Research the phytoplankton dynamics regimes depending on nutrient transformation processes in coastal systems

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Abstract. The paper describes the construction of a three-dimensional mathematical model of biogeochemical processes, considering the salinity and temperature influence on the phytoplankton populations' development. The paper proposes a new difference scheme for solving convection-diffusion-reaction problems at large values of the Peclet grid number ($2<Pe\leq20$), which is a linear combination of the central and the upwind leapfrog difference schemes. The three-layer difference scheme is more accurate than the traditional upwind leapfrog difference scheme for problems where convection prevails over diffusion. The construction of discrete equations for solving the problem of biogeochemical cycles on the basis of the scheme considering the filling of cells is described. The stationary regimes of phytoplankton dynamics problem were researched considering the transformation of phosphorus, nitrogen and silicon forms. Results of software complex, which allows to simulate biogeochemical processes in the Azov Sea, were described. The software package allows to forecast the dynamics of the Azov Sea ecosystem development in the conditions of modern salinization.

1. Introduction

To predict the situation of shallow waters, mathematical models are constructed, considering the unique features of the researched water object – climatic factors and hydrodynamic regimes. Among the papers of Russian scientists devoted to the research and forecast of aquatic ecosystems can be identified the papers of G.I. Marchuk, G.G. Matishov, Yu.A. Dombrovsky, S.V. Berdnikov, Yu.V. Tyutyunov, E.V. Yakushev, V.G. Ilyichev, etc. [1-8] The development of models, software and information systems for monitoring and forecasting the situation of water ecosystems is performed by leading foreign research centers and organizations such as Sweden's Meteorelogical and Hydrological Institute, Center for Water Research, National Oceanic and Atmospheric Administration, Centre for Ecology and Hydrology [9-11].

Examples of existing software systems that allow to simulate hydrodynamic and biogeochemical processes occurring in the researched waters, as well as to predict the situation of water ecosystems, can be: software complex SALMO; complex CHARISMA; software package "MARS3D"; software package CHTDM; CARDINAL; packages for simulation various aerohydrodynamics processes; PHOENICS software; Ecointegrator application.

The existing software do not consider the spatially inhomogeneous motion of the water environment, do not have the necessary accuracy for simulation the vortex structures of currents, are not conservative, do not consider the complex shape of the bottom and shore relief, evaporation, river flows, salinity, temperature and other factors, exhibit instability with significant depth differences and changes in the density of the water environment.

Problems of substances transport are based on the advection-diffusion equations, for solving of which it requires a separate development of qualitative approximations of advective terms. Application of standard finite difference schemes with large values of the grid Peclet number leads to a loss of precision. One way to solve this problem is to reduce the steps on the space-time grid; but this leads to an increase in labor intensity. To solve a class of problems in which advection prevails over diffusion, different schemes are used, for example, upwind leapfrog difference scheme. The upwind leapfrog difference schemes were developed to solve problems of aeroacoustics. In the paper of V.Y. Glotov, V.M. Goloviznin and etc. [12] to solve the transfer problem, it is proposed to use a scheme representing a linear combination of upwind and standard leapfrog difference schemes with weight coefficients. Minimizing the approximation error, it is possible to obtain optimal values of the weight coefficients, as shown in the researches [13-19]. This class of schemes practically does not have a grid viscosity and on its basis, it is possible to model complex flow structures, for example, vortices, quite accurately. At present, many authors use similar schemes to simulate turbulent flows. Employees of leading foreign research organizations, such as Stanford University, Imperial College London, etc., as well as employees of the Institute of computational mathematics of the Russian Academy of Sciences E.M. Volodin, A.V. Glazunov, A.S. Gritsun, N.G. Yakovlev and etc. [20-23] wrote a number of works in which mathematical modeling of climate change, atmospheric processes, hydrodynamic processes is based on vortex-resolving schemes.

2. Problem statement

The model of biogeochemical cycles is based on a system of non-stationary convection-diffusion-reaction equations of parabolic type with nonlinear source functions and lower derivatives, the form of which for each model block F_i as

$$\frac{\partial q_i}{\partial t} + u\frac{\partial q_i}{\partial x} + v\frac{\partial q_i}{\partial y} + w\frac{\partial q_i}{\partial z} = div(k\mathrm{grad}q_i) + R_{q_i}, \quad (1)$$

where q_i is the concentration of i-th component, [мg/l]; i∈M, M={F_1, F_2, F_3, PO_4, POP, DOP, NO_3, NO_2, NH_4, Si}; $\mathbf{V} = \{u, v, w\}$ is the water flow velocity vector, [m/s]; k is the coefficient of turbulent exchange, [m^2/s]; R_{q_i} is the function-source of nutrients, [mg/(l·s)].

