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Perspective Article

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Application of Methods of Observational Data Assimilation to Model the Spread of Pollutants in a Reservoir and Manage Sustainable Development

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Abstract

Introduction. Mathematical models and methods are widely used to study natural phenomena, replacing more expensive field experiments. However, one of the main challenges in modeling processes in complex systems is the lack of available input data and difficulty in selecting model parameters. The use of observational data assimilation methods is one of the ways to provide mathematical models with input data and parameter values. The aim of this study was to predict the development of complex natural systems under conditions of pollution using mathematical modeling techniques. To achieve this, several tasks were completed: a method for assimilating observational data was selected, a mathematical model for biological kinetics was updated, it was integrated with a hydrodynamic model, and a software package was developed. The significance of the work lies in the to the implementation of a model of the dynamics of phytoplankton populations (eutrophication) of the Azov Sea in the presence of pollutants, based on the use of variational methods for assimilating data obtained during expeditionary research.

Materials and Methods. The spread of pollutants was modeled using a three-dimensional mathematical model based on a system of convection — diffusion — reaction equations. The vector of movement of the aquatic environment was the input data for the model. The components of the current velocity vector in the coastal system were calculated using a mathematical model of hydrodynamics, based on three equations of motion and the equation of continuity. The software package developed based on these models received full-scale data collected during expeditionary research as input, and allowed us to refine the model of pollution in the aquatic environment and biota using variational methods for data assimilation.

Results. A short-term forecast for the spread of pollutants at the outlet of the Taganrog Bay was developed. The conducted computational experiment reflected the dynamics of pollutant spread from sources of contamination over a period of 3 to 12 days.

Discussion and Conclusion. The variational methods of assimilating observational data discussed in this study allow for the refinement and supplementation of mathematical models of phytoplankton population dynamics and pollutant spread. The software based on these mathematical models enables the creation of short- and medium-term forecasts for the spread of harmful substances, assessment of their impact on the growth of major phytoplankton species in the Azov Sea, and determination of strategies for sustainable development management.

Keywords: eutrophication model, hydrodynamics model, variational methods, dangerous phenomena, assimilation of observational data

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Статья-перспектива

Применение методов усвоения данных наблюдений для моделирования распространения загрязняющих веществ в водоеме и управления устойчивым развитием

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Аннотация
Введение. Математические модели и методы повсеместно используются для исследования природных объектов, заменяя более дорогие натурные эксперименты. Одними из трудностей, возникающих при моделировании процессов в сложных системах, являются наличие входных данных и подбор параметров модели. Применение методов усвоения данных наблюдений является одним из способов оснащения математических моделей входными данными и значениями параметров. Цель настоящего исследования состоит в прогнозировании на основе методов математического моделирования развития сложных природных систем в условиях загрязнения вредными веществами. Для достижения цели были решены следующие задачи: выбран метод усвоения данных наблюдений, актуализирована математическая модель биологической кинетики, данная модель скомплексирована с моделью гидродинамики, разработан программный комплекс. Актуальность работы заключается в применении нового подхода к реализации модели динамики фитопланктонных популяций (эвтрофикации) Азовского моря при наличии загрязняющих примесей, основанного на применении вариационных методов усвоения данных, полученных в ходе экспедиционных исследований.
Материалы и методы. Распространение загрязняющих веществ моделируется на основе трехмерной математической модели, основанной на системе уравнений конвекции — диффузии — реакции. На входе модели подается вектор движения водной среды. Составляющие вектора скорости течений в прибрежной системе рассчитываются на основе математической модели гидродинамики, базирующейся на трех уравнениях движения и уравнении неразрывности. Разработанный на основе описанных моделей программный комплекс получает на входе натурные данные, собранные в ходе экспедиционных исследований, и позволяет уточнять модель загрязнения водной среды и биоты благодаря применению вариационных методов усвоения данных.
Результаты исследования. Построен краткосрочный прогноз распространения загрязняющих веществ на выходе из Таганрогского залива. Проведенный вычислительный эксперимент отражает динамику распространения загрязняющих веществ от источников заражения на временном интервале от 3 до 12 дней.
Обсуждение и заключение. Рассмотренные в данном исследовании вариационные методы усвоения данных наблюдений позволяют уточнять и дополнять математические модели динамики фитопланктонных популяций и распространения загрязняющих веществ. Программное обеспечение, основанное на описанных в данной работе математических моделях, дает возможность строить кратко- и среднесрочные прогнозы распространения вредных примесей, оценивать их влияние на развитие основных видов фитопланктонных популяций в Азовском море и определять стратегии управления устойчивым развитием.

