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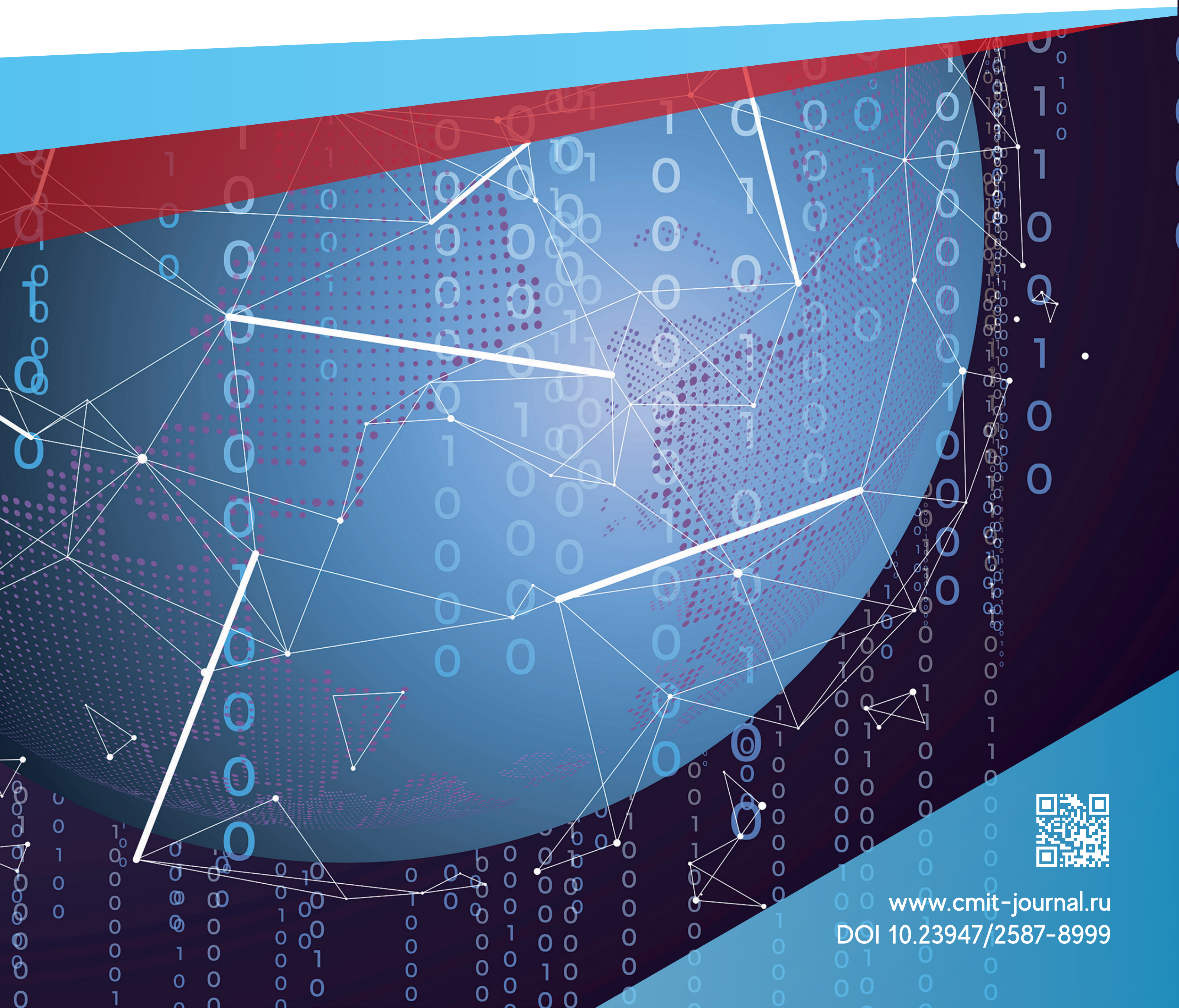

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ANNIVERSARY OF THE SCIENTIST
ЮБИЛЕЙ УЧЕНОГО

Valentin Dymnikov, Academician member of the Russian Academy of Sciences, is 85 years old

Valentin Dymnikov, Academician of the Russian Academy of Sciences, Doctor of Physical and Mathematical Sciences, Professor, turned 85 on November 26, 2023. Valentin Dymnikov is an outstanding figure of Russian science, a specialist in the field of mathematical models and numerical methods in the field of problems of geophysical hydro-aerohydrodynamics, ocean-atmosphere interaction. He is responsible for the fundamental development of global models of atmospheric processes, climate and the creation of a scientific basis for studying the predictability of its changes.

V.P. Dymnikov was born in the village of Yurino, Mari ASSR. In 1955, with a silver medal, he graduated from the 11th men's secondary school in Yoshkar-Ola, and in 1961 — the Moscow Engineering Physics Institute. He is a student of Academician G.I. Marchuk, the last President of the USSR Academy of Sciences, founder of the Institute of Computational Mathematics of the Russian Academy of Sciences.

V.P. Dymnikov headed the Institute of Computational Mathematics of the Russian Academy of Sciences (now Marchuk institute of numerical mathematics of the Russian Academy of Sciences) in the period from 2000 to 2010. Under his leadership, a galaxy of young promising doctors and candidates of sciences has been educated. V.P. Dymnikov is the author of more than 200 scientific papers, including 15 monographs and textbooks.

He is a member of the editorial boards of a number of authoritative journals: "Izvestia RAS. Physics of the Atmosphere and Ocean", "Reports of the Academy of Sciences", "Russian Journal of Numerical Analysis and Mathematical Modelling", "Ecological Bulletin of the Scientific Centers of the Black Sea Economic Cooperation", member of the publishing council "Synergetics".

V.P. Dymnikov is a member of a number of international scientific committees and commissions, in particular, the International Commission on Dynamic Meteorology, the Steering Scientific Committee of the international TOGA program (Tropical Ocean and Global Atmosphere), the steering scientific committee of the World Climate Program. Member of the American Meteorological Society. In 2004, he was elected a member of the European Academy of Sciences. V.P. Dymnikov was awarded the Order of Honor, is a Laureate of the State Prize of the Russian Federation. Awarded the A.A. Prize. Friedman RAS for a series of works on the theory of large-scale atmospheric processes and climate theory.

The editorial staff of "Computational Mathematics and Information Technologies", colleagues of Valentin Dymnikov cordially congratulate the dear and deeply respected hero of the day on his 85th birthday, wish him good health, new ideas and creative achievements in the field of computational mathematics, solving problems of climate and geophysical hydro-aerohydrodynamics, great human happiness!

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Brief information about the main scientific achievements of Academician of the Russian Academy of Sciences V.P. Dymnikov

The academician obtained fundamental scientific results in a number of areas of modern geophysics and mathematical modelling. In the field of transfer of humidity fields in the atmosphere, he investigated the microphysical processes of adaptation of humidity and cloud fields, formulated a new equation for the transfer of these fields, and also proposed methods for solving it, solved the problem of parametrization of torn clouds, proposed a method for parametrization of wet convection, etc.

Under the leadership of V.P. Dymnikov, a fully automated weather forecasting system for a limited area was developed and put into operational practice. The works carried out under his leadership together with a specially created laboratory at the Hydrometeorological Center of Russia were accepted in 2007 for implementation into the operational practice of Roshydromet.

In the field of the theory of hydrodynamic stability, he solved the problem of the development of baroclinic instability in the atmosphere in the presence of condensation, and investigated the problem of approximation by spectrum. The problem of symmetry of Lyapunov exponents for regular systems with Rayleigh friction, the problem of instability of zonal-asymmetric atmospheric flows, etc. is studied.

V.P. Dymnikov proposed and justified a dynamic-stochastic equation to describe the low-frequency variability of atmospheric circulation and investigated the relationship of the singular vectors of the dynamic operator with the eigenvectors of the covariance matrix, investigated the most correlated distributions of ocean surface temperature and atmospheric circulation characteristics.

In the field of numerical methods for solving differential equations, a method for constructing absolutely stable difference schemes for atmospheric hydrothermodynamics equations is proposed, which has an exact analogue of the quadratic law of conservation of energy based on the symmetrization of the original system of equations. A method for constructing difference schemes with a given set of integral conservation laws based on the use of conjugate equations is proposed.

Under the leadership of V.P. Dymnikov, original global models of the general circulation of the atmosphere, zonal-averaged models of the general circulation of the atmosphere and the ocean were developed, and a number of important results on modelling the modern climate and its changes were obtained.

A new direction in climate theory has been formed — the mathematical theory of climate, the basis of which is the study of the structure of the attractors of climate change models, their stability and sensitivity to changes in parameters. The structure of the attractors of atmospheric models is investigated, the dissipation-fluctuation relations are applied to construct the operator of the response of models to small external influences, which makes it possible to investigate the sensitivity of a real climate system.