For system (1), the initial boundary value problem is posed in the cylindrical region G. We assume that the boundary Σ of the cylindrical domain G is a piecewise smooth surface; $= \Sigma_H \cup \Sigma_o \cup \sigma$, where Σ_H is the surface of the water bottom, Σ_o is the undisturbed surface of the aqueous medium, σ is the lateral (cylindrical) surface. Let $u_{\mathbf{n}}$ be the normal component of the water flow velocity vector with respect to Σ and, $\mathbf{n}$ be the vector of the external normal to Σ. For concentrations q_i we assume at the lateral boundary σ:

$$q_i = 0 \text{ on } \sigma, \text{ if } u_{\mathbf{n}} < 0, i\text{∈M}; \quad (2)$$

$$\frac{\partial q_i}{\partial n} = 0 \text{ on } \sigma, \text{ if } u_{\mathbf{n}} < 0, i\text{∈M}; \quad (3)$$

$$\frac{\partial q_i}{\partial z} = 0 \text{ on } \Sigma_o \text{ the water surface, } i\text{∈M}; \quad (4)$$

$$\frac{\partial q_i}{\partial z} = \varepsilon_{1,i} q_i,\ i \in \{F_1, F_2, F_3\};$$

on the bottom Σ_H:

$$\frac{\partial q_i}{\partial z} = \varepsilon_{2,i} q_i,\ i \in \{PO_4, \mathrm{POP}, \mathrm{DOP}, NO_3, NO_2, NH_4, Si\}, \quad (5)$$

where $\varepsilon_{1,i}$, $\varepsilon_{2,i}$ are non-negative constants; $\varepsilon_{1,i}$, $i \in \{F_1, F_2, F_3\}$ consider the dipping algae to the bottom and their flooding; $\varepsilon_{2,i}$, , $i \in \{PO_4, \mathrm{POP}, \mathrm{DOP}, NO_3, NO_2, NH_4, Si\}$ consider the absorption of nutrients by bottom sediments.

Chemical-biological reactions are described by the following equations:

$$\mathrm{R_{F_i}} = \mathrm{C_{F_i}}\left(1 - \mathrm{K_{F_iR}}\right)\mathrm{q_{F_i}} - \mathrm{R_{F_iD}}\mathrm{q_{F_i}} - \mathrm{K_{F_iE}}\mathrm{q_{F_i}}, \mathrm{i} = \overline{1,3},$$

$$R_{POP} = \sum_{i=1}^{3} s_P K_{F_iD} q_{F_i} - K_{PD} q_{POP} - K_{PN} q_{POP},$$

$$R_{DOP} = \sum_{i=1}^{3} s_P K_{F_iE} q_{F_i} + K_{PD} q_{POP} - K_{DN} q_{DOP},$$

$$R_{PO_4} = \sum_{i=1}^{3} s_P C_{F_i} (K_{F_iR} - 1) q_{F_i} + K_{PN} q_{POP} - K_{DN} q_{DOP},$$

$$R_{NH_4} = \sum_{i=1}^{3} s_N C_{F_i} (K_{F_iR} - 1) \frac{f_N^{(2)}(q_{NH_4})}{f_N(q_{No_3}, q_{No_2}, q_{NH_4})} q_{F_i} + \sum_{i=1}^{3} s_N (K_{F_iD} + K_{F_iE}) q_{F_i} - K_{42} q_{NH_4},$$

$$R_{NO_2} = \sum_{i=1}^{3} s_N C_{F_i} (K_{F_iR} - 1) \frac{f_N^{(1)}(q_{No_3}, q_{No_2}, q_{NH_4})}{f_N(q_{No_3}, q_{No_2}, q_{NH_4})} \cdot \frac{q_{No_2}}{q_{No_3} + q_{No_2}} q_{F_i} + K_{42} q_{NH_4} - K_{23} q_{NO_2},$$

$$R_{NO_3} = \sum_{i=1}^{3} s_N C_{F_i} (K_{F_iR} - 1) \frac{f_N^{(1)}(q_{No_3}, q_{No_2}, q_{NH_4})}{f_N(q_{No_3}, q_{No_2}, q_{NH_4})} \cdot \frac{q_{No_3}}{q_{No_3} + q_{No_2}} q_{F_i} + K_{23} q_{NO_2},$$

