

# INFORMATION TECHNOLOGIES ИНФОРМАЦИОННЫЕ ТЕХНОЛОГИИ



Original article



UDC 004.93'1, 004.932, 004.942

<https://doi.org/10.23947/2587-8999-2023-7-4-54-65>

## Forecasting the Coastal Systems State using Mathematical Modelling Based on Satellite Images

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### Abstract

**Introduction.** Coastal systems of Southern Russia are constantly exposed to biotic, abiotic and anthropogenic factors. In this regard, there is a need to develop non-stationary spatially inhomogeneous interconnected mathematical models that make it possible to reproduce various scenarios for the dynamics of biological and geochemical processes in coastal systems. There is also the problem of the practical use of mathematical modelling, namely its equipping with real input data (boundary, initial conditions, information about source functions). An operational source of field information can be data received from artificial Earth satellites. Therefore, the problem arises of identifying phytoplankton populations in images of reservoirs, which, as a rule, have a spotty structure, with low image contrast relative to the background, as well as determining the boundaries of their location.

**Materials and Methods.** This work is based on the correct application of modern mathematical analysis methods, mathematical physics and functional analysis, the theory of difference schemes, as well as methods for solving grid equations. Biogeochemical processes are described based on convection-diffusion-reaction equations. Linearization of the constructed model is carried out on a time grid with step  $\tau$ . A method for recognizing the boundaries of spotted structures is being developed based on Earth remote sensing data. A combination of methods is considered as image processing algorithms: local binary patterns (LBP) and a two-layer neural network.

**Results.** The developed software-algorithmic tools for space image recognition are presented, based on a combination of methods — local binary patterns (LBP) and neural network technologies, focused on the subsequent input of the obtained initial conditions for the problem of phytoplankton dynamics into a mathematical model. Regarding the necessary mathematical model, a continuous linearized model has been proposed and studied, and on its basis a linearized discrete model of biogeochemical cycles in coastal systems, for which practically acceptable time step values have been established for numerical (predictive) modelling of problems of the dynamics of planktonic populations and biogeochemical cycles, including in the event of death phenomena, which makes it possible to reduce the time of operational forecasting. At the same time, for the constructed discrete model, properties that are practically significant for discrete models are guaranteed to be satisfied: stability, monotonicity and convergence of the difference scheme, which is important for reliable forecasts of adverse and dangerous phenomena.

In the process of work, referring to satellite images, which make it possible to obtain the state of coastal systems with high accuracy, initial conditions are entered into the mathematical (computer) model. The model analyzes satellite image data and determines levels of “pollution”, the formation of extinction zones and other factors that may threaten nature.

**Discussion and Conclusion.** Discussion and conclusions. Using this model, it is possible to predict possible changes in coastal ecosystems and develop strategies to protect them. The results obtained make it possible to significantly reduce the time of forecast calculations (by 20–30 %) and increase the likelihood of early detection of unfavorable and dangerous phenomena, such as intense “blooming” of the aquatic environment and the formation of extinction zones in coastal systems.

**Keywords:** mathematical model, biogeochemical cycles, remote sensing data, neural network-LBP

**Acknowledgements.** The author thanks his scientific supervisor Alexander Ivanovich Sukhinov (corresponding member of the Russian Academy of Sciences, Doctor of Physical and Mathematical Sciences, professor, head of the department of Don State Technical University) for his invaluable help and advice.

**Funding information.** The study was supported by a grant from the Russian Science Foundation (project no. 21–71–20050).

**For citation.** Panasenko N.D. Forecasting the coastal systems state using mathematical modelling based on satellite images. *Computational Mathematics and Information Technologies*. 2023;7(4):54–65. <https://doi.org/10.23947/2587-8999-2023-7-4-54-65>

Научная статья

## Прогноз состояния прибрежных систем с помощью математического моделирования на основе космических снимков

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### Аннотация

**Введение.** Прибрежные системы Юга России постоянно подвергаются воздействию биотических, абиотических и антропогенных факторов. В связи с этим возникает необходимость разработки нестационарных пространственно-неоднородных взаимосвязанных математических моделей, позволяющих «проигрывать» различные сценарии динамики биологических и геохимических процессов в прибрежных системах. Также существует проблема практического использования математического моделирования, а именно его оснащения реальными входными данными (граничными и начальными условиями, информацией о функциях-источниках). Оперативным источником натурной информации могут стать данные, получаемые от искусственных спутников Земли. Поэтому возникает задача идентификации и определения границ расположения фитопланктонных популяций (имеющих, как правило, пятнистую структуру) на снимках водоемов при малом контрасте изображений по отношению к фону.

**Материалы и методы.** Автором используются методы математического анализа, математической физики, функционального анализа, теории разностных схем, а также методов решения сеточных уравнений. Биогеохимические процессы описаны на основе уравнений конвекции-диффузии-реакции; линеаризация построенной модели производится на временной сетке с шагом  $\tau$ . Строится метод распознавания границ пятнистых структур на основе данных дистанционного зондирования Земли. В качестве алгоритмов обработки изображений рассматривается комбинация методов локальных бинарных шаблонов (LBP) и двухслойной нейронной сети.

**Результаты исследования.** Разработан программно-алгоритмический инструментарий распознавания космических снимков, основанный на комбинации методов локальных бинарных шаблонов (LBP) и технологий нейронных сетей, ориентированный на последующий ввод полученных начальных условий для задачи динамики фитопланктона в математическую модель. Предложена и исследована непрерывная линеаризованная математическая модель, а на ее основе — линеаризованная дискретная модель биогеохимических циклов в прибрежных системах. Установлены практически допустимые значения шага по времени при численном (прогностическом) моделировании задач динамики планктонных популяций и биогеохимических циклов, в том числе при возникновении заморных явлений, что позволяет сократить время оперативного прогноза. При этом для построенной дискретной модели гарантированно выполняются практически значимые для дискретных моделей свойства: устойчивость, монотонность и сходимость разностной схемы, что важно для достоверных прогнозов неблагоприятных и опасных явлений. В процессе работы, обращаясь к космическим снимкам, которые позволяют получить состояние прибрежных систем с высокой точностью, вносятся начальные условия в математическую (компьютерную) модель. Модель анализирует данные спутниковых изображений и определяет уровни «загрязнения», образование зон заморов и другие факторы, которые могут угрожать природе.