The applicability of conjugate equations of nonlinear hydrodynamic systems for the construction of known integral conservation laws is investigated and proved, new conservation laws are obtained. A method for constructing optimal excitation of large-scale components of atmospheric circulation is proposed, a problem of potential predictability of the first kind is formulated and a method for solving it is proposed based on the reduction of a dynamic system to a dynamic-stochastic one.

Under the leadership of V.P. Dymnikov, a global mathematical model of the world-class climate has been developed at the INM RAS, which makes it possible to assess future climate changes based on joint interactive models of the general circulation of the atmosphere, ocean, cryosphere and land. As part of the project to create a model of the Earth system, original models of the upper atmosphere and ionosphere have been developed. In order to introduce the developed models into operational practice, V.P. Dymnikov organized an ionosphere modeling laboratory at the E.K. Fedorov Institute of Applied Geophysics.

V.P. Dymnikov is the head of the leading scientific school “Mathematical Modelling of Climate”, supported by a grant from the President of Russia. On the initiative of Academician V.P. Dymnikov and under his scientific guidance, since 2001, a school of young scientists “Computing and information technologies in environmental science” has been regularly held in various cities of Western Siberia. He has trained 8 doctors and 12 candidates of sciences. The scientist is the head of the seminar “Mathematical modelling of geophysical processes”, co-head of the seminar “Global changes in the natural environment and climate”.

COMPUTATIONAL MATHEMATICS
ВЫЧИСЛИТЕЛЬНАЯ МАТЕМАТИКА

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Two Dimensional Hydrodynamics Model with Evaporation for Coastal Systems

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Abstract

Introduction. The use of two-dimensional (2D) hydrodynamic models is relevant, despite the development of numerical methods of marine hydrodynamics focused on the use of three-dimensional spatial models. This is due to the modelling of hydrodynamic processes in shallow and coastal systems in solving practically important problems of predicting the transport of pollutants in suspended and dissolved forms. Evaporation for the Southern of Russia marine coastal systems (the Azov Sea, the Northern Caspian, etc.), and even more so in the coastal areas of the Red Sea, is a significant factor that affects not only the balance of water masses, but also makes changes in the momentum of the system and the distribution of the velocity vector of the aquatic environment. This effect is significant for coastal currents and shallow-water systems.

Materials and Methods. The traditional method of converting the terms of the Navier-Stokes equations containing differentiation by horizontal spatial variables was used, involving the rearrangement of differentiation operations by horizontal spatial coordinates and integration by vertical coordinate when constructing a spatially two-dimensional model of hydrodynamics of marine coastal systems when integrated by vertical coordinate. This made it possible to avoid the appearance of non-physical sources of energy and momentum in the spatially two-dimensional model, which can be essential in traditional 2D models with significant depth differences characteristic of coastal systems. The implementation of the analogue of the law of conservation of the total mechanical energy of the system for the constructed 2D model is investigated.

Results. Using the correct transformation of the 3D model (integration of the Navier-Stokes equations and continuity along a vertical coordinate, taking into account evaporation from a free surface), spatially two-dimensional models of hydrodynamics are constructed, for which the basic conservation laws, including mass and total mechanical energy of the system, are fulfilled. The implementation of an analogue of the law of conservation of total mechanical energy for various types of boundary conditions, including at the bottom, is investigated. The evaporation from the free surface is correctly accounted for not only in the continuity equation, but also in the equations of motion taking into account wind and waves.

Discussion and Conclusion. 2D model of hydrodynamics has been constructed and studied, taking into account evaporation not only in the mass balance equation (continuity), but also in the Navier-Stokes equations of motion. The proposed model can be used for predictive modelling of hydrophysical processes, including the spread of pollutants in the aquatic environment of coastal systems and shallow reservoirs in relation to marine systems such as the Azov Sea, the Northern Caspian Sea, coastal areas of the Red Sea, etc. Spatially two-dimensional models of marine hydrodynamics, without replacing three-dimensional models, can serve as a model basis for operational forecasting of situations in coastal systems and shallow-water objects using computing systems with relatively low performance and a moderate amount of RAM (5–10 Tflops, 2–4 TB, respectively).

Keywords: Coastal Systems, Evaporation, 2D Hydrodynamics Models, Mass Conservation Law, Mechanical Energy Conservation Law

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Научная статья

Двумерная гидродинамическая модель прибрежных систем, учитывающая испарение

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Аннотация

Введение. Несмотря на развитие численных методов морской гидродинамики, ориентированных на использование пространственно-трехмерных моделей, применение двумерных гидродинамических моделей по-прежнему остается актуальным. Прежде всего это касается моделирования гидродинамических процессов в мелководных и прибрежных системах при решении практически важных задач прогнозирования переноса загрязняющих веществ во взвешенной и растворенной формах. Испарение для морских прибрежных систем, располагающихся на Юге России (Азовское море, Северный Каспий и др.), а тем более в прибрежных районах Красного моря, является существенным фактором, который влияет не только на баланс водных масс, но и вносит изменения в импульс системы и распределение вектора скорости водной среды. Этот эффект заметен для прибрежных течений и мелководных систем.

Материалы и методы. В данной работе при построении пространственно-двумерной (2D) модели гидродинамики морских прибрежных систем при интегрировании по вертикальной координате не применялась традиционная методика преобразования членов уравнений Навье-Стокса, содержащих дифференцирование по горизонтальным пространственным переменным, предполагающая перестановку операций дифференцирования по горизонтальным пространственным координатам и интегрирование по вертикальной координате. Это позволило избежать появления в пространственно-двумерной модели нефизических источников энергии и импульса, которые могут иметь существенное значение в традиционных 2D-моделях при значительных перепадах глубин, характерных для прибрежных систем. Дополнительно в работе исследовано выполнение аналога закона сохранения полной механической энергии системы для построенной 2D-модели.

Результаты исследования. С помощью корректного преобразования 3D-модели (интегрирования уравнений Навье-Стокса и неразрывности по вертикальной координате с учетом испарения со свободной поверхности) построены пространственно-двумерные модели гидродинамики, для которых выполняются основные законы сохранения, в том числе массы и полной механической энергии системы. Исследовано выполнение аналога закона сохранения полной механической энергии для различных типов граничных условий, в том числе на дне. Выполнен корректный учет испарения со свободной поверхности не только в уравнении неразрывности, но и в уравнениях движения с учетом ветра и волн.

Обсуждение и заключение. Построена и исследована двумерная модель гидродинамики, учитывающая испарение не только в уравнении баланса масс (неразрывности), но и в уравнениях движения (Навье-Стокса). Предложенная модель может быть использована для прогнозного моделирования гидрофизических процессов, в том числе распространения загрязняющих веществ в водной среде прибрежных систем и мелководных водоемов применительно к таким морским системам, как Азовское море, Северный Каспий, прибрежные районы Красного моря и др. Пространственно-двумерные модели морской гидродинамики, не заменяя трехмерных моделей, могут служить модельной основой для оперативного прогнозирования ситуаций в прибрежных системах и мелководных объектах с использованием вычислительных систем с относительно невысокой производительностью и умеренным объемом оперативной памяти (5–10 Тфлопс, 2–4 ТБ соответственно).

Ключевые слова: прибрежные морские системы, испарение, 2D-модели гидродинамики, законы сохранения массы и полной механической энергии

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Introduction. The use of 2D hydrodynamic models is in demand despite the development of numerical methods of marine hydrodynamics focused on the use of three-dimensional spatial models, the use of two-dimensional hydrodynamic models remains in demand [1‒4]. First of all, this concerns hydrodynamic processes in shallow and coastal systems when solving practically important tasks of operational forecasting of the spread of pollutants in suspended and dissolved forms, the movement of sediments and sediments. Evaporation for Southern Russia marine coastal systems (the Azov Sea, the Northern Caspian, etc.), and even more so for coastal areas of the Red Sea, is a significant factor that affects not only the balance of water masses, but also makes changes in the momentum of the system and the distribution of the velocity vector of the aquatic environment. This effect is very noticeable for coastal currents and shallow-water systems [5‒8]. The aim of the work is to construct a conservative spatially two-dimensional hydrodynamic model for which the laws of conservation of mass balance and total mechanical energy are fulfilled, taking into account the evaporation of water from the free surface of a water body.

Coastal systems are characterized by high intensity of movement of the aquatic environment, large depth differences, a complex shape of the coastline, and in some cases — the presence of various hydraulic structures. Industrial pollution causes the greatest harm to water resources [9‒10]. As a result of the activities of coastal enterprises and the navy, polychlorinated biphenyls, heavy metals, surfactants, easily oxidized organics, polyaromatic hydrocarbons, etc. enter the water. Waste from the petrochemical and oil refining industries is particularly dangerous. Oil pollution is one of the most harmful and intractable emergencies [11–12].