Ключевые слова: модель эвтрофикации, модель гидродинамики, вариационные методы, опасные явления, усвоение данных наблюдений

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Introduction. Mathematical models and methods have been successfully used for decades in conducting research in various fields of science and engineering. These models provide fast, convenient, and relatively inexpensive tools for studying and predicting processes in complex natural systems, compared to expeditions and field experiments. They are used to solve a wide range of scientific and practical problems, such as predictive modeling of siltation of shipping lanes, which is important for safe navigation, as well as predicting the consequences of emergencies and man-made disasters. An example is the severe storm on November 11, 2007 in the Azov-Black Sea basin, as a result of which more than 20 ships were wrecked, and the Kerch Strait area became the site of an environmental disaster. Several tons of fuel oil and sulfur got into the water, as a result of which the coastline and sediment layer were contaminated with petroleum compounds. Its consequences were observed for several more years. Another example of adverse processes is the transport of bottom materials from the mouth of the Don River to the Taganrog Bay, which affects the habitats of aquatic organisms, promotes intensive eutrophication and leads to the reproduction of *Chironomidae Newman*.

According to Decree of the Government of the Russian Federation No. 2451 dated December 31, 2020[1], researchers, decision makers, and representatives of water protection services have only four hours from the moment of detection or from the moment of receipt of information about a spill in a reservoir to calculate changes in the concentration of oil and petroleum products and their localization. According to the above and other regulatory documents adopted by the Government of the Russian Federation, responsible persons and structures must make a decision and take actions to eliminate a dangerous environmental situation of a natural and man-made nature within a few hours or days. Based on this, the time for making forecasts and scenarios for the development of an emergency situation is limited. This requirement determines the relevance of developing a set of mathematical models of hydrodynamics and hydrobiology that would take into account the features of coastal systems (the effect of winds on the structure of currents, the Coriolis force, the complex geometry of the computational domain, turbulent exchange, evaporation, wind-driven effects, river flows, etc.) and make it possible to obtain forecasts in a minimum time.

When forecasting the development of natural systems and describing a real physical phenomenon through mathematical modeling, it is not enough to simply construct a function of the process state. The use of conjugate problems for mathematical models and algorithms based on variational principles can increase the accuracy of solutions. These principles allow us to establish a connection between the model and field data [1]. This methodology is effective for solving applied problems, including computationally intensive tasks, such as variational and optimization problems in mathematical and nuclear physics [2]. G.I. Marchuk and his colleagues used conjugate equations [3], which made it possible to improve the efficiency of solving problems of aero- and hydrophysics for the atmosphere and deep-water reservoirs. The theory of building conjugate operators for linear and nonlinear models has also been improved [4].

A variational approach to solving combined direct and conjugate problems using assimilation methods has improved the relationship between mathematical models and field data. Methods of data assimilation, which have been developing since the 1960s, are based on the construction of inverse and optimization problems using two approaches: the classical Lagrange variational principle using conjugate problems [4] and optimization methods such as weighted least squares [5].

The assimilation of observational data is a tool that can significantly improve the accuracy of predictive modeling of natural processes. It has long been successfully used by the scientific community [6]. Here, the urgent task is to develop new methods that would significantly reduce the calculation time.

Materials and Methods. When building models for predicting natural phenomena and processes, one of the main problems was the correspondence of the solution obtained using a mathematical model to the real process occurring in the natural system and reducing the percentage of uncertainties.

When constructing mathematical models of hydrodynamic and hydrobiological processes, information about the initial conditions and parameters of the model was required, which could be obtained using observational data. Thus, when constructing predictive scenarios of natural or man-made emergencies, it was very important to assess the adequacy of the mathematical model itself. The next stage of modeling included checking the correctness and stability of the task. The study of a mathematical model at a continuous level involved the study of the influence of input data on the solution of a model problem. The perturbation of the right-hand sides of the equation used or the system of partial differential equations in the Cauchy problem under consideration made it possible, with known operators, to investigate the properties of the constructed mathematical model. The study of stationary and special points of a continuous function or several functions — solutions to the task, for example, the concentration of one or more pollutants in the aquatic environment, allowed us to develop scenarios, from pessimistic to optimistic ones, in order to develop measures for effective management of a complex aquatic ecosystem.

For the first time, the method of polynomial interpolation of data from a constantly replenished database of environmental measurements in the two-dimensional case was used to analyze field data. Areas of influence have been identified for observations. When implementing the algorithm for calculating the current background, the data from the previously received forecast was used as input information.