**Обсуждение и заключение.** С помощью разработанной модели можно предсказывать изменения в прибрежных экосистемах и разрабатывать стратегии по их защите. Полученные результаты позволяют существенно сократить время прогностических расчетов (на 20–30 %) и повысить вероятность заблаговременного обнаружения неблагоприятных и опасных явлений, таких как интенсивное «цветение» водной среды и образование зон заморов в прибрежных системах.

**Ключевые слова:** математическая модель, биогеохимические циклы, данные дистанционного зондирования, нейросеть-LBP

**Благодарности:** автор благодарит своего научного руководителя Сухинова Александра Ивановича (члена-корреспондента РАН, д-ра физ.-мат. наук, профессора, заведующего кафедрой Донского государственного технического университета) за бесценную помощь и советы.

**Финансирование.** Исследование выполнено при поддержке гранта Российского научного фонда (проект № 21–71–20050).

**Для цитирования.** Панасенко Н.Д. Прогноз состояния прибрежных систем с помощью математического моделирования на основе космических снимков. *Computational Mathematics and Information Technologies*. 2023;7(4):54–65. <https://doi.org/10.23947/2587-8999-2023-7-4-54-65>

**Introduction.** Coastal systems play an important role in the ecosystem of our planet, providing conditions for the life of many species of plants and animals. However, due to negative and catastrophic events, coastal systems may be under threat. Here are some excerpts from sources [1, 2]: “... the overfishing in July 2020 in the southeastern sector of the Azov Sea caused significant damage to the reproduction process of commercial fish; extensive zones of hypoxia and hydrogen sulfide contamination occurred in the eastern part of the Azov Sea in 2001; a catastrophic storm in November 2006, storm surges in 2007, 2014; shallowing of the Azov Sea the shores of Taganrog (Rostov region) and the Don River in 2019, 2021, 2022”. Since changes in the systems occur within a few weeks, prompt forecasting of adverse events is required. Therefore, mathematical modeling, in particular based on satellite images, can be a useful tool for predicting the state of coastal systems and evaluating the effectiveness of conservation measures.

**Materials and Methods.** The problem of forecasting the dynamics of phyto- and zooplankton is relevant for marine and coastal systems. On the one hand, they make up more than 95 % of the biomass of marine and coastal systems and are the foundation of the trophic pyramid (the basis of nutrition for its higher levels). On the other hand, an excess of plankton leads to blooming and overseas phenomena, and an extremely large excess of nutrients ceases to be a food base for plankton, being a toxicant for the living environment.

These problems, in relation to the Sea of Azov and similar marine and coastal systems, are reduced to a system of 10 diffusion-convection-reaction equations, with functions of the right parts that depend non-linearly on the desired solutions. Direct decomposition of these problems is impossible, and for the subsequent numerical solution, correct linearization of the corresponding initial boundary value problem on the right sides is required. Despite the large number of works devoted to this problem, some important stages of their research and numerical implementation do not have a satisfactory solution at this time. Among the insufficiently studied problems of constructing mathematical models of phytoplankton dynamics and their application for operational forecasting, it should be noted the development and study of a linear continuous mathematical model of biogeochemical processes approximating the original nonlinear problem, the construction of a discrete analogue for it with the properties of monotony, approximation, stability and convergence, as well as the creation of a program for recognizing the boundaries of plankton populations (boundary contours) on satellite images, having improved characteristics of their identification in conditions of low contrast objects.

This task is computationally time-consuming, since the grid equations obtained as a result of approximation have dimensions from several million to hundreds of millions. Solving real tasks of forecasting biogeochemical processes in an acceptable time (tens of minutes — tens of hours), it is necessary to quickly and reliably recognize remote sensing data — the location and boundaries of plankton populations and other substances.

Figure 1 schematically shows the process of studying the dynamics of marine and coastal water systems. For early decision-making, valid models and data are needed that allow these models to work reliably.

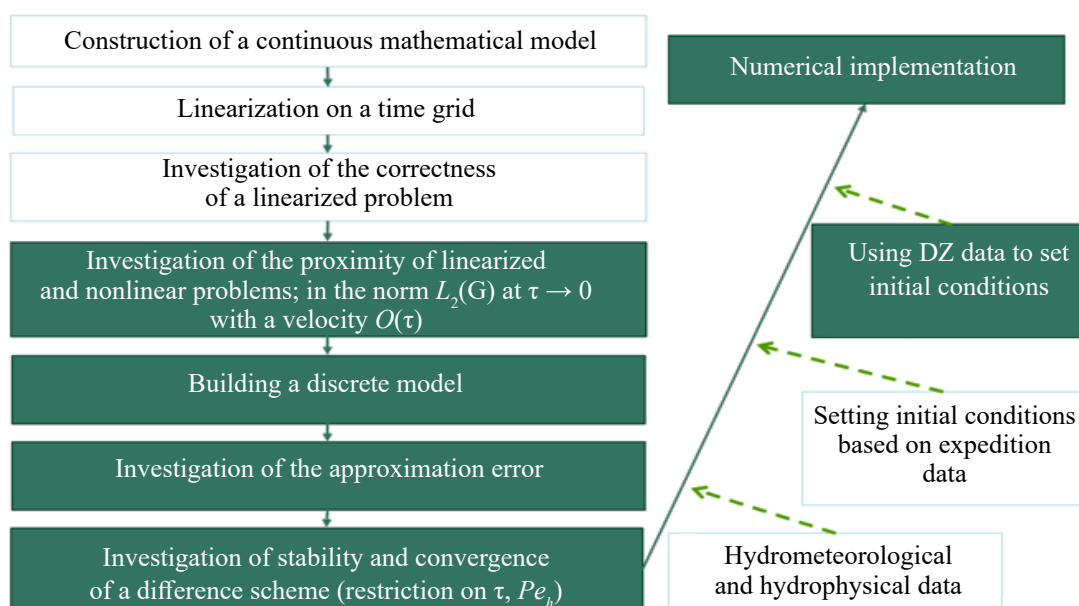


Fig. 1. Research scheme of continuous and discrete mathematical models

## Results

**Object recognition program “neural network-LBP”.** The use of mathematical models requires the presence of real input data (boundary and initial conditions, information about source functions), which make it possible to correctly set initial boundary value problems for systems of nonlinear partial differential equations, as well as to determine various functional dependencies included in the constructed models. In the decision-making process related to dangerous natural phenomena and disasters, up to 50 % of the total computer forecasting time can be occupied by recognizing the situation, namely, determining the location and size of the plankton blooming spot and other initial data.

The available source of natural information for mathematical modelling can be remote sensing data of the Earth. Their recognition and input as initial and boundary conditions is a very time-consuming procedure and requires the development of appropriate algorithms.