Evaporation is an important process in most oil spills. Light oil changes very dramatically from liquid to viscous. In conditions when the boundary layer of air is stationary (there is no wind) or has low turbulence, the air directly above the water is quickly saturated and evaporation slows down [13]. When the wind speed increases, the evaporation rate increases significantly and is a non-linearly dependent function of wave height. In this paper, a relatively simple evaporation model is used, which allows us to take these effects into account.

Another feature of the obtained spatially two-dimensional models of hydrodynamics is the consideration of the fact that the operations of differentiation by spatial variables in horizontal directions are not, as shown by A.I. Sukhinov, commutative with respect to the operation of integration along a vertical spatial coordinate. In the case of coastal systems, where there is a significant difference in depth, an arbitrary change in the order of these operations, performed for the “convenience and simplicity” of obtaining spatially two-dimensional equations of motion of the aquatic environment, can lead to the appearance of fictitious, physically unreasonable sources of momentum in the Navier-Stokes equations. The method of constructing two-dimensional equations of motion proposed by the authors makes it possible to exclude this negative effect.

Materials and Methods. To simulate the hydrodynamic process with evaporation in an open water area, the equations of conservation of mass, momentum and energy describing the transfer of both liquid and gas phases are used. A rectangular Cartesian coordinate system is introduced. The axis Oz is directed opposite to the direction g from some point on the undisturbed surface of the liquid, the axis Ox is to the east, the axis Oy is to the north. Since the contribution of the centrifugal force is ≈ 0.2 % of the contribution of the gravitational force of attraction to the Earth, the angle ϑ between the vector of the angular velocity of rotation of the Earth and the vertical Oz can be considered complementary to $\pi/2$ the latitude of the place.

Results. Let’s perform the integration of the 3D continuity equation in the derivation of the 2D model of hydrodynamics

$$u'_x + v'_y + w'_z = 0$$

and the 3D Navier-Stokes equations

$$u'_t + \left(u^2\right)'_x + \left(uv\right)'_y + \left(uw\right)'_z = -\rho^{-1} p'_x - \varphi'_x + \eta\rho^{-1}\left(u''_{xx} + u''_{yy} + u''_{zz}\right) + 2\Omega\left(v\sin\vartheta - w\cos\vartheta\right),$$

$$v'_t + \left(uv\right)'_x + \left(v^2\right)'_y + \left(vw\right)'_z = -\rho^{-1} p'_y - \varphi'_y + \eta\rho^{-1}\left(v''_{xx} + v''_{yy} + v''_{zz}\right) - 2\Omega\, u\sin\vartheta,$$

$$w'_t + \left(uw\right)'_x + \left(vw\right)'_y + \left(w^2\right)'_z = -\rho^{-1} p'_z - \varphi'_z + \eta\rho^{-1}\left(w''_{xx} + w''_{yy} + w''_{zz}\right) + 2\Omega\, u\cos\vartheta$$

for viscous (in linear approximation) incompressible (density) liquid rotating at an angular velocity

$$\mathbf{\Omega} = \Omega\left(\mathbf{j}\cos\vartheta + \mathbf{k}\sin\vartheta\right),$$

where **i, j, k** are the unit orts; $u = u\,(x, y, z, t)$, $v = v\,(x, y, z, t)$, $w = w\,(x, y, z, t)$ are the components of the liquid velocity vector at point (x, y, z) at time t; p is the total hydrostatic pressure; φ is the gravitational potential; η is the first viscosity coefficient in a homogeneous gravity field $\nabla\varphi = -\mathbf{g} = -g\mathbf{k} = \text{const}$; $p_a = p_a\,(x, y, t)$; is the atmospheric pressure,

$p = p_a + + \rho g(\xi - z)$, $\nabla p = g\left(\zeta_x' \mathbf{i} + \zeta_y' \mathbf{j} - \mathbf{k}\right), -h \le z \le \xi$, where $\xi = \xi\ (x, y, z)$ is the elevation of the level of the free surface of the liquid with respect to the undisturbed state;
$h = h\ (x, y, z)$ is the height of the liquid column under the undisturbed surface.

Substituting the expressions for the gravitational potential and pressure into the 3D Navier-Stokes equations, we obtain:

$$u_x' + v_y' + w_z' = 0,$$

$$u_t' + \left(u^2\right)_x' + (uv)_y' + (uw)_z' = -g\zeta_x' - \rho^{-1}(p_a)_x' + \eta\rho^{-1}\left(u_{xx}'' + u_{yy}'' + u_{zz}''\right) + 2\Omega\left(v\sin\vartheta - w\cos\vartheta\right),$$

$$v_t' + (uv)_x' + \left(v^2\right)_y' + (vw)_z' = -g\zeta_y' - \rho^{-1}(p_a)_y' + \eta\rho^{-1}\left(v_{xx}'' + v_{yy}'' + v_{zz}''\right) - 2\Omega u\sin\vartheta,$$

$$w_t' + (uw)_x' + (vw)_y' + \left(w^2\right)_z' = \eta\rho^{-1}\left(w_{xx}'' + w_{yy}'' + w_{zz}''\right) + 2\Omega u\cos\vartheta.$$

We integrate the obtained equations along the vertical coordinate z from $-h$ to ξ taking into account the relations for differentiable functions $f = f(x, y, z, t)$, $\xi = \xi\ (x, y, t)$, $h = h\ (x, y, t)$:

$$\int_{-h}^{\zeta} f_t' dz = \left(\int_{-h}^{\zeta} f dz\right)_t' - f_s\zeta_t' + f_b\left(-h_t'\right),$$

$$\int_{-h}^{\zeta} f_x' dz = \left(\int_{-h}^{\zeta} f dz\right)_x' - f_s\zeta_x' + f_b\left(-h_x'\right),$$

$$\int_{-h}^{\zeta} f_y' dz = \left(\int_{-h}^{\zeta} f dz\right)_y' - f_s\zeta_y' + f_b\left(-h_y'\right),$$

$$\int_{-h}^{\zeta} f_z' dz = f_s - f_b,$$

where $f_s = f(x, y, \xi, t)$, $f_b = f(x, y, -h, t)$, are the values of the function f on the surface and bottom, respectively.

We obtain the following equations:

$$\left(U_x' - u_s\zeta_x' - u_b h_x'\right) + \left(V_x' - v_s\zeta_y' - v_b h_y'\right) + \left(w_s - w_b\right) = 0,$$

$$\left(U_t' - u_s\zeta_t' - u_b h_t'\right) + \left(\left(\int_{-h}^{\zeta} u^2 dz\right)_x' - u_s^2\zeta_x' - u_b^2 h_x'\right) + \left(\left(\int_{-h}^{\zeta} uv dz\right)_y' - u_s v_s\zeta_y' - u_b v_b h_y'\right) + \left(u_s w_s - u_b w_b\right) =$$

$$= -gH\zeta_x' - \frac{H}{\rho}(p_a)_x' + \frac{\eta}{\rho}\left(\left(\left(\int_{-h}^{\zeta} u_x' dz\right)_x' - \left(u_x'\right)_s\zeta_x' - \left(u_x'\right)_b h_x'\right) + \left(\left(\int_{-h}^{\zeta} u_y' dz\right)_y' - \left(u_y'\right)_s\zeta_y' - \left(u_y'\right)_b h_y'\right) +\right.$$

$$\left. + \left(\left(u_z'\right)_s - \left(u_z'\right)_b\right)\right) + 2\Omega\left(V\sin\vartheta - W\cos\vartheta\right), \tag{1}$$

$$\left(V_t' - v_s\zeta_t' - v_b h_t'\right) + \left(\left(\int_{-h}^{\zeta} uv dz\right)_x' - u_s v_s\zeta_x' - u_b v_b h_x'\right) + \left(\left(\int_{-h}^{\zeta} v^2 dz\right)_y' - v_s^2\zeta_y' - v_b^2 h_y'\right) + \left(v_s w_s - v_b w_b\right) =$$

$$= -gH\zeta_y' - \frac{H}{\rho}(p_a)_y' + \frac{\eta}{\rho}\left(\left(\left(\int_{-h}^{\zeta} v_x' dz\right)_x' - \left(v_x'\right)_s\zeta_x' - \left(v_x'\right)_b h_x'\right) + \left(\left(\int_{-h}^{\zeta} v_y' dz\right)_y' - \left(v_y'\right)_s\zeta_y' - \left(v_y'\right)_b h_y'\right) +\right.$$