$$R_{Si} = s_{Si} C_{F_3} (K_{F_3R} - 1) q_{F_3} + s_{Si} K_{F_3D} q_{F_3}.$$

Here K_{F_iR} is the specific rate of phytoplankton respiration; K_{F_iD} is the specific rate of phytoplankton death; K_{F_iE} is the specific rate of phytoplankton excretion; K_{PD} is the specific rate of autolysis *POP*; K_{PN} is the coefficient of phosphatification *POP*; K_{DN} is the coefficient of phosphatification *DOP*; K_{42} is the specific rate of ammonium oxidation to nitrites during nitrification; K_{23} is the specific rate nitrite oxidation to nitrates during nitrification; s_P, s_N, s_{Si} are normalization coefficients between the content of *N, P, Si* in organic matter.

For the system of equations, it is necessary to set the water flow velocity vector, the salinity and temperature fields, as well as the initial values of the q_i functions at any time:

$$q_i(x, y, z, 0) = q_{0i}(x, y, z), \quad (x, y, z) \in \bar{G}, t = 0, i \in \mathrm{M}, \tag{6}$$
$$\mathbf{V}(x, y, z, 0) = \mathbf{V}_0(x, y, z), T(x, y, z, 0) = T_0(x, y, z), S(x, y, z, 0) = S_0(x, y, z).$$

3. Solution method of model problems

The solution of the substances transport problems based on the advection-diffusion equations requires a separate development of qualitative approximations of advective terms, since the use of standard schemes at large values of the grid Peclet numbers leads to a loss of accuracy.

To solve such problems, a difference scheme is developed, which is a linear combination of the central and the upwind leapfrog difference schemes. The stability and accuracy of the obtained difference scheme are investigated. A discrete analogue of the model of biogeochemical cycles in shallow waters was constructed on the basis of the proposed difference scheme, considering the filling of cells. We introduced a uniform rectangular grid:

$$w_h = \left\{ t^n = n\tau,\ x_i = ih, n = \overline{0, N_t},\ i = \overline{0, N_x},\ \ N_t\tau = T,\ N_x h = l \right\},$$

where n, i are indices; τ is the time step; h is space step; $N_x \times N_t$ time-space grid points; T, l are the time and space areas.

The difference scheme, which is a linear combination of the central and the upwind leapfrog difference schemes, for the approximation of the unsteady one-dimensional convection equation has the form:

$$\frac{q_i^{n+1} - q_i^n}{\tau} + \frac{q_{i-1}^n - q_{i-1}^{n-1}}{2\tau} + u \frac{q_{i+1}^n + 4q_i^n - 5q_{i-1}^n}{4h} = 0. \tag{7}$$

Figure 1 shows the results of numerical solution of the problem of propagation of a perturbation of the “step” type – the advective transfer equation by standard difference schemes and the scheme (7). It is shown that the front “blurs” on several steps in space at approximation by the left difference scheme. At approximation by the central and the upwind leapfrog difference schemes, the solution is unstable, oscillations (entropy perturbations) occur. The scheme (7) gives the most accurate

approximation of the function describing the motion of the perturbation front. Line 1 represents a numerical solution, line 2 – an exact solution.

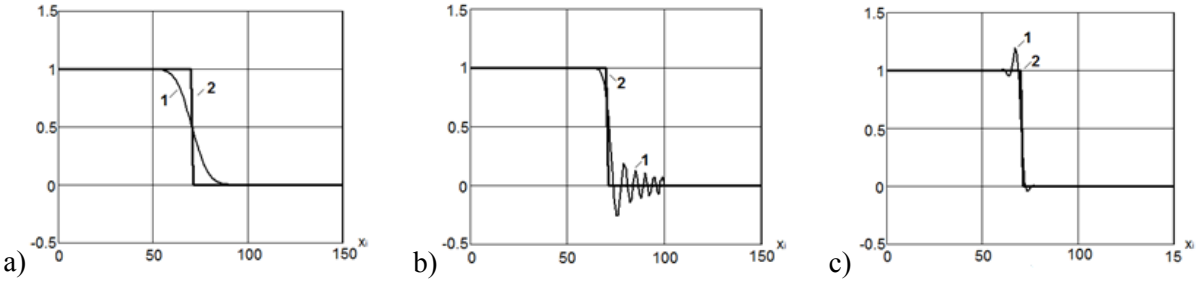

Figure 1. Approximation of the function describing the particle front motion by the left difference scheme (a), the upwind leapfrog difference scheme (b), a new scheme – a linear combination of the central and upwind leapfrog difference schemes (c).