In the course of the study, an algorithm was developed for identifying planktonic populations with a complex structure and low contrast (differences in shades of green) of the background and the region — “neural network-LBP”. A detailed description of this algorithm can be found in [3–5].

The software module (based on the algorithm “neural network-LBP”) is included in the research predictive complex (RPC) “Azov3d”, developed at the scientific school of A.I. Sukhinov. It allows you to get initial data for predictive modelling. Fig. 2 presents the results of numerical experiments with a software module, using the example of the Taganrog Bay.

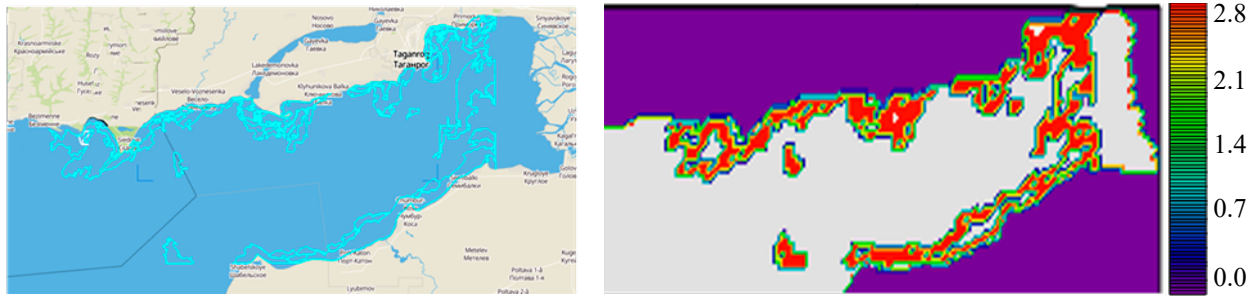


Fig. 2. Determination of the initial modeling of the dynamics of phytoplankton concentrations of RPC “Azov3d”

The data obtained using the neural “network-LBP” software modules and the biogeochemical cycles included in the “Azov3d” RPC make it possible to predict the dynamics of changes in the concentrations of the three most common phytoplankton species and seven biogenic substances in the summer period.

**Mathematical model.** The dynamics of planktonic populations should be considered in connection with the dynamics of the main biogenic substances: phosphates, organic phosphorus in suspension, dissolved phosphorus, dissolved oxygen, nitrates, nitrites, ammonium (ammonium nitrogen), total organic nitrogen, dissolved inorganic silicon (including silica and silicates), hydrogen sulfide (including elemental sulfur).

Let us consider the constructed mathematical model of the dynamics of biogeochemical cycles, including the equations of the dynamics of phytoplankton populations and basic nutrients [5–8]:

$$\frac{\partial q_i}{\partial t} + u \frac{\partial q_i}{\partial x} + v \frac{\partial q_i}{\partial y} + w \frac{\partial q_i}{\partial z} = \text{div}(\vec{k} \cdot \text{grad } q_i) + R_{q_i}, \quad (x, y, z) \in G, \quad 0 < t \leq T, \quad (1)$$

where  $q_i$  is the concentration of the corresponding component numbered  $i$ ,  $i \in M$ ,  $M = \{F_1, F_2, F_3, PO_4, POP, DOP, O_2, NO_3, NO_2, NH_4, N, Si, H_2S\}$ ;  $F_1$  is the concentration of green algae,  $F_2$  is the concentration of blue-green algae and  $F_3$  is the concentration of diatoms.

The biogenic components are listed below:  $PO_4$  means that the component belongs to phosphates,  $POP$  belongs to organic phosphorus in suspension,  $DOP$  belongs to dissolved phosphorus,  $O_2$  belongs to dissolved oxygen,  $NO_3$  belongs to nitrates,  $NO_2$  belongs to nitrites,  $NH_4$  belongs to ammonium (ammonium nitrogen),  $N$  belongs to total organic nitrogen,  $Si$  belongs to dissolved inorganic silicon (including silica and silicates),  $H_2S$  belongs to hydrogen sulfide (including elemental sulfur).

$\vec{V} \equiv (u, v, w)^T$  is three-dimensional velocity vector of the aquatic medium,  $u$ ,  $v$ ,  $w$  are the components of the vector  $\vec{V}$ , directed along the coordinate axes  $Ox$ ,  $Oy$  and  $Oz$  respectively. It is assumed that the axis  $Ox$  is directed to the north,  $Oy$  — to the east,  $Oz$  — vertically down, so that the given coordinate system forms the right triple of vectors. The origin of the coordinate system is located on the undisturbed surface of the water  $\vec{k} = (K_h, K_h, K_v)^T$  is the coefficient of turbulent exchange (turbulent diffusion), where  $K_h$  is the coefficient of turbulent diffusion in each of the coordinate directions  $Ox$  and  $Oy$ , which for simplicity we will consider constant,  $K_v$  is the coefficient of turbulent exchange in the vertical direction  $Oz$ .

Let's formulate a mathematical model in relation to the Taganrog Bay and the Azov Sea. Note that it is described by 10 equations of the form (1), i. e. the diffusion-convection equations of the functions of the right parts  $R_{qi} = R_{qi}(x, y, z, t)$ , depending on the desired solutions, on the temperature of the aqueous medium ( $T_{\text{temp}}$ ) and its salinity ( $S$ ) in accordance with the equations (2)–(14) [8]:

$$R_{Fi} = C_{Fi}(1 - K_{FiR})q_{Fi} - K_{FiD}q_{Fi} - K_{FiE}q_{Fi}, \quad i = \overline{1,3}, \quad (2)$$

$$R_{POP} = \sum_{i=1}^3 S_P K_{FiD} q_{Fi} - K_{PD} q_{POP} - K_{PN} q_{POP}, \quad (3)$$

$$R_{DOP} = \sum_{i=1}^3 S_P K_{FiE} q_{Fi} + K_{PD} q_{POP} - K_{DN} q_{DOP}, \quad (4)$$

$$R_{PO_4} = \sum_{i=1}^3 S_P C_{Fi} (K_{FiR} - 1) q_{Fi} + K_{PN} q_{POP} + K_{DN} q_{DOP}, \quad (5)$$

$$R_{NH_4} = \sum_{i=1}^3 S_N C_{Fi} (K_{FiR} - 1) \frac{f_N^{(2)}(q_{NH_4})}{f_N(q_{NO_3}, q_{NO_2}, q_{NH_4})} q_{Fi} + \sum_{i=1}^3 S_N (K_{FiD} + K_{FiE}) q_{Fi} - K_{42} q_{NH_4}, \quad (6)$$