$$\left. + \left(\left(v_z'\right)_s - \left(v_z'\right)_b\right)\right) - 2\Omega U\sin\vartheta, \tag{2}$$

$$\left(W_t' - w_s\zeta_t' - w_b h_t'\right) + \left(\left(\int_{-h}^{\zeta} uw dz\right)_x' - u_s w_s\zeta_x' - u_b w_b h_x'\right) + \left(\left(\int_{-h}^{\zeta} vw dz\right)_y' - v_s w_s\zeta_y' - v_b w_b h_y'\right) +$$

$$+\left(w_s^2-w_b^2\right)=\frac{\eta}{\rho}\left(\left(\left(\int_{-h}^{\zeta}w'_x dz\right)'_x-\left(w'_x\right)_s\zeta'_x-\left(w'_x\right)_b h'_x\right)+\left(\left(\int_{-h}^{\zeta}w'_y dz\right)'_y-\left(w'_y\right)_s\zeta'_y-\left(w'_y\right)_b h'_y\right)+\right.$$

$$\left.+\left(\left(w'_z\right)_s-\left(w'_z\right)_b\right)\right)+2\Omega U\cos\vartheta, \tag{3}$$

where e $U=\int_{-h}^{\zeta}udz,\ V=\int_{-h}^{\zeta}vdz,\ W=\int_{-h}^{\zeta}wdz$; is the full depth.

By rearranging the terms, we get:

$$U'_x+V'_y+\left(-u_s\zeta'_x-v_s\zeta'_y+w_s\right)-\left(u_bh'_x+v_bh'_y+w_b\right)=0,$$

$$U'_t+\left(\int_{-h}^{\zeta}u^2dz\right)'_x+\left(\int_{-h}^{\zeta}uvdz\right)'_y-u_s\left(\zeta'_t+u_s\zeta'_x+v_s\zeta'_y-w_s\right)-u_b\left(h'_t+u_bh'_x+v_bh'_y+w_b\right)=$$

$$=-gH\zeta'_x+\frac{\eta}{\rho}\left(\left(U'_x-u_s\zeta'_x-u_bh'_x\right)'_x+\left(U'_y-u_s\zeta'_y-u_bh'_y\right)'_y\right)+\left(F_s\right)_x+\left(F_b\right)_x+2\Omega\left(V\sin\vartheta-W\cos\vartheta\right),$$

$$V'_t+\left(\int_{-h}^{\zeta}uvdz\right)'_x+\left(\int_{-h}^{\zeta}v^2dz\right)'_y-v_s\left(\zeta'_t+u_s\zeta'_x+v_s\zeta'_y-w_s\right)-v_b\left(h'_t+u_bh'_x+v_bh'_y+w_b\right)=$$

$$W'_t+\left(\int_{-h}^{\zeta}uwdz\right)'_x+\left(\int_{-h}^{\zeta}vwdz\right)'_y-w_s\left(\zeta'_t+u_s\zeta'_x+v_s\zeta'_y-w_s\right)-w_b\left(h'_t+u_bh'_x+v_bh'_y+w_b\right)=$$

$$=\frac{\eta}{\rho}\left(\left(W'_x-w_s\zeta'_x-w_bh'_x\right)'_x+\left(W'_y-w_s\zeta'_y-w_bh'_y\right)'_y\right)+\left(F_s\right)_z+\left(F_b\right)_z+2\Omega U\cos\vartheta,$$

where the boundary viscous stresses on the surface of the liquid are attributed to the friction force of the wind on the surface

$$\mathbf{F}_s=\left(F_s\right)_x\mathbf{i}+\left(F_s\right)_y\mathbf{j}+\left(F_s\right)_z\mathbf{k}=\left(-H\rho^{-1}\left(p_a\right)'_x+\eta\rho^{-1}\left(-\left(u'_x\right)_s\zeta'_x-\left(u'_y\right)_s\zeta'_y+\left(u'_z\right)_s\right)\right)\mathbf{i}+$$

$$+\left(-H\rho^{-1}\left(p_a\right)'_y+\eta\rho^{-1}\left(-\left(v'_x\right)_s\zeta'_x-\left(v'_y\right)_s\zeta'_y+\left(v'_z\right)_s\right)\right)\mathbf{j}+\left(\eta\rho^{-1}\left(-\left(w'_x\right)_s\zeta'_x-\left(w'_y\right)_s\zeta'_y+\left(w'_z\right)_s\right)\right)\mathbf{k},$$

and viscous stresses at the bottom are attributed to the friction force on the bottom

$$\mathbf{F}_b=\left(F_b\right)_x\mathbf{i}+\left(F_b\right)_y\mathbf{j}+\left(F_b\right)_z\mathbf{k}=\eta\rho^{-1}\left(\left(-\left(u'_x\right)_bh'_x-\left(u'_y\right)_bh'_y-\left(u'_z\right)_b\right)\mathbf{i}+\right.$$

$$\left.+\left(-\left(v'_x\right)_s\zeta'_x-\left(v'_y\right)_s\zeta'_y+\left(v'_z\right)_s\right)\mathbf{j}+\left(-\left(w'_x\right)_s\zeta'_x-\left(w'_y\right)_s\zeta'_y+\left(w'_z\right)_s\right)\mathbf{k}\right).$$

Taking into account the kinematic conditions on the surface and bottom

$$-u_s\zeta'_x-v_s\zeta'_y+w_s=\zeta'_t+\omega\rho^{-1},\ u_bh'_x+v_bh'_y+w_b=-h'_t,$$

where $\omega\rho^{-1}$ is the layer of liquid evaporating per unit of time, we get

$$H'_t+U'_x+V'_y+\frac{\omega}{\rho}=0.$$

The following empirical equation was used to determine the evaporation rate from a unit area:

$$\omega\left(\frac{g}{h}\right)=e\left(P_{us}-P_{set}\right),$$

where P_{us} is the vapor pressure of saturated air, mbar; P_{set} is the partial pressure of water vapor at a given temperature and humidity, mbar; e is the empirical coefficient, g/m^2/h/ mbar, which depends on the intensity of spray formation in the pool.

Consider the two-dimensional problem of determining the evaporation rate from the surface of water when air moves at a constant speed at wind speed V, air humidity f, air temperature T_a, water temperature T_w. The evaporation rate from the surface of the pool W is determined in g/sec/m^2 (Fig. 1).

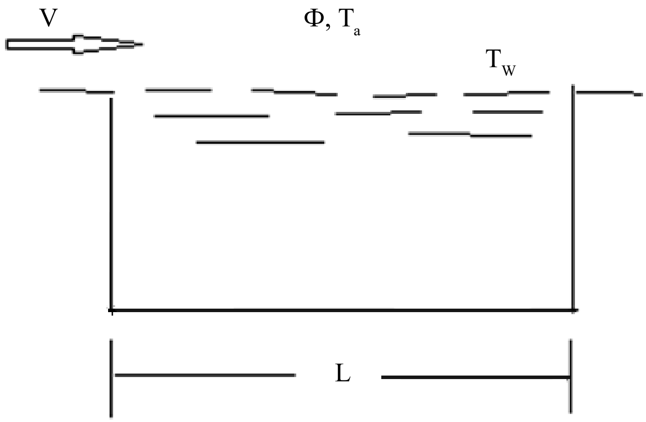

Fig. 1. The boundary between water and air

Let us determine the empirical dependencies for calculating the evaporation rate according to the formula based on the unit area based on experimental data:

$$\omega = \frac{\left(A + B \cdot V\right)\left(P_w - \varphi \cdot P_a\right)}{r_w},$$

where P_w is the saturated steam pressure at water temperature; P_a is the saturated steam pressure at air temperature; r_w is the heat of vaporization (r_w = 2.2582 J/kg at normal atmospheric pressure); A and B are empirical constants. The spread of evaporation rates across different sources is +100 % –80 %.

There are a number of standards that give similar results in the middle of this range: WMO (1966) USSR, Sartori (1989), McMillan (1971), etc. According to the WMO standard (1966) of the USSR, the coefficients A = 0.0369, B = 0.0266. It should be noted that the evaporation rate calculated according to the specified standard for V = 0 m/s is consistent with the evaporation rate determined according to the VDI 2089 standard for a fixed (undisturbed) surface, with an accuracy of 10–15 %.

