12.2023

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Все авторы прочитали и одобрили окончательный вариант рукописи.