$$R_{NO_2} = \sum_{i=1}^3 S_N C_{Fi} (K_{FiR} - 1) \frac{f_N^{(1)}(q_{NO_3}, q_{NO_2}, q_{NH_4})}{f_N(q_{NO_3}, q_{NO_2}, q_{NH_4})} \cdot \frac{q_{NO_2}}{q_{NO_2} + q_{NO_3}} q_{Fi} + K_{42} q_{NH_4} - K_{23} q_{NO_2}, \quad (7)$$

$$R_{NO_3} = \sum_{i=1}^3 S_N C_{Fi} (K_{FiR} - 1) \frac{f_N^{(1)}(q_{NO_3}, q_{NO_2}, q_{NH_4})}{f_N(q_{NO_3}, q_{NO_2}, q_{NH_4})} \cdot \frac{q_{NO_3}}{q_{NO_2} + q_{NO_3}} q_{Fi} + K_{23} q_{NO_2}, \quad (8)$$

$$R_{Si} = S_{Si} C_{Fi} (K_{FiR} - 1) q_{Fi} + S_{Si} K_{FiD} q_{Fi}, \quad (9)$$

where  $K_{FiR}$  is the specific rate of respiration of phytoplankton;  $K_{FiD}$  is the specific rate of death of phytoplankton;  $K_{FiE}$  is the specific rate of excretion of phytoplankton;  $K_{PD}$  is the specific rate of autolysis  $POP$ ;  $K_{PN}$  is the phosphatification coefficient  $POP$ ;  $K_{DN}$  is phosphatification coefficient  $DOP$ ;  $K_{42}$  is the specific rate of oxidation of ammonium to nitrites during nitrification;  $K_{23}$  is the specific rate of oxidation of nitrites to nitrates during nitrification;  $S_P, S_N, S_{Si}$  are normalization coefficients between the content of  $N, P, Si$  in organic matter [6].

The growth rate of phytoplankton is determined by the expressions:

$$C_{Fi,2} = K_{NF_{1,2}} f_{T_{\text{temp}}}(T_{\text{temp}}) f_S(S) \min\{f_P(q_{PO_4}), f_N(q_{NO_3}, q_{NO_2}, q_{NH_4})\}, \quad (10)$$

$$C_{Fi,3} = K_{NF_3} f_{T_{\text{temp}}}(T_{\text{temp}}) f_S(S) \min\{f_P(q_{PO_4}), f_N(q_{NO_3}, q_{NO_2}, q_{NH_4}), f_{Si}(q_{Si})\}, \quad (11)$$

where  $C_{Fi}$  is the maximum specific growth rate of phytoplankton.

Functions of the growth rate of hydrobionts dependence on temperature and salinity:

$$f_{T_{\text{temp}}}(T_{\text{temp}}) = \exp(-a_l \{(T_{\text{temp}} - T_{\text{opt}})/T_{\text{opt}}\}^2), \quad l = \overline{1,3}, \quad (12)$$

$$f_S(S) = \exp(-b_l \{(S - S_{\text{opt}})/S_{\text{opt}}\}^2), \quad l = 2,3, \quad (13)$$

$$f_S(S) = \begin{cases} k_s, & \text{для } S \leq S_{\text{opt}}, \\ \exp(-b_1 \{(S - S_{\text{opt}})/S_{\text{opt}}\}^2), & \text{для } S > S_{\text{opt}}, \end{cases} \quad (14)$$

where  $k_s = 1$ ;  $T_{\text{opt}}, S_{\text{opt}}$  are optimal temperature and salinity for a given type of phytoplankton;  $a_l > 0, b_l > 0$  are defined as coefficients of the width of the range of tolerance of phytoplankton to temperature and salinity, respectively.

The boundary and initial conditions for the system of equations are formulated by equations (15)–(17):

$$q_i = 0, \text{ at } \sigma \text{ if } u_n < 0; \quad \frac{\partial q_i}{\partial n} = 0, \text{ at } \sigma, \text{ if } u_n \geq 0; \quad (15)$$

$$\frac{\partial q_i}{\partial z} = 0, \text{ at } \Sigma_o; \quad \frac{\partial q_i}{\partial z} = -\varepsilon_i q_i \text{ at the bottom } \Sigma_H, \quad (16)$$



$$\begin{aligned} q_i(x, y, z, 0) &= q_{0i}(x, y, z), \vec{V}(x, y, z, 0) = \vec{V}_0(x, y, z), t = 0, i \in M, \\ T_{\text{temp}}(x, y, z, 0) &= T_{\text{temp}0}(x, y, z), S(x, y, z, 0) = S_0(x, y, z), (x, y, z) \in \bar{G}, \end{aligned} \quad (17)$$

where  $\epsilon_i$  are non-negative constants;  $i \in M$ ;  $\epsilon_i$  takes into account the lowering of algae to the bottom and their flooding for  $i \in \{F_1, F_2, F_3\}$  and takes into account the absorption of nutrients by bottom sediments for  $i \in \{PO_4, POP, DOP, O_2, NO_3, NO_2, NH_4, N, Si, H_2S\}$ ,  $u_{\vec{n}}$  is the component of the velocity vector of the water flow normal with respect to the boundary surface,  $\vec{n}$  is the vector of the external normal to the boundary surface,  $T_{\text{temp}}$  is the temperature of the aqueous medium,  $S$  is salinity.

Figure 3 graphically shows this process. Note that the right-hand sides of positive constants are supposed to be used in functions.

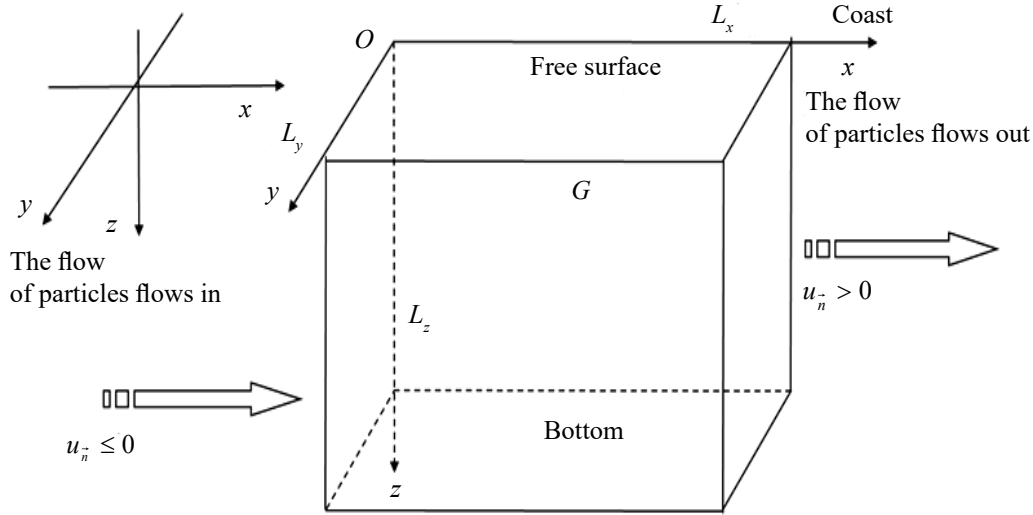


Fig. 3. Schematic representation of the considered area

For clarity, we present the model and the structure of the connections of the considered mathematical model of biological kinetics and geochemical cycles in the form of a block diagram (Fig. 4).