[1] *On Approval of the Rules for the Organization of Measures to Prevent and Eliminate Oil and Petroleum Product Spills on the Territory of the Russian Federation, with the Exception of the Internal Sea Waters of the Russian Federation and the Territorial Sea of the Russian Federation.* Decree of the Government of the Russian Federation No. 2451 dated 31.12.2020. URL: https://docs.cntd.ru/document/573319208 (accessed: 21.05.2024). (In Russ.)

The OI (Optimal Interpolation) method has brought a new level of sophistication to the methodology for solving problems of data assimilation. This method was based on statistical interpolation techniques.

The next stage in the development of the considered methods was associated with the development and implementation of variational methods, including the theory of optimal control. These methods were based on minimizing the functionality built in a special way, with the help of which a connection was established between solutions and observations (field measurements, expedition data, GIS geographic information system databases).

This theory and methods were widely used in the implementation of the tasks of meteorology [5] and dynamic oceanography [7]. In the process of minimizing the constructed functional, it was necessary to calculate its gradient, for which conjugate equations were successfully applied, which was described in [8, 9].

Model of the Dynamics of Phytoplankton Populations. A mathematical model of the dynamics of phytoplankton populations describes the process of active growth of microalgae in the presence of a sufficient number of biogenic elements. If the development of phytoplankton populations becomes too intense, it is referred to as the process of eutrophication. The causes of eutrophication can be both natural (climatic changes) and anthropogenic in nature (the entry of a significant amount of nutrients into the reservoir from river drains). System C_i contains the concentration values of the i-th substance [10, 11]:

$$\frac{\partial C_k}{\partial t}+\frac{\partial (uC_k)}{\partial x}+\frac{\partial (vC_k)}{\partial y}+\frac{\partial ((w+w_{C,k})C_k)}{\partial z}=\frac{\partial}{\partial x}\left(\mu_k\frac{\partial C_k}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu_k\frac{\partial C_k}{\partial y}\right)+\frac{\partial}{\partial z}\left(\nu_k\frac{\partial C_k}{\partial z}\right)+\psi_k, \qquad (1)$$

where $\mathbf{u}=\{u, v, w\}$ — velocity vector of the medium (water flow); $w_{C,k}$ — gravitational deposition of the k-th component, if it is in a suspended state; μ_k, ν_k — horizontal and vertical components of the coefficient of turbulent exchange for the k-th componen; ψ_k — chemical-biological source (drain) or term describing aggregation (sticking-splitting), if the corresponding component is a suspension, index k indicates the type of substance, $k=\overline{1,15}$:

1 — hydrogen sulfide (H_2S);
2 — element sulfur S;
3 — thiosulfates (and sulfites);
4 — sulfates (SO_4);
5 — total organic nitrogen (N);
6 — ammonium (NH_4 — ammonium nitrogen);
7 — nitrates (NO_3);
8 — nitrites (NO_2);
9 — phytoplankton;
10 — zooplankton;
11 — silicates (SiO_3 — metasilicate; SiO_4 — orthosilicate);
12 — dissolved oxygen (O_2);
13 — ferrum (Fe^{2+});
14 — phosphates (PO_4);
15 — silicic acid (H_2SiO_4, H_2SiO_3 — orthosilicic and metasilicic acids, respectively);
16 — microplastic.

System (1) contains equations that can be attributed to the convection — diffusion — reaction type. As a computational domain, let us consider enclosed basin G. Undisturbed surface of basin Σ_0 is bounded from above by G, $\Sigma_b=\Sigma_b(x, y)$ — bottom surface from below, σ — cylindrical surface limits G from the side. We will use the following notation: $\Sigma=\Sigma_0\cup\sigma\cup\Sigma_b$ — piecewise smooth boundary of domain G, time interval $0<t\le T_0$. We assume that $\mathbf{n}$ and $\mathbf{u_n}$ — vector of external normal and is the normal component $\mathbf{u}$ to surface Σ.

We consider that initial conditions of system (1) are as follows: $C_k|_{t=0}=C_{k0}(x, y, z)$, $k=\overline{1,15}$.

We combine (1) with the following combined boundary conditions:

for σ: if $\mathbf{u_n}<0$, then $C_k=0$; if $\mathbf{u_n}\ge 0$, then $\frac{\partial C_k}{\partial \mathbf{n}}=0$; for Σ_0: $\frac{\partial C_k}{\partial z}=g(C_k)$; at the bottom Σ_b: $\frac{\partial C_k}{\partial z}=-\varepsilon_k C_k$, $k=\overline{1,16}$, we define ε_k as the coefficient of absorption of the k-th impurity by bottom sediments.