The stability of the difference scheme (7) was investigated by the harmonic method. The scheme is stable at the Courant numbers in the interval [0, 0.75].

The proposed difference scheme, which is a linear combination of the central and upwind leapfrog difference schemes, for the approximation of the non-stationary one-dimensional convection-diffusion equation has the form:

$$\frac{q_i^{n+1}-q_i^n}{\tau}+\frac{q_{i-1}^n-q_{i-1}^{n-1}}{2\tau}+u\frac{q_{i+1}^n+4q_i^n-5q_{i-1}^n}{4h}-3\mu\frac{q_{i+1}^n-2q_i^n+q_{i-1}^n}{2h^2}=0. \quad (8)$$

Figure 2 shows the results of the numerical solution of the problem of propagation of the perturbation of the type “step” – the convection-diffusion equation by the scheme (8) at different values of the grid Peclet number (Pe=2, Pe=25, Pe→∞). It is shown that the scheme (8) provides the more accurate approximation compared to the left difference scheme at large values of the grid Peclet number (Pe>2).

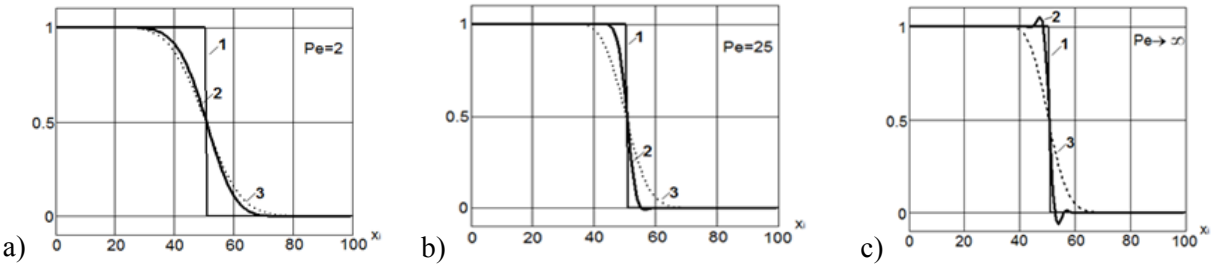

Figure 2. Graphs 1 – the function describing the particle front motion; 2 – the approximate solution using the proposed difference scheme; 3 – the approximate solution using the left difference scheme for the values of the grid Peclet numbers: (a) Pe=2, (b) Pe=25, (c) Pe→∞.

The research of the approximation error of the proposed difference scheme was performed with the help of Fourier series. It is shown that this scheme approximates the convective transport operator with the third order of accuracy in space. It can be concluded that the scheme (8), which is a linear combination of the central and the upwind leapfrog difference schemes, is effective at solving the convection-diffusion problems, in which the convective transport prevails over the diffusion and the values of the grid Peclet number are in the range 2<Pe<20.

On the example of solving the model unsteady two-dimensional convection-diffusion problem in the limiting case ($Pe\to\infty$), it is shown that the error of numerical solution of model problem on the basis of the proposed difference scheme is 2.248 times less than the error at solving with the help of the upwind leapfrog difference scheme.

As a result of the analysis of iterative methods, an adaptive modified alternately triangular iterative method was used to solve the problem, since it requires the least number of iterations for a given accuracy at solving problems with a skew-symmetric operator. Two- and three-layer iterative schemes are also compared. It is shown that three-layer iterative methods converge significantly faster than

two-layer ones. It is also proved that a four-layer iterative scheme for solving grid equations transforms to a three-layer one, and therefore has no advantages.

The case of spatially uniform distribution of substances (phytoplankton, forms of phosphorus, nitrogen and silicon) is considered to clarify the parameters of the system and determine the initial concentrations. The system of ordinary differential equations was solved, and the values of parameters and concentrations at which stationary regimes occur were determined under the assumption that the development of phytoplankton is limited by a single nutrient element.

4. Program complex and results of experimental researches

The developed software complex was designed to construct three-dimensional fields of phytoplankton concentrations and nutrients-biochemical compounds of phosphorus, nitrogen and silicon, as well as to forecast the dynamics of the development of ecosystems of shallow waters on the example of the Azov Sea at increasing the salinity level.