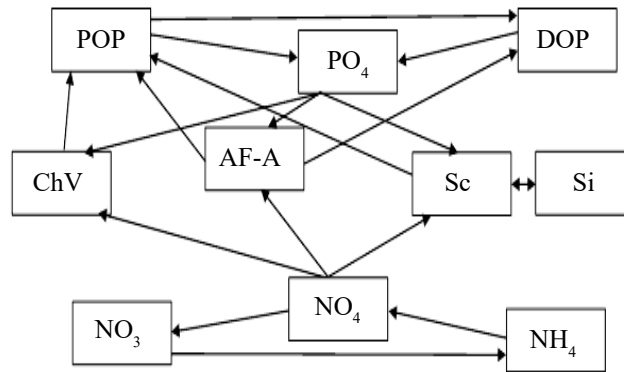


Fig. 4. Structure of the model of biogeochemical transformation of phosphorus, nitrogen and silicon forms

This structure was developed at the P.P. Shirshov Institute of Oceanology of the Russian Academy of Sciences by E.V. Yakushev [9–11], and also improved in the works of A.I. Sukhinov, A.V. Nikitina, Yu.V. Belova [2, 3, 5–8]. Comparison with numerous field data confirmed the validity of the structure of relationships between individual elements of the model.

Further, the existence and uniqueness of the solution of the initial-boundary value problem of the dynamics of biogeochemical cycles, linearized along the right sides, was investigated under natural restrictions on the smoothness of the input data [6–8].

The idea of linearization is that the nonlinear right-hand sides are taken with a delay relative to the simulated time step. It is proposed to implement the linearization of the right parts using a uniform time grid  $\omega_\tau$  in time increments  $\tau$ :

$$\omega_\tau = \{t_n = n\tau, n = 0, 1, \dots, N; N\tau = T\}.$$

At each time step  $t_{n-1} < t < t_n$  we will consider the equations (1) linearized by the functions of the right-hand sides  $R_{q_i}$  ( $i \in M$ ), the solutions of which are functions  $\tilde{q}_i^n$  ( $n = 1, 2, \dots, N$ ) of the form:

$$\frac{\partial \tilde{q}_i^n}{\partial t} + \operatorname{div}(\vec{V} \cdot \tilde{q}_i^n) = \operatorname{div}\left(k_h \frac{\partial \tilde{q}_i^n}{\partial x} + k_h \frac{\partial \tilde{q}_i^n}{\partial y} + k_v \frac{\partial \tilde{q}_i^n}{\partial z}\right) + \tilde{R}_{q_i}^n. \quad (18)$$

After that, we can proceed to the study of the proximity of solutions of the linearized and initial initial boundary value problems [8].

**Investigation of the proximity of linearized and original initial boundary value problems solutions.** Take equations (1) and (18) with the corresponding boundary and initial conditions. Subtracting the corresponding equations (1) from equations (18) and introducing the linearization error function, we obtain a problem that has the form characteristic of a linearized problem, where instead of the functions of the right part there is an error in approximating the right parts of the original continuous problem:

$$\begin{aligned} \frac{\partial z_i^n}{\partial t} + u \frac{\partial z_i^n}{\partial x} + v \frac{\partial z_i^n}{\partial y} + w \frac{\partial z_i^n}{\partial z} - \operatorname{div}(\vec{k} \cdot \operatorname{grad} z_i^n) &= \tilde{R}_{q_i}^n - R_{q_i}^n, \\ i &= 1, \dots, 10, n = 1, \dots, N, (x, y, z) \in G, t_{n-1} < t < t_n. \end{aligned} \quad (19)$$

We add the corresponding initial and boundary conditions to the system.

We will assume that each of the  $q_i$  functions is integrable “with a square” in the domain  $G$ . We introduce a scalar product of functions such that for any selected interval from 0 to  $T$  there exist and are bounded integrals, each of which is a continuously differentiable function of the variable  $t$ .

Let’s introduce the norm:

$$\|\xi\|_{L_2(x,y,z)} = (\xi, \xi)^{\frac{1}{2}} = \left( \iiint_G \xi^2(x, y, z) dx dy dz \right)^{\frac{1}{2}}.$$

Obviously, each such norm is a non-negative function of a variable continuously differentiable by this variable. Multiplying both parts of equation (19) by the linearization error function, and then integrating first over the domain  $G$ , and then over the time variable  $t$ , we obtain an integral equality, which is a quadratic functional:

$$\begin{aligned} \int_{t_{n-1}}^{t_n} \left( \iiint_G z_i^n \cdot \frac{\partial z_i^n}{\partial t} dG \right) dt + \int_{t_{n-1}}^{t_n} \left( \iiint_G z_i^n \cdot \operatorname{div}(\vec{V} \cdot z_i^n) dG \right) dt - \int_{t_{n-1}}^{t_n} \left( \iiint_G z_i^n \cdot \operatorname{div}(\vec{k} \cdot \operatorname{grad} z_i^n) dG \right) dt = \\ = \int_{t_{n-1}}^{t_n} \left( \iiint_G (\tilde{R}_{q_i}^n - R_{q_i}^n) z_i^n dG \right) dt. \end{aligned}$$