Calculations can be performed in both laminar and turbulent formulations with calibration of the Schmidt number S_c and the turbulent Schmidt number Sc_t. This number is calibrated depending on the difference in water and wind speeds in the area of the interface between the media. Based on the available tools of the STAR-CCM hydrodynamics package, the velocity in the interface area can be determined as

$$V_b = \nabla V \cdot G^{(1/3)},$$

where ∇V is the velocity gradient determined from the current velocity field; $G^{1/3}$ is the characteristic cell size calculated from its volume. The dependence of the turbulent Schmidt number on the velocity in the interface region for predicting the evaporation rate on waves. For example, with a wave height of 1.5 m, a length of 10 m, and a speed of 3 m/s, we get:

$$Sc_t(V_B) = (-0.333\, V_B^2 + 6.667\, V_B + 3) \cdot 3.5\,.$$

The above formula is used to predict the evaporation rate in the presence of waves. We do not consider further refinement of the evaporation process and will continue to obtain a 2D model:

$$U'_t + \left(\int_{-h}^{\zeta} u^2 dz\right)'_x + \left(\int_{-h}^{\zeta} uvdz\right)'_y + \frac{\omega}{\rho}u_s = -gH\zeta'_x + \frac{\eta}{\rho}\left(\left(U''_{xx} - u_s\zeta''_{xx} - u_b h''_{xx}\right) + \left(U''_{yy} - u_s\zeta''_{yy} - u_b h''_{yy}\right)\right) +$$
$$+\left(\left(F_s\right)_x - \frac{\eta}{\rho}\left(\left(u_s\right)'_x\zeta'_x + \left(u_s\right)'_y\zeta'_y\right)\right) + \left(\left(F_b\right)_x - \frac{\eta}{\rho}\left(\left(u_b\right)'_x h'_x + \left(u_b\right)'_y h'_y\right)\right) + 2\Omega\left(V\sin\vartheta - W\cos\vartheta\right),$$

$$V'_t + \left(\int_{-h}^{\zeta} uvdz\right)'_x + \left(\int_{-h}^{\zeta} v^2 dz\right)'_y + \frac{\omega}{\rho}v_s = -gH\zeta'_y + \frac{\eta}{\rho}\left(\left(V''_{xx} - v_s\zeta''_{xx} - v_b h''_{xx}\right) + \left(V''_{yy} - v_s\zeta''_{yy} - v_b h''_{yy}\right)\right) +$$
$$+\left(\left(F_s\right)_y - \frac{\eta}{\rho}\left(\left(v_s\right)'_x\zeta'_x + \left(v_s\right)'_y\zeta'_y\right)\right) + \left(\left(F_b\right)_y - \frac{\eta}{\rho}\left(\left(v_b\right)'_x h'_x + \left(v_b\right)'_y h'_y\right)\right) - 2\Omega U\sin\vartheta,$$

$$W'_t + \left(\int_{-h}^{\zeta} uwdz\right)'_x + \left(\int_{-h}^{\zeta} vwdz\right)'_y + \frac{\omega}{\rho}w_s = \frac{\eta}{\rho}\left(\left(W''_{xx} - w_s\zeta''_{xx} - w_b h''_{xx}\right) + \left(W''_{yy} - w_s\zeta''_{yy} - w_b h''_{yy}\right)\right) +$$
$$+\left(\left(F_s\right)_z - \frac{\eta}{\rho}\left(\left(w_s\right)'_x\zeta'_x + \left(w_s\right)'_y\zeta'_y\right)\right) + \left(\left(F_b\right)_z - \frac{\eta}{\rho}\left(\left(w_b\right)'_x h'_x + \left(w_b\right)'_y h'_y\right)\right) + 2\Omega U\cos\zeta\,.$$

Isolating in derivatives

$$(f_s)'_x = (f'_x)_s + (f'_z)_s \zeta'_x, \quad (f_b)'_x = (f'_x)_b - (f'_z)_b h'_x,$$
$$(f_s)'_y = (f'_y)_s + (f'_z)_s \zeta'_y, \quad (f_b)'_y = (f'_y)_b - (f'_y)_b h'_y,$$

of complex functions $f_s = f(x, y, \xi, t), t)$, $f_b = f(x, y, -h(x, y, t)\ t)$ terms having the form and dimension of viscous stresses, therefore, changing continuously when crossing the boundaries of the "atmosphere — liquid" and "liquid — bottom" interface, and attributing them to the generalized forces of friction of wind on the surface $\mathbf{F}_s^*$ and liquid on the bottom $\mathbf{F}_b^*$, we obtain:

$$H'_t + U'_x + V'_y + \frac{\omega}{\rho} = 0,$$

$$U'_t + \left(\int_{-h}^{\zeta} u^2 dz\right)'_x + \left(\int_{-h}^{\zeta} uvdz\right)'_y + \frac{\omega}{\rho} u_s = -gH\zeta'_x + \frac{\eta}{\rho}\left(\left(U''_{xx} + U''_{yy}\right) - u_s\left(\zeta''_{xx} + \zeta''_{yy}\right) - u_b\left(h''_{xx} + h''_{yy}\right)\right) +$$
$$+ \left(F_s^*\right)_x + \left(F_b^*\right)_x + 2\Omega\left(V \sin\vartheta - W\cos\vartheta\right), \tag{4}$$

$$V'_t + \left(\int_{-h}^{\zeta} uvdz\right)'_x + \left(\int_{-h}^{\zeta} v^2 dz\right)'_y + \frac{\omega}{\rho} v_s = -gH\zeta'_y + \frac{\eta}{\rho}\left(\left(V''_{xx} + V''_{yy}\right) - v_s\left(\zeta''_{xx} + \zeta''_{yy}\right) - v_b\left(h''_{xx} + h''_{yy}\right)\right) +$$
$$+ \left(F_s^*\right)_y + \left(F_b^*\right)_y - 2\Omega U \sin\vartheta, \tag{5}$$

$$W'_t + \left(\int_{-h}^{\zeta} uwdz\right)'_x + \left(\int_{-h}^{\zeta} vwdz\right)'_y + \frac{\omega}{\rho} w_s = \frac{\eta}{\rho}\left(\left(W''_{xx} + W''_{yy}\right) - w_s\left(\zeta''_{xx} + \zeta''_{yy}\right) - w_b\left(h''_{xx} + h''_{yy}\right)\right) +$$
$$+ \left(F_s^*\right)_z + \left(F_b^*\right)_z + 2\Omega U \cos\vartheta, \tag{6}$$

where

$$\mathbf{F}_s^* = \left(\left(F_s\right)_x - \eta\rho^{-1}\left(\left(u'_x\right)_s \zeta'_x + \left(u'_y\right)_s \zeta'_y + \left(u'_z\right)_s\left(\left(\zeta'_x\right)^2 + \left(\zeta'_y\right)^2\right)\right)\right)\mathbf{i} +$$
$$+ \left(\left(F_s\right)_y - \eta\rho^{-1}\left(\left(v'_x\right)_s \zeta'_x + \left(v'_y\right)_s \zeta'_y + \left(v'_z\right)_s\left(\left(\zeta'_x\right)^2 + \left(\zeta'_y\right)^2\right)\right)\right)\mathbf{j} +$$
$$+ \left(\left(F_s\right)_z - \eta\rho^{-1}\left(\left(w'_x\right)_s \zeta'_x + \left(w'_y\right)_s \zeta'_y + \left(w'_z\right)_s\left(\left(\zeta'_x\right)^2 + \left(\zeta'_y\right)^2\right)\right)\right)\mathbf{k},$$
$$\mathbf{F}_b^* = \left(\left(F_b\right)_x - \eta\rho^{-1}\left(\left(u'_x\right)_b h'_x + \left(u'_y\right)_b h'_y + \left(u'_z\right)_b\left(\left(h'_x\right)^2 + \left(h'_y\right)^2\right)\right)\right)\mathbf{i} +$$
$$+ \left(\left(F_b\right)_y - \eta\rho^{-1}\left(\left(v'_x\right)_b h'_x + \left(v'_y\right)_b h'_y + \left(v'_z\right)_b\left(\left(h'_x\right)^2 + \left(h'_y\right)^2\right)\right)\right)\mathbf{j} +$$
$$+ \left(\left(F_b\right)_z - \eta\rho^{-1}\left(\left(w'_x\right)_b h'_x + \left(w'_y\right)_b h'_y + \left(w'_z\right)_b\left(\left(h'_x\right)^2 + \left(h'_y\right)^2\right)\right)\right)\mathbf{k},$$

they are equal in magnitude and directed opposite to the forces acting from the side of the column of liquid on the column of atmospheric air above it and the section of the bottom below it. The terms that change abruptly when crossing the boundaries of the "atmosphere — liquid" and "liquid — bottom" interface are left to the account of the forces of internal viscous friction.