The program considers factors and processes such as Coriolis force, turbulent exchange, complex geometry of the bottom and coastline, evaporation, river flows, wind currents and friction on the bottom. The computational domain corresponds to the physical dimensions of the Azov Sea: the length is 355 km; the width is 233 km; the step across the space in the horizontal direction is 1000 m; the time interval is 30 days. As a result of the numerical experiment, we obtained a picture of the distribution of concentrations of three species of phytoplankton (green, blue-green and diatoms), phosphorus, nitrogen and silicon compounds. Figures 3-12 show the effect of salinity and temperature on the development of three species of phytoplankton, the uptake of phosphates and nitrogen forms by phytoplankton, the transition of phosphorus and nitrogen forms from one to another, and the uptake of silicon by diatoms. The figures show that at this level of salinity in the Taganrog Bay dominated by green and blue-green algae (salinity 0-9‰), and in the main part of the Azov Sea – diatoms (salinity 9-12‰), which coincides with the natural data.

From 2007 to the present, there is salinization of the Azov Sea. This is due to the decrease of the Don River flow in 35.6% compared to the 1998-2006. Decrease of flow directly affects nutrient concentrations, which in turn depends on the development of phytoplankton in the Azov Sea and especially in the Taganrog Bay. Also, the salinization of the sea affects the change in the species composition of biota; freshwater species are displaced by marine ones.

On the basis of the developed software complex, the predictive simulation of the dynamics of changes in the concentration of phytoplankton and nutrients populations in the Azov Sea over time with an increase in sea salinity has been performed.

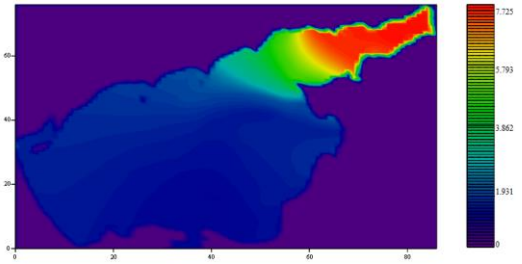

Figure 3. Distribution of the *Chlorella vulgaris* (green algae) concentration.

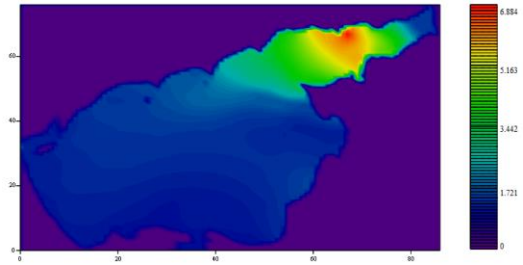

Figure 4. Distribution of the *Aphanizomenon flos-aquae* (blue-green algae) concentration.

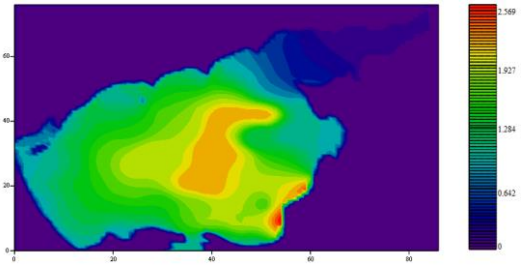

Figure 5. Distribution of the *Sceletonema costatum* (diatoms) concentration.

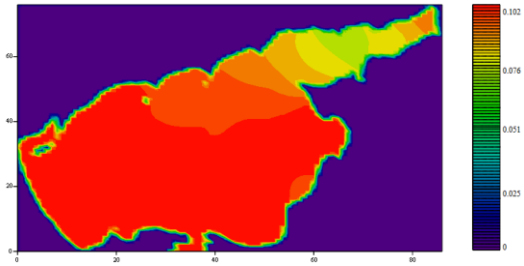

Figure 6. Distribution of phosphate concentration.

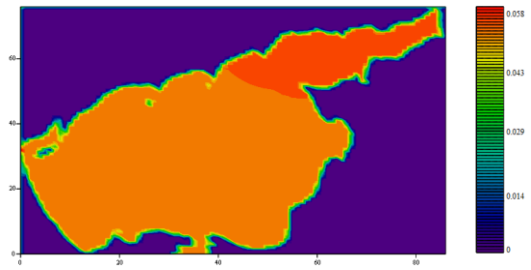

Figure 7. Distribution of suspended organic phosphorus concentration.