When there is no wind, especially in summer, almost anaerobic conditions may occur in the bottom layers of shallow reservoirs, such as, for example, the Azov Sea, the Taganrog Bay, and the Gelendzhik Bay. The reduction of water-saturated surface sludge entails the release of iron, phosphates, sulfates, manganese, ammonium and silicates, as well as organic compounds into the solution. Complexed models of type (1) (developed by the team of authors the model of hydrodynamics [12]) were used to study the mechanisms of manganese oxidation and reduction, NH_4 assimilation, nitrification, nitrate reduction (denitrification), ammonification, H_2S oxidation, sulfate reduction, etc. Experiments with model (1) made it possible to study biogenic and oxygen regimes of the coastal system, to analyze the mechanism of formation due to anthropogenic eutrophication of marine phenomena of fish and other aquatic organisms.

Variational Approach for a Three-Dimensional Spatial Mathematical Model of Water Eutrophication. Let us write down mathematical model (1) for the computational domain (the Azov Sea) in the form of an operator equation:

$$L(C,\mathbf{Y}) \equiv D\frac{\partial C}{\partial t} + J(C,\mathbf{Y}) - \boldsymbol{\psi} - \mathbf{r} = 0, \tag{2}$$

we define **C** as a vector function of the state of the studied aquatic ecosystem $\mathbf{C} = \left\{C_k(\mathbf{x},t), k = \overline{1,16}\right\}$, $\mathbf{C} = \mathbf{C}(\mathbf{x},t) \in Q(Ц_t)$, $Ц_t = G \times (0,T_0)$, $(\mathbf{x},t) \in Ц_t$; $J(\mathbf{S},\mathbf{Y})$ — differential nonlinear spatial operator; D — diagonal matrix; $\boldsymbol{\psi} = \left\{\psi_k(\mathbf{x},t), k = \overline{1,16}\right\}$ — vector the components of which are source functions; $\mathbf{r} = \left\{r_k(\mathbf{x},t), k = \overline{1,16}\right\}$ — vector the components of which contain functions of uncertainties and errors of mathematical model (1) with initial and boundary conditions. Dependencies (observation models), coefficients and parameters $w_{C,k}$, μ_k, u, v, w, v_k, input data of initial and boundary conditions for model (2), $k = \overline{1,16}$; internal parameters of the operators are included in $\mathbf{Y} \in R(Ц_t)$.

Let $t = 0$, then the initial conditions for (2) take the form:

$$\mathbf{C} = \mathbf{C}_a^0 + \xi, \ \mathbf{Y} = \mathbf{Y}_a^0 + \zeta, \tag{3}$$

where $\mathbf{C}_a^0$ and $\mathbf{Y}_a^0$ — a priori estimates of the vector function of the state and the vector of parameters, respectively; the uncertainty functions are denoted using ξ and ζ.

Let us consider the integral identity:

$$I(\mathbf{C},\mathbf{Y},\mathbf{C}^*) \equiv \int\limits_{Ц_t} \left(L(\mathbf{C},\mathbf{Y}),\mathbf{C}^*\right) dGdt = 0, \tag{4}$$

here $\mathbf{C}^*$ — functions conjugate to $\mathbf{C}(\mathbf{C}^* \in Q^*(Ц_t))$. (4) is a variational formulation of model problem (2), (3), or an energy-type functional. Let us rewrite (4) in the following form:

$$I(\mathbf{C},\mathbf{Y},\mathbf{C}^*) \equiv \sum_{k=1}^{16} \left\{ \left(\Lambda\mathbf{C},\mathbf{C}^*\right)_k - \int\limits_{Ц_t} (\psi_k + r_k)\mathbf{C}_k^* dGdt \right\} = 0. \tag{5}$$

The operators of turbulent exchange and transfer are included in terms ($\Lambda\mathbf{C}$, $\mathbf{C}^*$).

Hydrodynamics model [12] will be considered as a model of the process. In hydrobiology models, parameterization of parameters and the resulting functional dependencies, for example, for describing production and destruction processes or the growth of phyto- or zooplankton, will be considered submodels, or observation models. Let us define the relationship between measurements and state functions:

$$\boldsymbol{\varphi}_m = \left[\mathbf{W}(\mathbf{C})\right]_m + \boldsymbol{\eta}(\mathbf{x},t), \tag{6}$$

where $[\mathbf{W}(\mathbf{C})]_m$ — vector of submodels (observation models); $\boldsymbol{\eta}(\mathbf{x}, t)$ — vector of errors and uncertainties; $\boldsymbol{\varphi}_m$ — values that we are monitoring.

Let us define $\boldsymbol{\varphi}_m$ on $Ц_t^m \in Ц_t$. In (6), the operation of transferring information from $Ц_t$ to $Ц_t^m$ is indicated by square brackets.