Using the Ostrogradsky-Gauss theorem, Green’s formula and Poincare inequalities, we arrive at an estimate (20):

$$\begin{aligned} \|z_1^n(x, y, z, t_n)\|_{L_2(G)}^2 &\leq \|z_1^{n-1}(x, y, z, t_{n-1})\|_{L_2(G)}^2 + \\ &+ 2[K_{NF_1}(1 - K_{F_1R}) - K_{F_1D} - K_{F_1E} - 4\left[k_h\left(\frac{1}{H_x^2} + \frac{1}{H_y^2}\right) + k_{v\min} \frac{1}{H_z^2}\right]] \cdot \int_{t_{n-1}}^{t_n} \left( \iiint_G (z_1^n(x, y, z, t))^2 dG \right) dt, \end{aligned} \quad (20)$$

guaranteeing the proximity (convergence at  $\tau \rightarrow 0$ ) of solutions of a linearized and nonlinear problem. For the substance  $F_1$  (the original function  $q_{F_1} \equiv q_1$ ) in  $L_2(G)$  on a sequence of grids, if the expression in square brackets is non-negative, we obtain:

$$\omega_\tau(\tau \rightarrow 0): \quad \|z_1^n(x, y, z, t_n)\|_{L_2(G)} \leq C_1 \tau, \quad n=1, 2, \dots, N$$

$C_1 = \text{const} > 0$

By a similar method of estimation, it is possible to prove the proximity of the linearized and initial equations for the remaining substances (biogenic components). After the conducted research, the basis for constructing a correct difference scheme appears.

Investigation of the difference scheme for the problem of dynamics of biogeochemical cycles. When constructing a discrete model, we will focus on the linearized chain of initial boundary value problems constructed earlier using equation (18). The construction is carried out in a standard way, however, a feature is the skew-symmetric notation of the convective transfer operator, which guarantees monotonicity when limited to time steps and grid space steps.

In the study of difference schemes, specific features in the assignment of the right parts are taken into account. In the subsequent analysis, restrictions will appear on the value of the permissible time step  $\tau$ , the more stringent the greater the positive value of the right part, which is responsible for the increase in the number (concentration) of the substance for phytoplankton populations. The remaining functions of the right parts ( $i = 4, \dots, 10$ ) provided that biogens enter the area under consideration, are non-positive and therefore an increase in concentrations is not observed in real problems.

Also, for simplicity of presentation, we will consider a parallelepiped as the selected area:

$$G = \{0 < x < L_x, 0 < y < L_y, 0 < z < L_z\}.$$

To set the grid functions of concentrations of plankton populations and biogenic substances, we will construct a uniform space-time grid  $\overline{\omega}_t \times \overline{\omega}$ , and use the template of the difference scheme (control volume) (Fig. 5).

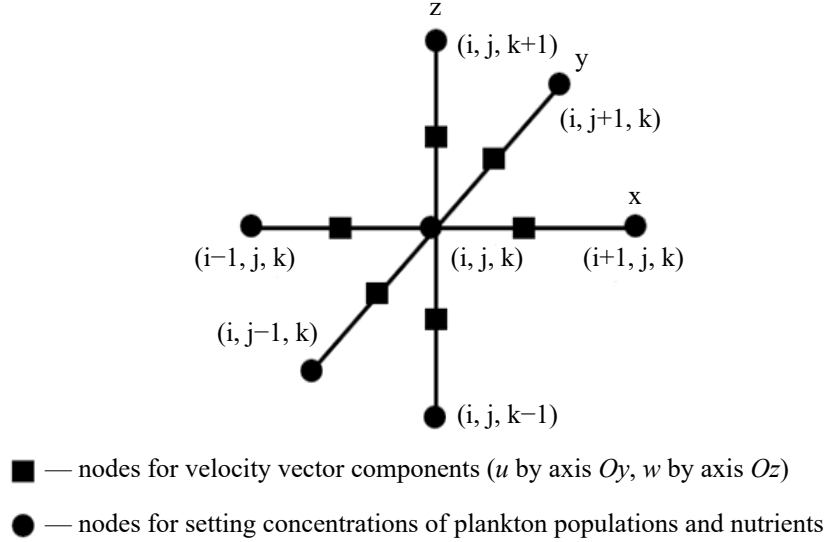


Fig. 5. Schematic designation of the control volume and the scheme template

All unknown functions are set and calculated at the nodes of the template, and the velocity functions, since they are input data that are calculated at the stage of hydrodynamic modeling, are calculated in the middle of the edges of the template of the difference scheme. To correctly set the boundary conditions of the second and third genera in the difference scheme, we will use an expanded spatial difference grid, with a deviation from all nodes in the direction of the normal (perpendicular) outward by a distance of one grid step in the corresponding direction. For brevity, we omit this stage.

Based on the symmetric form of representation of the convective transfer operator, we come to this operator in a skew-symmetric form:  $(x, y, z) \in \omega$ ,  $i = 1, \dots, 10$ :

$$C_0 \overline{q}_i^n \equiv \left( (u_{r+0,5}^n \overline{q}_{i,r+1}^n - u_{r-0,5}^n \overline{q}_{i,r-1}^n) / 2h_x \right) + \left( (v_{r+0,5}^n \overline{q}_{i,r+1}^n - v_{r-0,5}^n \overline{q}_{i,r-1}^n) / 2h_y \right) + \left( (w_{r+0,5}^n \overline{q}_{i,r+1}^n - w_{r-0,5}^n \overline{q}_{i,r-1}^n) / 2h_z \right). \quad (21)$$

And to the type of diffusion transfer operator:

$$Dq_i^n = \left( (k_{h,r+0,5} ((q_{i,r+1}^n - q_i^n) / h_x) - k_{h,r-0,5} ((q_i^n - q_{i,r-1}^n) / h_x)) / h_x \right) + \left( (k_{h,r+0,5} ((q_{i,r+1}^n - q_i^n) / h_y) - k_{h,r-0,5} ((q_i^n - q_{i,r-1}^n) / h_y)) / h_y \right) + \left( (k_{v,r+0,5} ((q_{i,r+1}^n - q_i^n) / h_z) - k_{v,r-0,5} ((q_i^n - q_{i,r-1}^n) / h_z)) / h_z \right). \quad (22)$$

In the direction of the  $Ox$  and  $Oy$  approximations, Neumann boundary conditions (of the second kind) take place. At the bottom of the reservoir ( $Oz$ ), we present the results of approximation of boundary conditions of the third kind. Here and further, for brevity, we will omit them. These approximations are valid for grid nodes and have an approximation error for the corresponding continuous (differential) operators  $O(h^2)$ .