In case of

$$W\cos\vartheta << V\sin\vartheta$$

the solutions of equations (4) and (5) do not depend on the solution of equation (6), which we exclude

$$H'_t + U'_x + V'_y + \frac{\omega}{\rho} = 0, \tag{7}$$

$$U'_t + \left(\int_{-h}^{\zeta} u^2 dz\right)'_x + \left(\int_{-h}^{\zeta} uvdz\right)'_y + \frac{\omega}{\rho} u_s = -gH\zeta'_x + \frac{\eta}{\rho}\left(\Delta U - u_s\Delta\zeta - u_b\Delta h\right) +$$
$$+ \left(F_s^*\right)_x + \left(F_b^*\right)_x + 2\Omega V \sin\vartheta,$$

$$V'_t + \left(\int_{-h}^{\zeta} uvdz\right)'_x + \left(\int_{-h}^{\zeta} v^2 dz\right)'_y + \frac{\omega}{\rho} v_s = -gH\zeta'_y + \frac{\eta}{\rho}\left(\Delta V - v_s\Delta\zeta - v_b\Delta h\right) +$$
$$+ \left(F_s^*\right)_y + \left(F_b^*\right)_y - 2\Omega U \sin\vartheta, \tag{8}$$

where $\Delta = \partial^2 / \partial x^2 + \partial^2 / \partial y^2$ is two-dimensional Laplace operator.

Introducing coefficients C_{uu}, C_{uv}, C_{vv}, C_u, C_v:

$$\int_{-h}^{\zeta} u^2 dz = C_{uu} H^{-1} U^2, \quad \int_{-h}^{\zeta} uv dz = C_{uv} H^{-1} UV, \quad \int_{-h}^{\zeta} v^2 dz = C_{vv} H^{-1} V^2, \; u_s = C_u H^{-1} U, \; v_s = C_v H^{-1} V,$$

equations (7)–(9) can be rewritten as

$$H'_t + U'_x + V'_y + (\omega/\rho) = 0,$$

$$U'_t + \left(C_{uu} U^2/H\right)'_x + \left(C_{uv} UV/H\right)'_y + (\omega/\rho) C_u (U/H) = -gH\zeta'_x + (\eta/\rho)\left(\Delta U - C_u (U/H)\Delta\zeta - u_b \Delta h\right) +$$
$$+ \left(F^*_s\right)_x + \left(F^*_b\right)_x + 2\Omega V \sin\vartheta,$$

$$V'_t + \left(C_{uv} UV/H\right)'_x + \left(C_{vv} V^2/H\right)'_y + (\omega/\rho) C_v (V/H) = -gH\zeta'_y + (\eta/\rho)\left(\Delta V - C_v (V/H)\Delta\zeta - v_b \Delta h\right) +$$
$$+ \left(F^*_s\right)_y + \left(F^*_b\right)_y - 2\Omega U \sin\vartheta. \tag{9}$$

Due to the Cauchy-Bunyakovsky inequality, there are the following restrictions for the coefficients C_{uu} and C_{vv}:

$$U^2 = \left(\int_{-h}^{\zeta} u dz\right)^2 \le H \int_{-h}^{\zeta} u^2 dz \Rightarrow C_{uu} \ge 1, \;\; V^2 = (v)^2 \le H \int_{-h}^{\zeta} v^2 dz \Rightarrow C_{vv} \ge 1,$$

and due to the positive semi-definiteness of the quadratic form

$$H \int_{-h}^{\zeta} (u - v)^2 dz = H\left(\int_{-h}^{\zeta} u^2 dz - 2\int_{-h}^{\zeta} uv dz + \int_{-h}^{\zeta} v^2 dz\right) = C_{uu} U^2 - 2C_{uv} UV + C_{vv} V^2 \ge 0,$$

— restriction for C_{uv}

$$C_{uv}^{\;2} \le C_{uu} C_{vv}.$$

The next stage of the study is to obtain and analyze the balance equation of total mechanical energy with certain simplifications.

When $C_{uu} \equiv C_{uv} \equiv C_{vv} \equiv 1$ for a simplified model, we get:

$$H'_t + U'_x + V'_y + (\omega/\rho) = 0,$$

$$U'_t + \left(U^2/H\right)'_x + \left(UV/H\right)'_y + (\omega/\rho) C_u (U/H) = -gH\zeta'_x + (\eta/\rho)\left(\Delta U - C_u (U/H)\Delta\zeta - u_b \Delta h\right) +$$
$$+ \left(F^*_s\right)_x + \left(F^*_b\right)_x + 2\Omega V \sin\vartheta, \tag{10}$$

$$V'_t + \left(UV/H\right)'_x + \left(V^2/H\right)'_y + (\omega/\rho) C_v (V/H) = -gH\zeta'_y + (\eta/\rho)\left(\Delta V - C_v (V/H)\Delta\zeta - v_b \Delta h\right) +$$
$$+ \left(F^*_s\right)_y + \left(F^*_b\right)_y - 2\Omega U \sin\vartheta. \tag{11}$$

The law of conservation of total mechanical energy is fulfilled — the sum of the potential energy in the resulting gravity field and the positive definite quadratic form of the integrals U and V, acceptable as an estimate of the kinetic energy of a column of liquid.

Multiplying (10) by U/H:

$$(U/H)U'_t + (U/H)\left(U^2/H\right)'_x + (U/H)\left(UV/H\right)'_y + (\omega/\rho) C_u \left(U^2/H^2\right) + gU\zeta'_x =$$
$$= (\eta/\rho)(U/H)\left(\Delta U - C_u (U/H)\Delta\zeta - u_b \Delta h\right) + (U/H)\left(\left(F^*_s\right)_x + \left(F^*_b\right)_x\right) + 2\Omega \sin\vartheta\,(UV/H),$$

multiplying (11) by V/H:

$$(V/H)V'_t + (V/H)\left(UV/H\right)'_x + (V/H)\left(V^2/H\right)'_y + (\omega/\rho) C_v \left(V^2/H^2\right) + gV\zeta'_y =$$
$$= (\eta/\rho)(V/H)\left(\Delta V - C_v (V/H)\Delta\zeta - v_b \Delta h\right) + (V/H)\left(\left(F^*_s\right)_y + \left(F^*_b\right)_y\right) - 2\Omega \sin\vartheta\,(UV/H)$$

and taking into account the ratios

$$(U/H)U'_t = \left(U^2/(2H)\right)'_t + \left(U^2/\left(2H^2\right)\right)H'_t,$$

$$(V/H)V'_t = \left(V^2/(2H)\right)'_t + \left(V^2/\left(2H^2\right)\right)H'_t,$$

$$(U/H)\left(U^2/H\right)'_x = \left(U^2/\left(2H^2\right)\right)U'_x + \left((U/H)\left(U^2/(2H)\right)\right)'_x,$$

$$(U/H)(UV/H)'_y = (U^2/(2H^2))V'_y + ((V/H)(U^2/(2H)))'_y,$$
$$(V/H)(UV/H)'_x = (V^2/(2H^2))U'_x + ((U/H)(V^2/(2H)))'_x,$$
$$(V/H)(V^2/H)'_y = (V^2/(2H^2))V'_y + ((V/H)(V^2/(2H)))'_y,$$

we will get

$$\begin{gathered}(U^2/(2H))'_t + ((U/H)(U^2/(2H)))'_x + ((V/H)(U^2/(2H)))'_y + (U^2/(2H^2))(H'_t + U'_x + V'_y + (\omega/\rho)) + \\ + (\omega/\rho)(C_u - 1/2)(U/H)^2 + g\left((U\zeta)'_x - \zeta U'_x\right) = \\ = (\eta/\rho)(U/H)(\Delta U - C_u(U/H)\Delta\zeta - u_b\Delta h) + (U/H)((F_s^*)_x + (F_b^*)_x) + 2\Omega\sin\vartheta(UV/H),\end{gathered} \tag{12}$$

$$\begin{gathered}(V^2/(2H))'_t + ((U/H)(V^2/(2H)))'_x + ((V/H)(V^2/(2H)))'_y + (V^2/(2H^2))(H'_t + U'_x + V'_y + (\omega/\rho)) + \\ + (\omega/\rho)(C_v - 1/2)(V/H)^2 + g\left((V\zeta)'_y - \zeta V'_y\right) = \\ = (\eta/\rho)(V/H)(\Delta V - C_v(V/H)\Delta\zeta - v_b\Delta h) + (V/H)((F_s^*)_y + (F_b^*)_y) - 2\Omega\sin\vartheta(UV/H).\end{gathered} \tag{13}$$

Adding (12) and (13), we come to

$$\begin{gathered}((U^2+V^2)/(2H))'_t + ((U/H)((U^2+V^2)/(2H) + gH\zeta))'_x + ((V/H)((U^2+V^2)/(2H) + gH\zeta))'_y + \\ + (\omega/(\rho H))((2C_u-1)U^2 + (2C_v-1)V^2)/(2H) - g\zeta(U'_x + V'_y) = \\ = (\eta/\rho)\left((U/H)\Delta U + (V/H)\Delta V - \left(C_u(U/H)^2 + C_v(V/H)^2\right)\Delta\zeta - ((U/H)u_b + (V/H)v_b)\Delta h\right) + \\ + \left(U((F_s^*)_x + (F_b^*)_x) + V((F_s^*)_y + (F_b^*)_y)\right)/H.\end{gathered}$$