Let us expand the modeling system with data from field measurements (we consider them close to accurate), while the "quality" functionality will have a look:

$$\Phi_0(\mathbf{C}) = \left\{ \left(\boldsymbol{\varphi}_m - \left[\mathbf{W}(\mathbf{C})\right]_m\right)^\tau M\chi_0 \left(\boldsymbol{\varphi}_m - \left[\mathbf{W}(\mathbf{C})\right]_m\right) \right\}_{Ц_t^m} \equiv \left(\boldsymbol{\eta}^\tau C_1 \boldsymbol{\eta}\right), \tag{7}$$

we define χ_0 as a weight function for determining the configuration of the observation carrier $Ц_t^m$ in $Ц_t$ and the integrals over domain $Ц_t$, representing a measure for (7) in the form $C_1 = M\chi_0(\mathbf{x}, t)$, where M — weight matrix.

Let us consider functionals representing generalized characteristics of hydrobiogeocenosis behavior:

$$\Phi_k(\mathbf{C}) = \int\limits_{Ц_t} F_k(\mathbf{C})\chi_k(\mathbf{x},t)dGdt \equiv (F_k,\chi_k), \ \chi_k \subset Q^*(Ц_t), \ k = \overline{1,K}.$$

$F_k(\mathbf{C})$ — limited and differentiable relative to $\mathbf{C} \in Q(Ц_t)$ functions that we will evaluate.

Let us define a functional to minimize uncertainties:

$$\tilde{\Phi}_k^h(\mathbf{C}) = \Phi_k^h(\mathbf{C}) + \left\{ \left(\boldsymbol{\eta}^\tau C_1 \boldsymbol{\eta}\right)_{Ц_t^m}^h + \left(\mathbf{r}^\tau C_2 \mathbf{r}\right)_{Ц_t^m}^h + \left(\left(\mathbf{C}^0 - \mathbf{C}_a^0\right)^\tau C_3 \left(\mathbf{C}^0 - \mathbf{C}_a^0\right)\right)_{Ц_t^m}^h + \right.$$
$$\left. + \left(\left(\mathbf{Y}^0 - \mathbf{Y}_a^0\right)^\tau C_4 \left(\mathbf{Y}^0 - \mathbf{Y}_a^0\right)\right)_{R^h\left(Ц_t^m\right)}^h \right\} / 2 + I^h\left(\mathbf{C}, \mathbf{Y}, \mathbf{C}^*\right), k \ge 1. \tag{8}$$

We assume that C_i — weight matrices, $i = \overline{1,4}$. Let us consider the system:

$$\frac{\partial \tilde{\Phi}_k^h}{\partial \mathbf{C}^*} \equiv D\Lambda_t \mathbf{C} + J^h\left(\mathbf{C}, \mathbf{Y}\right) - \boldsymbol{\psi} - \mathbf{r} = 0; \tag{9}$$

$$\frac{\partial \tilde{\Phi}_k^h}{\partial \mathbf{C}} \equiv \left(D\Lambda_t\right)^\tau \mathbf{C}_k^* + A^\tau\left(\mathbf{C}, \mathbf{Y}\right)\mathbf{C}_k^* + \mathbf{d}_k = 0;$$

$$\mathbf{C}_k^*\left(\mathbf{x}\right)\Big|_{t=T_0} = 0;\ \mathbf{d}_k = \frac{\partial}{\partial \mathbf{C}}\left(\tilde{\Phi}_k^h\left(\mathbf{C}\right) + 0{,}5\left(\boldsymbol{\eta}^\tau C_1 \boldsymbol{\eta}\right)\right);$$

$$\mathbf{C}^0 = \mathbf{C}_a^0 + C_3^{-1}\mathbf{C}_k^*\left(0\right),\ t = 0;\ \mathbf{r}\left(\mathbf{x}, t\right) = C_2^{-1}\mathbf{C}_k^*\left(\mathbf{x}, t\right);$$

$$\mathbf{Y} = \mathbf{Y}_a + C_4^{-1}\Gamma_k;\ \Gamma_k = \frac{\partial}{\partial \mathbf{Y}} I^h\left(\mathbf{C}, \mathbf{Y}, \mathbf{C}_k^*\right);$$

$$A\left(\mathbf{C}, \mathbf{Y}\right)\mathbf{C}' = \frac{\partial}{\partial \alpha}\left\{J^h\left(\mathbf{C} + \alpha\mathbf{C}', \mathbf{Y}\right)\right\}\Big|_{\alpha=0},\ k \ge 1.$$

$A^\tau(\mathbf{C}', \mathbf{Y})$, Λ_t we define as operators of the conjugate problem and derivatives or their discrete approximations in time; $\boldsymbol{\Gamma}_k$ — functions of the sensitivity of models to changes in parameters; $\mathbf{C}' \equiv \delta\mathbf{C}$; α — set number.