The constructed relations guarantee that the error of approximation of the difference scheme on the grid in norm  $C$  is limited and estimated by the inequality:



$$\max_{1 \leq n \leq N_T} \left\{ \max_{(x,y,z) \in \omega_h} |\Psi(x,y,z,t_n)| \right\} \leq M \cdot (h^2 + \tau), \quad h^2 \equiv h_x^2 + h_y^2 + h_z^2, \quad M \equiv \text{const} > 0. \quad (23)$$

It is assumed that on the expanded grid, which was mentioned above, there is an aquatic environment in horizontal directions and these values can be determined in the hydrodynamic block of the combined model “hydrodynamics, phytoplankton populations and biogens”.

Sufficient conditions for monotonicity and convergence to the solution of a linearized problem. When proving the monotonicity of the difference scheme and its convergence at  $|h| \rightarrow 0$  and  $\tau \rightarrow 0$  we apply the maximum grid principle and its corollary — an estimate of the solution of an inhomogeneous grid equation in norm  $C$ . For the convenience of subsequent calculations, we present a template of the difference scheme (Fig. 6) with the designation of nodes that will be used in the canonical form of writing grid equations of a general form.

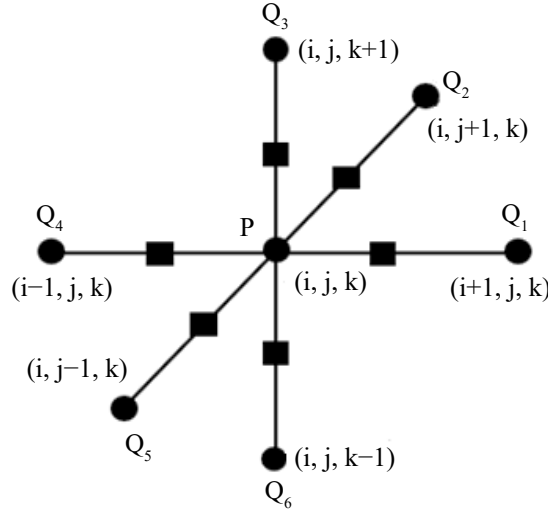


Fig. 6. The template of the difference scheme with the designation of nodes

On the previously constructed spatial grid, we will consider (on the upper time layer) the grid equation in canonical form:

$$A(P) \cdot Y(P) = \sum_{\substack{Q_m \in III'(P) \\ m=1,2,\dots,6}} B(P, Q_m) \cdot Y(Q_m) + F(P), \quad (24)$$

$$P \in \omega, \quad P \equiv (x_i, y_j, z_k), \quad Y(P) \equiv \bar{q}^n(x_i, y_j, z_k).$$

The values of the coefficients, as well as the right parts, will be generated for the internal and boundary nodes separately. It should be noted that the values of the velocity vector component determined in half-integer grid nodes in the hydrodynamic block of the model participate in the formation of all coefficients of the grid equation.

When the condition (inequality) of the Courant and the restriction on the grid number of Pecles are met, we determine the permissible values of time steps of the order of 20 seconds for coastal systems:

$$10^{-4} \leq \frac{|u^n(x_i \pm 0.5h_x, y_j, z_k)| h_x}{k_h(x_i \pm 0.5h_x, y_j, z_k)} \leq 1, \quad \tau \leq \frac{10^2}{6 \cdot 1 \text{ M/c}} \cong 16,6 [\text{c}], \quad (25)$$

$$10^{-4} \leq \frac{|v^n(x_i, y_j \pm 0.5h_y, z_k)| h_y}{k_h(x_i, y_j \pm 0.5h_y, z_k)} \leq 1, \quad \tau \sim 16,6 [\text{c}], \quad (26)$$

$$10^{-4} \leq \frac{|w^n(x_i, y_j, z_k \pm 0.5h_z)| h_z}{k_v(x_i, y_j, z_k \pm 0.5h_z)} \leq 1, \quad \tau \leq \frac{10^{-1}}{6 \cdot 10^{-3} \text{ M/c}} \cong 16,6 [\text{c}]. \quad (27)$$

For further studies of the stability of the difference scheme and convergence, an assessment of the coefficients will be required. We formulate a theorem in relation to the problem under consideration, using the theorem of estimating the solution of an inhomogeneous grid equation:

$$z^n(x_i, y_j, z_k) \equiv z^n(P) = 0, \quad P \in \bar{\omega}^* \setminus \bar{\omega}.$$

For ease of use, we use an extended grid on which the conditions of the theorem are fulfilled.

The theorem. If:

$$D(P) \equiv A(P) - \sum_{\substack{Q_m \in \mathcal{M}^*(P) \\ m=1,2,\dots,6}} B(P, Q_m) > 0, B(P, Q_m) \geq 0, m = 1, 2, \dots, 6,$$

in all nodes of the connected grid  $\bar{\omega}$ , then to solve the problem:

$$A(P)z^n(P) - \sum_{\substack{Q_m \in \mathcal{M}^*(P) \\ m=1,2,\dots,6}} B(P, Q_m)z^n(Q_m) = F(P), -P \in \bar{\omega}, z^n(P) = 0, P \in \Upsilon_n^* \equiv \bar{\omega}^* \setminus \bar{\omega},$$

is fair assessment:

$$\|z^n\|_{C(\bar{\omega})} \leq \left\| \frac{\Psi(x, y, z, t_n)}{D(x, y, z, t_n)} \right\|_{C(\bar{\omega})}.$$

Focusing on the canonical form of the grid equation for the constructed difference scheme in the inner and boundary nodes of the main grid, when the condition (inequality) of the Courant and the restriction on the grid number of Peclet are met, when estimating for  $D(P)$  from below:

$$D(P) \equiv A(P) - \sum_{m=1}^6 B(P, Q_m) \geq \frac{1}{\tau} - \frac{1}{4\tau} - \frac{1}{2\tau} = \frac{1}{4\tau},$$

we guarantee monotony and stability.

Thus, it is possible to return to the error estimation based on the constructed discrete model. When switching from the time layer of the number “ $n-1$ ” to the time layer “ $n$ ” in accordance with the **Theorem**, we obtain:

$$\|z^n\|_{C(\bar{\omega})} \leq \left\| \frac{\Psi(x, y, z, t_n)}{D(x, y, z, t_n)} \right\| \leq 4M(h^2 + \tau)\tau,$$

$$\|z^n\|^T \leq \|z^{N_T}\| \leq 4 \sum_{n=1}^{N_T} M(h^2 + \tau)\tau = 4MN_T\tau(h^2 + \tau) \leq 4MT(h^2 + \tau) \equiv K(h^2 + \tau),$$

where  $K \equiv 4MT$  is constant.

Taking into account the obtained estimate of the approximation error  $O(|h|^2 + \tau)$ . The resulting system of grid equations for all substances (concentrations of phytoplankton, as well as biogenic substances) has a high dimension in real problems.