Above the fixed ($h_0' \equiv 0$) bottom is performed

$$\begin{gathered}-g\zeta(U'_x + V'_y) = g\zeta(\zeta'_t + (\omega/\rho)) = \left(g(\zeta^2 - h^2)/2\right)'_t + (\omega/(\rho H))gH\zeta = \\ = (gH(\zeta - h)/2)'_t + (\omega/(\rho H))(gH(\zeta - h)/2 + gH^2/2).\end{gathered}$$

As a result, we come to an equation that is an analogue of the equation of the balance of total mechanical energy in differential form

$$\begin{gathered}(\mathrm{K}+\Pi)'_t + ((U/H)(\mathrm{K}+\Pi+P))'_x + ((V/H)(\mathrm{K}+\Pi+P))'_y + (\omega/(\rho H))(\Pi + P) + \\ + (\omega/(\rho H))((2C_u-1)U^2 + (2C_v-1)V^2)/(2H) = \\ = (\eta/\rho)\left((U/H)\Delta U + (V/H)\Delta V - \left(C_u(U/H)^2 + C_v(V/H)^2\right)\Delta\zeta - ((U/H)u_b + (V/H)v_b)\Delta h\right) + \\ + \left(U((F_s^*)_x + (F_b^*)_x) + V((F_s^*)_y + (F_b^*)_y)\right)/H,\end{gathered} \tag{14}$$

where $K = (U^2+V^2)/(2H)$, $\Pi = gH(\xi - h)/2$, $\mathrm{P} = gH^2/2$, $\Pi + P = gH\xi$.

For a positive function $E = E(x, y, t) > 0$, satisfying the transfer equation

$$E'_t + (U/H)E'_x + (V/H)E'_y = 0,$$

equation (4) is also valid for generalizing estimates of kinetic energy

$$K = E \cdot (U^2 + V^2)/(2H).$$

If we consider the boundary ∂G of the region G to be fixed then

$$\iint_G (\mathrm{K}+\Pi)'_t\,dxdy = \left(\iint_G (\mathrm{K}+\Pi)\,dxdy\right)'_t,$$

using the Green function

$$\iint_G \left(((U/H)(\mathrm{K}+\Pi+P))'_x + ((V/H)(\mathrm{K}+\Pi+P))'_y\right)dxdy = \oint_{\partial G} (\mathrm{K}+\Pi+P)(Udx - Vdy)/H =$$

$$= \oint_{\partial G} (\mathrm{K} + \Pi + P)(U\mathbf{i} + V\mathbf{j}, \mathbf{n}) dl / H,$$

$$\iint_G ((U/H)\Delta U + (V/H)\Delta V) dxdy =$$

$$= \oint_{\partial G} (\nabla \mathrm{K}, \mathbf{n}) dl - \iint_G H \left(|\nabla (U/H)|^2 + |\nabla (V/H)|^2 \right) dxdy + \iint_G (\mathrm{K}/H) \Delta H dxdy,$$

where $\mathbf{n}$ is the external normal to the boundary ∂G of the region G and assuming $C_u \equiv C_v \equiv C$, we obtain the balance equation of the analogue of the total mechanical energy of the liquid in integral form:

$$\left(\iint_G (\mathrm{K} + \Pi) dxdy \right)'_t + \oint_{\partial G} (\mathrm{K} + \Pi + P)(U\mathbf{i} + V\mathbf{j}, \mathbf{n}) dl / H + \iint_G (\omega/(\rho H))((2C-1)\mathrm{K} + \Pi + P) dxdy = \tag{15}$$

$$= (\eta/\rho) \left(\oint_{\partial G} (\nabla \mathrm{K}, \mathbf{n}) dl - \iint_G H \left(|\nabla (U/H)|^2 + |\nabla (V/H)|^2 \right) dxdy - (2C-1) \iint_G (\mathrm{K}/H) \Delta \zeta dxdy + \right.$$

$$\left. + \iint_G ((\mathrm{K}/H) - ((U/H) u_b + (V/H) v_b)) \Delta h dxdy \right) +$$

$$+ \iint_G \left(U \left((F_s^*)_x + (F_b^*)_x \right) + V \left((F_s^*)_y + (F_b^*)_y \right) \right) dxdy / H.$$

If the conditions of «sticking» are met on the bottom surface

$$u_b \equiv v_b \equiv w_b \equiv 0,$$

then the term

$$\iint_G ((U/H) u_b + (V/H) v_b) \Delta h dxdy = 0$$

there is no balance equation (15), and above the bottom surface, which is a harmonic function

$$\Delta h \equiv 0 \tag{16}$$

there is also no term

$$\iint_G (\mathrm{K}/H) \Delta h dxdy = 0$$

and the model

$$\zeta'_t + U'_x + V'_y + (\omega/\rho) = 0 \ \text{ or } \ H'_t + U'_x + V'_y + (\omega/\rho) = 0, \tag{17}$$

$$U'_t + \left(U^2/H\right)'_x + \left(UV/H\right)'_y + (\omega/\rho) C (U/H) = -gH\zeta'_x + (\eta/\rho)(\Delta U - C(U/H)\Delta\zeta) + \tag{18}$$

$$+ (F_s^*)_x + (F_b^*)_x + 2\Omega V \sin\vartheta,$$

$$V'_t + \left(UV/H\right)'_x + \left(V^2/H\right)'_y + (\omega/\rho) C (V/H) = -gH\zeta'_y + (\eta/\rho)(\Delta V - C(V/H)\Delta\zeta) + \tag{19}$$

$$+ (F_s^*)_y + (F_b^*)_y - 2\Omega U \sin\vartheta$$

turns out to be strictly dissipative due to the action of internal viscous friction forces.

The corresponding (17)–(19) system of equations in averaged values of velocities $\bar{u} = U/H$ and $\bar{v} = V/H$ will have the form:

$$\zeta'_t + \left(H\bar{u}\right)'_x + \left(H\bar{v}\right)'_y + (\omega/\rho) = 0 \ \text{ or } \ H'_t + \left(H\bar{u}\right)'_x + \left(H\bar{v}\right)'_y + (\omega/\rho) = 0, \tag{20}$$

$$\left(H\bar{u}\right)'_t + \left(H\bar{u}^2\right)'_x + \left(H\bar{u}\bar{v}\right)'_y + (\omega/\rho) C\bar{u} = -gH\zeta'_x + (\eta/\rho)(\Delta(H\bar{u}) - C\bar{u}\Delta\zeta) + \tag{21}$$

$$+ (F_s^*)_x + (F_b^*)_x + 2\Omega H\bar{v} \sin\vartheta,$$

$$\left(H\bar{v}\right)'_t + \left(H\bar{u}\bar{v}\right)'_x + \left(H\bar{v}^2\right)'_y + (\omega/\rho) C\bar{v} = -gH\zeta'_y + (\eta/\rho)(\Delta(H\bar{v}) - C\bar{v}\Delta\zeta) + \tag{22}$$

$$+\left(F_s^*\right)_y+\left(F_b^*\right)_y-2\Omega H\overline{u}\sin\vartheta$$

or, by virtue of the continuity equation:

$$\zeta_t'+\left(H\overline{u}\right)'_x+\left(H\overline{v}\right)'_y+\left(\omega/\rho\right)=0 \text{ or } H_t'+\left(H\overline{u}\right)'_x+\left(H\overline{v}\right)'_y+\left(\omega/\rho\right)=0, \quad (23)$$

$$\overline{u}_t'+\overline{u}\overline{u}_x'+\overline{v}\overline{u}_y'+\left(\omega/\rho\right)\left(C-1\right)\left(\overline{u}/H\right)=-g\zeta_x'+\left(\eta/\left(\rho H\right)\right)\left(\Delta\left(H\overline{u}\right)-C\overline{u}\Delta\zeta\right)+ \quad (24)$$
$$+\left(\left(F_s^*\right)_x+\left(F_b^*\right)_x\right)/H+2\Omega\overline{v}\sin\vartheta,$$

$$\overline{v}_t'+\overline{u}\overline{v}_x'+\overline{v}\overline{v}_y'+\left(\omega/\rho\right)\left(C-1\right)\left(\overline{v}/H\right)=-g\zeta_y'+\left(\eta/\left(\rho H\right)\right)\left(\Delta\left(H\overline{v}\right)-C\overline{v}\Delta\zeta\right)+ \quad (25)$$
$$+\left(\left(F_s^*\right)_y+\left(F_b^*\right)_y\right)/H-2\Omega\overline{u}\sin\vartheta.$$

Other spatially two-dimensional hydrodynamic models of coastal systems and shallow waters can also be obtained.