Let us consider algorithms for assimilation of data from successive observations coming from various observational tools into a real-time modeling system. To do this, we will use the methods of splitting and decomposition:

$$Ц_t^h = \sum_{n=1}^{N_t - 1} Ц_{tn}^h;\ Ц_{tn}^h = G^h \times \left[t_{n-1}, t_n\right];\ \tilde{\Phi}^h\left(\mathbf{C}, \mathbf{C}^*, \mathbf{Y}, \boldsymbol{\varphi}\right) = \sum_{n=1}^{N_t - 1}\sum_{l=1}^{p} \tilde{\Phi}_{nl}^h, \tag{10}$$

here $\tilde{\Phi}_{nl}^h$ — part of functional (9) for $[t_{n-1}, t_n]$ on the l-th stage of splitting, $n = \overline{1, N_t}$, p we define as the total number of splitting steps. We will carry out the discretization on the basis of additive-averaged splitting schemes. We will use an algorithm to find a solution in domain $Ц_t^h$ with regular uniform time grid $\overline{\omega}_t^h \equiv \left\{t_n, n = \overline{0, N_t}\right\}$. For research, we will use a structure with phase spaces:

$$\left\{\mathbf{C}_l^n,\ \mathbf{C}_l^{*n},\ \mathbf{r}_l^n, l = \overline{1, p}\right\} = \bigcup_{l=1}^{p} Q_l^h\left(Ц_t^h\right) \subset Q^h\left(Ц_t^h\right).$$

Method of Solving the Problem. For solution (9), we consider that $n = \overline{1, N_t}$. Let us describe the algorithm of the method used step by step.

1. Switch to the subgrid decomposition structure, while $t = t_{n-1}$:

$$\left\{\mathbf{C}^{n-1} \in Q^h\left(Ц_t^h\right)\right\},\ \bigcup_{l=1}^{p}\left\{\mathbf{C}_l^{n-1} \in Q_l^h\left(Ц_t^h\right)\right\},\ \mathbf{C}_l^{n-1} = \mathbf{C}^{n-1}.$$

2. In the subgrid structure, obtain solutions to direct and conjugate problems:

$$\Lambda_l^n \mathbf{C}_l^n - \boldsymbol{\psi}_l^n - \mathbf{r}_l^n = 0,\ l = \overline{1, p},\ p \ge 1.$$

$$\Lambda_l^{*n}\mathbf{C}_l^{*n} = \left[\frac{\partial \Phi_{kl}\left(\mathbf{C}\right)}{\partial \mathbf{C}} + U^\tau C_1\left(\boldsymbol{\varphi}_m - \left[\mathbf{W}\left(\mathbf{C}\right)\right]_m\right)\right]_l^{n-1},$$

$$\mathbf{C}_l^{*n+1} = 0,\ \mathbf{r}_l^n = \left(C_2^n\right)^{-1}\mathbf{C}_l^{*n},\ t_n \le t \le t_n.$$

Functions $\boldsymbol{\psi}_l^n$ include $\mathbf{C}_l^{n-1}$. $\mathbf{r}_l^n$ takes into account all the uncertainties in the step $[t_{n-1}, t_n]$.

3. Return to main structure $Q^h\left(Ц_t^h\right)$ at $t = t_n$:

$$\bigcup_{l=1}^{p}\left\{\mathbf{C}_l^n \in Q_l^h\left(\text{Ц}_t^h\right)\right\} \Rightarrow \left\{\mathbf{C}^n \in Q^h\left(\text{Ц}_t^h\right)\right\},\quad \mathbf{C}^n = \frac{1}{p}\sum_{l=1}^{p}\mathbf{C}_l^n .$$

We believe that the last stage of splitting can be implemented using formula:

$$\Lambda_{pn}\mathbf{C}^n - \boldsymbol{\psi}_p^n - \mathbf{r}_p^n = 0, \tag{11}$$

here $\Lambda_{pn}\mathbf{C}^n$ — approximation operator part of the model at the p-th stage; $\boldsymbol{\psi}_p^n$ — source functions; $\mathbf{r}_p^n$ — function of uncertainties of model (2) and the splits introduced into the discrete model at a step. We believe that matrices of weights C_{1n} and C_{2n} are known.