**On the numerical implementation of the constructed difference scheme.** The system of solved grid equations in operator form can be represented as:

$$\frac{\bar{q}_i^{n+1} - \bar{q}_i^n}{\tau} + C_0 q_i^{n+1} - D q_i^{n+1} - Q_i q_i^{n+1} = R_i^n, n = 0, 1, \dots, N \mp 1, i \in \{F_1, F_2, F_3, 4, \dots, 10\}.$$

Taking into account the special constructed difference scheme, due to the choice of a sufficiently small time step, and it is possible to use the Seidel method ( $D_i \neq D$ ).

Let

$$A_i \equiv A_i^- + D_i + A_i^+,$$

$$(A_i^- + D_i)\bar{q}_i^{n+1, S+1} = A_i^+ \bar{q}_i^{n+1, S} + R_i^n,$$

where the initial approximations on each time layer  $n = 1, 2, \dots, N_T$  are given based on the obtained “final” values of the iterative process for the desired grid function on the previous time layer, and for  $n = 0, n + 1 = 1, \bar{q}_i^{1,0}$  is determined based on the initial conditions for the initial boundary value problem.

The analysis shows that the denominator  $p$  of the geometric progression is included in the estimate:

$$\|z_i^{n+1, S+1}\|_{C(\bar{\omega})} \leq p \|z_i^{n+1, S}\|_{C(\bar{\omega})}.$$

The number of time steps for which these systems need to be solved will range from 103 to 105 iterations. These features of grid problems, especially in the operational forecast of the aquatic ecosystem, may require the use of high-performance computing systems with many thousands of processors, but this topic goes beyond the boundaries of this study, in which parallel algorithms are not considered.

Since the scheme is a system of grid equations with guaranteed diagonal predominance, it becomes possible to use a simple but rather effective Seidel method, which will converge when solving high-dimensional grid equations at a geometric progression rate with a denominator of 0.75–0.8.

**Discussion and Conclusion.** To check the correspondence of the compiled mathematical models of hydrodynamics and biological kinetics, the author used expedition data. The “Azov3d” software module, based on the initial data entered into the system automatically, simulates the dynamics of changes in concentrations of three types of phytoplankton and nutrients in the Taganrog Bay for a time interval of 30 days (06.08.2020–10.09.2020), (Fig. 7).

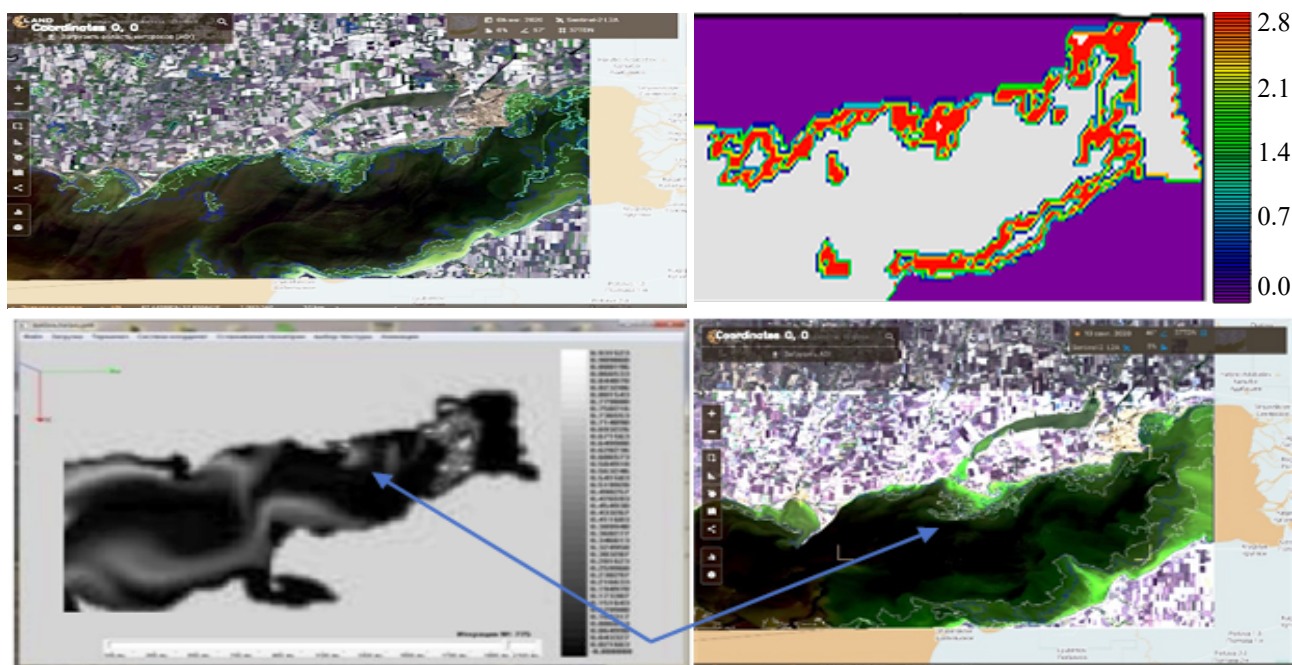


Fig. 7. Modelling the dynamics of phytoplankton concentrations of RPC “Azov3d”

The results of the work of the software module, which is part of the RPC “Azov3d”, clearly illustrate the possibilities of determining contours on the water surface and allow you to trace their change over time in the surface layer of the reservoir. Using this model, it is possible to predict possible changes in coastal ecosystems and develop strategies for their protection. The obtained results make it possible to significantly reduce the time of prognostic calculations (by 20–30 %) and increase the probability of early detection of adverse and dangerous phenomena, such as intensive “blooming” of the aquatic environment and the formation of zamor zones in coastal systems.

Mathematical modelling based on satellite images can be a useful tool for conducting research of coastal systems and developing strategies for the conservation of its ecosystem. However, in order to use this method effectively, it is necessary to continue to improve mathematical models and improve access to data collected by spacecraft.

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**Received** 10.10.2023

**Revised** 30.10.2023

**Accepted** 07.11.2023

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*Conflict of interest statement*

The author declares that there is no conflict of interest.

*The author read and approved the final version of the manuscript.*

**Поступила в редакцию** 10.10.2023

**Поступила после рецензирования** 30.10.2023

**Принята к публикации** 07.11.2023

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*Конфликт интересов*

Автор заявляет об отсутствии конфликта интересов.

*Автор прочитал и одобрил окончательный вариант рукописи.*