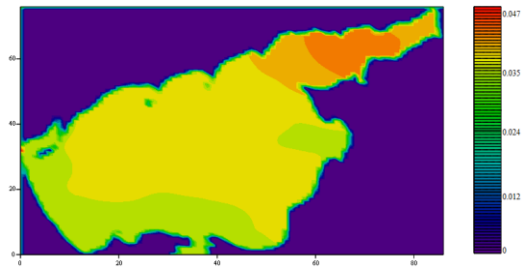

Figure 8. Distribution of dissolved organic phosphorus concentration.

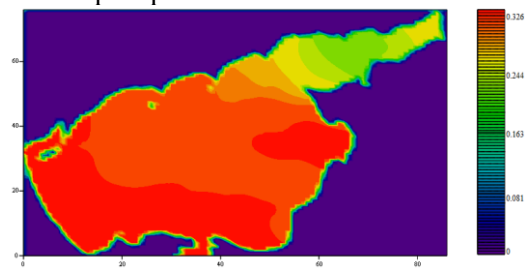

Figure 9. Distribution of nitrate concentration.

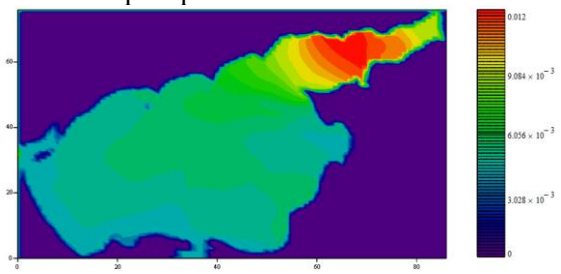

Figure 10. Distribution of nitrite concentration.

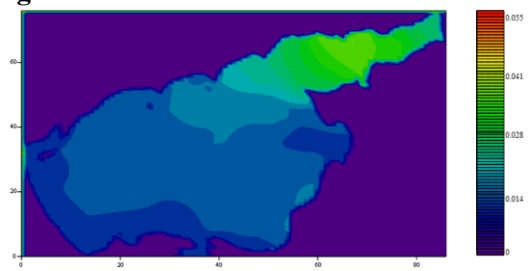

Figure 11. Distribution of ammonium concentration.

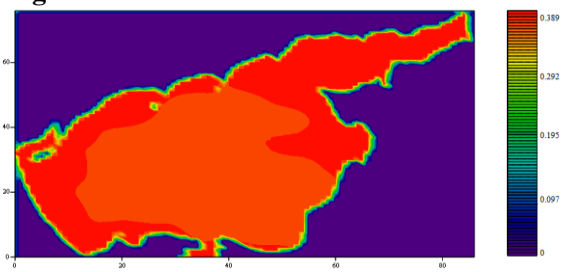

Figure 12. Distribution of dissolved inorganic silicon concentration.

It is shown that at increasing the salinity level, the green and blue-green algae populations develop in the area closer to the mouth of the Don, in the main part of the Azov Sea. The diatom concentration increases, and they penetrated into the Taganrog Bay.

5. Conclusion

Nonstationary spatially inhomogeneous models of biogeochemical cycles describing changes in concentrations of major nutrients (phosphorus, nitrogen and silicon), phytoplankton populations (blue-green (*Aphanizomenon flos-aquae*), green (*Chlorella Vulgaris*) and diatom (*Sceletonema costatum*) algae are developed taking into account the advective and microturbulent transport of water environment, effluents and sources at the boundary, uneven temperature distribution and salinity.

The developed model is an initial-boundary problem for ten diffusion-convection-reaction equations on the time grid. The linearization of nonlinear functions of sources was performed for developed model; the sufficient conditions for the uniqueness of solution of initial-boundary problems interconnected by initial and final conditions were obtained.

Difference schemes based on improved discretization of advective terms of linearized initial-boundary problems on the spatial grid were developed on the basis of linear combinations of the upwind leapfrog and central difference schemes. These schemes have better accuracy and increased margin of stability (applicable in a larger range of grid Peclet numbers) compared to the traditional difference schemes.

Software package has been developed that numerically implements non-stationary spatially inhomogeneous models of biogeochemical cycles describing changes in the concentrations of major nutrients (phosphorus, nitrogen and silicon), phytoplankton populations, considering advective and

microturbulent movement of the aquatic environment, effluents and sources at the boundary, uneven distribution of temperature and salinity.

The prognostic calculations of the main phytoplankton population distribution and nutrient concentrations in relation to the Azov Sea taking into account changes in salinity (salinization) were performed. Results of Earth satellite sensing data were used as input data, as well as the long-term average data about distribution of concentrations of major substances, temperatures and salinity by season. The simulation results are consistent with available observational data.

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