Let us consider the following task:

$$\Lambda_{pn}^*\mathbf{C}^{*n} = \alpha_{1n}C_{1n}\left(\boldsymbol{\varphi}^{n-1} - \mathbf{C}^{n-1}\right); \tag{12}$$

$$\mathbf{r}_p^n = \left(C_{2n}^{-1}/\alpha_{2n}\right)\mathbf{C}^{*n}. \tag{13}$$

For the solution, we will use the following method, the algorithm of which we will describe step by step:

1. Calculate $\mathbf{C}^{*n}$ using (12).

2. Find $\mathbf{r}_p^n$, using (13).

3. Find $\mathbf{C}^n$, using formula (11).

The problem that arises during the implementation of the algorithm of the system of linear equations method will be solved by the sweep method.

Let us consider the transformed algorithm:

$$\Lambda_{pn}^*\mathbf{C}^{*n} = \alpha_{1n}C_{1n}\left(\boldsymbol{\varphi}^n - \mathbf{C}^n\right), \tag{14}$$

$$\Lambda_{pn}\mathbf{C}^n - \boldsymbol{\psi}^n - \left(C_{2n}^{-1}/\alpha_{2n}\right)\mathbf{C}^{*n} = 0. \tag{15}$$

We will solve the system by the sweep method. For the modifications considered, the stability of the splitting schemes ensures the stability of the data assimilation schemes used. If in (8) $\mathbf{C}^* = const$, then it gives a balance ratio of the first order. If $\mathbf{C}^* = \mathbf{C}$, then we obtain the equation of the energy balance of the analyzed system.

Let us write out the quality functionality for the new subsequent modification:

$$\Phi_{0n}\left(\mathbf{C}\right) = 0,5\left[\alpha_1\left(\boldsymbol{\eta}_n^{\tau}W_{1n}\boldsymbol{\eta}_n\right) + \alpha_2\left(\mathbf{r}_n^{\tau}W_{2n}\mathbf{r}_n\right)\right], \tag{16}$$

$$\mathbf{r}_n = \Lambda_{pn}\mathbf{C}_n - \boldsymbol{\psi}_n;\ \boldsymbol{\eta}_n = \boldsymbol{\varphi}_n - \mathbf{C}_n;\ \alpha_1 + \alpha_2 = 1,\ \alpha_1, \alpha_2 > 0. \tag{17}$$

We find the minimum of the functional relative to function $\mathbf{C}^n$:

$$\Lambda_{pn}^*C_{1n}\left(\Lambda_{pn}\mathbf{C}^n - \boldsymbol{\Psi}^n\right) + \frac{\alpha_{1n}}{\alpha_{2n}}C_{2n}\left(\mathbf{C}^n - \boldsymbol{\varphi}^n\right) = 0. \tag{18}$$

We obtain a uniquely solvable system with a five-diagonal matrix. Let us solve the resulting system of linear equations using the sweep method.

A new class of real-time assimilation methods includes a scheme of additive sequential assimilation. Due to the large amount of computational work, the built modifications are focused on supercomputing systems, including cluster systems and graphics accelerators.

Measurements $\boldsymbol{\varphi}_m$ are used in the form of maps and digital images. This representation gives a significant density of data in domain Ц_t, measurements are information fields. The planning of observations is based on the values of the uncertainty function. If these values are high, additional field measurements or observations are scheduled.

Results. To solve the problem of modeling the eutrophication of the Azov Sea waters (1), a set of parallel programs has been developed, including:

– a module of hydrodynamic processes that calculates the flow field of a water stream based on a mathematical model for a shallow reservoir [12];

– a module for the spread of pollutants in the aquatic environment and changes in the concentration of basic aquatic organisms (1), which allows us to assess the effect of pollutants on the biological productivity of the water area;

– a map of depths of the Azov Sea for the construction of computational grids for the numerical implementation of the developed algorithms;

– a database of expedition data, which allows refining the model of pollution of the aquatic environment and the spread of biota through the use of methods of data assimilation described above.

The numerical experiment was conducted using the developed software. The velocity vector of the water flow was calculated using a hydrodynamic model with an easterly wind at a speed of 5 m/s and fed into the input for calculating the movement of pollutants containing microplastic particles based on convection-diffusion equations. Figure 1 *a* shows the results of the numerical experiment to calculate water flow current fields under specified meteorological conditions. Vortex structures of currents were observed in the region of spits, in the northeastern part of the sea in Taganrog Bay. The color gradient in Figure 1 *a* represents the distribution of water flow velocity, with the maximum value at 4.822 m/s. Figures 1 *b, c,* and *d* show the results of calculations for a hypothetical scenario of the spread of microplastic contamination in the aquatic environment, considering the input of microplastics into the Azov Sea through the drains of the Don and Kuban rivers and the presence of a source of hazardous substances including microplastics at the outlet of Taganrog Bay. The figures also include a short-term forecast for the spread of contaminants 3, 6, and 12 days after the initial input. The initial concentration of pollutants was 5 mg/L, and after 3 days, the maximum concentration at the Taganrog Bay outlet was 1.363 mg/L. After 6 days, it decreased to 0.83 mg/L and after 12 days, it dropped to 0.336 mg/L.

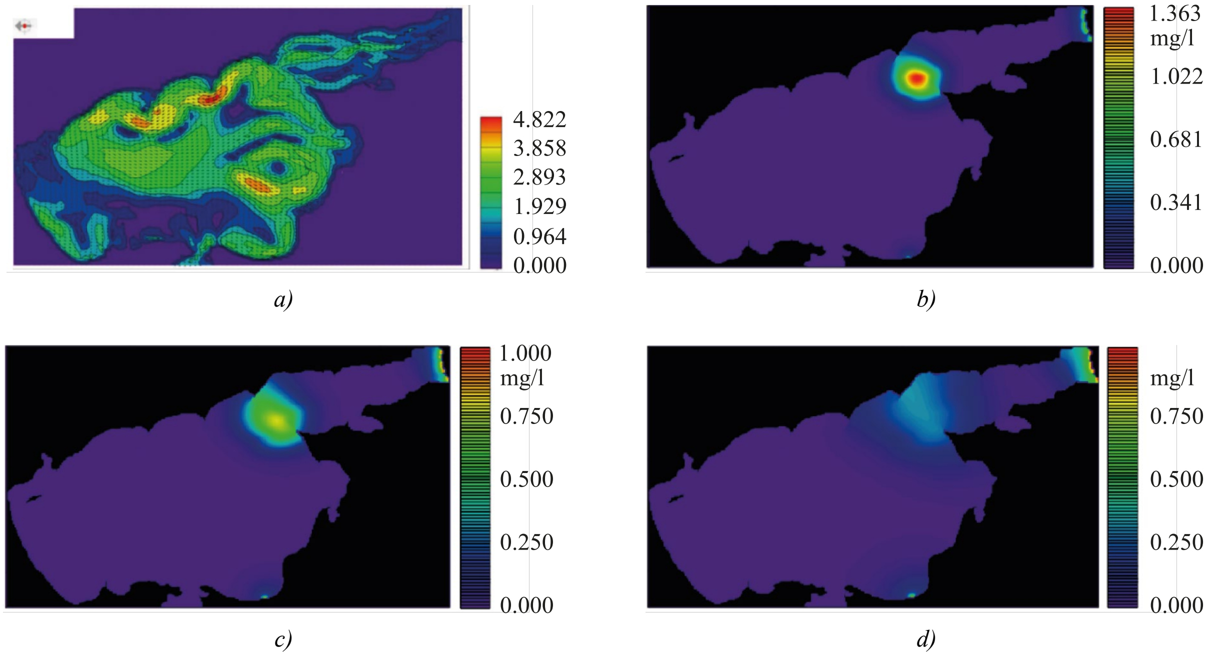

Fig. 1. Currents in the Azov Sea and the spread of pollutants, time interval:
a — initial concentration; *b* — 3 days; *c* — 6 days; *d* — 12 days

Discussion and Conclusion. The computational experiment shows that, despite the easterly wind, vortex structures in the currents captured pollutants and transported them to the Taganrog Bay. Stable vortices have the potential to capture and retain microplastic particles that enter the sea from river drains. They also contribute to the accumulation of pollutants in the lower layers due to biofouling by microplastic particles and their sinking.

As mentioned above, when creating mathematical models to predict natural phenomena and processes, one of the main challenges is to validate their accuracy by analyzing the outcomes obtained from them to ensure they match the behavior of the natural system under study. When creating mathematical models of hydrodynamic and hydrobiological processes, information on initial conditions and parameters (input data) is needed, which can be acquired through observations. Therefore, when creating predictive scenarios, it is essential not only to assess the quality of the developed mathematical model but also to incorporate observational data and investigate the sensitivity of these models to variations in input data.

The paper presents an approach to implementing a model of phytoplankton population dynamics (eutrophication) in the Azov Sea using variational methods for assimilating data obtained during field studies. The software package developed uses materials from the field studies, constantly updated environmental databases, and GIS, and allows refining the model of aquatic pollution and the spread of aquatic organisms using variational data assimilation techniques. The developed software makes it possible to forecast the spread of pollutants in the coastal system, including biogenic substances that act as a nutrient medium for the growth of dangerous microalgae, leading to eutrophication. This forecast enables the development of strategies for sustainable management of the natural system and its protection.

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