Introducing simplifications

$$\int_{-h}^{\zeta}u_x'dz\to H\left(U/H\right)'_x,\quad \int_{-h}^{\zeta}u_y'dz\to H\left(U/H\right)'_y,\quad \int_{-h}^{\zeta}v_x'dz\to H\left(V/H\right)'_x,\quad \int_{-h}^{\zeta}v_y'dz\to H\left(V/H\right)'_y$$

at stage (1)–(3) and reasoning similarly to the above, we come to the following model

$$\zeta_t'+U_x'+V_y'+\left(\omega/\rho\right)=0, \quad (26)$$

$$U_t'+\left(U^2/H\right)'_x+\left(UV/H\right)'_y+\left(\omega/\rho\right)C\left(U/H\right)=-gH\zeta_x'+\left(\eta/\rho\right)\left(\left(H\left(U/H\right)'_x\right)'_x+\left(H\left(U/H\right)'_y\right)'_y\right)+$$
$$+\left(F_s^*\right)_x+\left(F_b^*\right)_x+2\Omega V\sin\vartheta, \quad (27)$$

$$V_t'+\left(UV/H\right)'_x+\left(V^2/H\right)'_y+\left(\omega/\rho\right)C\left(V/H\right)=-gH\zeta_y'+\left(\eta/\rho\right)\left(\left(H\left(V/H\right)'_x\right)'_x+\left(H\left(V/H\right)'_y\right)'_y\right)+$$
$$+\left(F_s^*\right)_y+\left(F_b^*\right)_y-2\Omega U\sin\vartheta \quad (28)$$

or in averaged values of velocities

$$H_t'+\left(H\overline{u}\right)'_x+\left(H\overline{v}\right)'_y+\left(\omega/\rho\right)=0, \quad (29)$$

$$\overline{u}_t'+\overline{u}\overline{u}_x'+\overline{v}\overline{u}_y'+\left(\omega/\rho\right)\left(C-1\right)\left(\overline{u}/H\right)=-g\zeta_x'+\left(\eta/\left(\rho H\right)\right)\left(\left(H\overline{u}_x'\right)'_x+\left(H\overline{u}_y'\right)'_y\right)+$$
$$+\left(\left(F_s^*\right)_x+\left(F_b^*\right)_x\right)/H+2\Omega\overline{v}\sin\vartheta, \quad (30)$$

$$\overline{v}_t'+\overline{u}\overline{v}_x'+\overline{v}\overline{v}_y'+\left(\omega/\rho\right)\left(C-1\right)\left(\overline{v}/H\right)=-g\zeta_y'+\left(\eta/\left(\rho H\right)\right)\left(\left(H\overline{v}_x'\right)'_x+\left(H\overline{v}_y'\right)'_y\right)+$$
$$+\left(\left(F_s^*\right)_y+\left(F_b^*\right)_y\right)/H-2\Omega\overline{u}\sin\vartheta, \quad (31)$$

taking into account the equalities and assuming that the analogue of the total mechanical energy balance equation is fulfilled

$$\iint_G\left(\left(U/H\right)\left(\left(H\left(U/H\right)'_x\right)'_x+\left(H\left(U/H\right)'_y\right)'_y\right)+\left(V/H\right)\left(\left(H\left(V/H\right)'_x\right)'_x+\left(H\left(V/H\right)'_y\right)'_y\right)\right)dxdy=$$
$$=\oint_{\partial G}H\left(\nabla\left(\mathrm{K}/H\right),\mathbf{n}\right)dl-\iint_G H\left(\left|\nabla\left(U/H\right)\right|^2+\left|\nabla\left(V/H\right)\right|^2\right)dxdy,$$

in the form

$$\left(\iint_G\left(\mathrm{K}+\Pi\right)dxdy\right)'_t+\oint_{\partial G}\left(\mathrm{K}+\Pi+P\right)\left(U\mathbf{i}+V\mathbf{j},\mathbf{n}\right)dl/H+\iint\left(\omega/\left(\rho H\right)\right)\left(\left(2C-1\right)\mathrm{K}+\Pi+P\right)dxdy=$$
$$=\left(\eta/\rho\right)\left(\oint_{\partial G}H\left(\nabla\left(\mathrm{K}/H\right),\mathbf{n}\right)dl-\iint_G H\left(\left|\nabla\left(U/H\right)\right|^2+\left|\nabla\left(V/H\right)\right|^2\right)dxdy-\left(2C-1\right)\iint_G\left(\mathrm{K}/H\right)\Delta\zeta dxdy\right)+$$
$$+\iint_G\left(U\left(\left(F_s^*\right)_x+\left(F_b^*\right)_x\right)+V\left(\left(F_s^*\right)_y+\left(F_b^*\right)_y\right)\right)dxdy/H.$$

Another family of models can be obtained by leaving on account of the forces of internal viscous friction only the terms that do not interfere with obtaining a balance equation with strict dissipation of the analogue of the total mechanical energy of the system due to the action of internal viscous friction forces and transferring the remaining terms to the evaporation intensity, where an excess type term is added (under the surface of the liquid convex upwards) or insufficient (under the surface of the liquid convex downwards) Laplace pressure:

$$U'_t+\left(U^2/H\right)'_x+\left(UV/H\right)'_y+(\omega/\rho)^*C(U/H)=-gH\zeta'_x+(\eta/\rho)(\Delta U-(1/2)(U/H)\Delta H)+ \qquad (32)$$
$$+\left(F_s^*\right)_x+\left(F_b^*\right)_x+2\Omega V\sin\vartheta,$$

$$V'_t+\left(UV/H\right)'_x+\left(V^2/H\right)'_y+(\omega/\rho)^*C(V/H)=-gH\zeta'_y+(\eta/\rho)(\Delta V-(1/2)(V/H)\Delta H)+$$
$$+\left(F_s^*\right)_y+\left(F_b^*\right)_y-2\Omega U\sin\vartheta, \qquad (33)$$
$$H'_t+U'_x+V'_y+(\omega/\rho)^*-(\eta/\rho)\left(\left(1-(2C)^{-1}\right)\Delta H-\Delta h\right)=0$$

or

$$\zeta'_t+U'_x+V'_y+(\omega/\rho)^*-(\eta/\rho)\left(\left(1-(2C)^{-1}\right)\Delta\zeta-(2C)^{-1}\Delta h\right)=0.$$

The equation of the analogue of the total mechanical energy balance for the model (32)–(34) differs from (15) by replacing (ω/ρ) with

$$(\omega/\rho)^*-(\eta/\rho)\left(\left(1-(2C)^{-1}\right)\Delta H-\Delta h\right)=(\omega/\rho)^*-(\eta/\rho)\left(\left(1-(2C)^{-1}\right)\Delta\zeta-(2C)^{-1}\Delta h\right). \qquad (34)$$

In the course of the work, a two-dimensional model of the hydrodynamic process was constructed and studied, taking into account the essential features of coastal systems, based on the balance of mass, energy and momentum. The proposed model can be used for predictive modeling of hydrophysical processes, including the spread of pollutants in the aquatic environment of marine and coastal systems.

Discussion and Conclusion. The peculiarity of the obtained spatially two-dimensional models of hydrodynamics takes into account the fact that the operations of differentiation by spatial variables in horizontal directions are not commutative with respect to the operation of integration along a vertical spatial coordinate. In coastal systems, where there is a significant difference in depth, an arbitrary change in the order of these operations, performed to obtain spatially two-dimensional equations of motion of the aquatic environment, can lead to the appearance of fictitious, physically unreasonable sources of momentum in the Navier-Stokes equations. The method of constructing two-dimensional equations of motion developed by the authors makes it possible to eliminate this negative effect, and maintaining the order of operations ensures that evaporation from a free surface is correctly accounted for not only in the continuity equation, but also in the equations of motion taking into account wind and waves.

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Mathematical Modelling of Dust Transfer from the Tailings in the Alagir Gorge of the RNO-Alania

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Abstract
Introduction. Mathematical modelling of the aerodynamics of mountain gorges is an actual means of studying possible man-made emissions in various meteorological conditions that increase the transfer of pollutants in the direction of densely populated areas. Aerodynamics and climatic conditions are unique for various mountain gorges. This requires a separate study for each specific case. The paper studies the distribution of dust aerosol from the Unal tailings dump, located near the village of Verkhny Unal (Alagir Gorge, RNO-Alania, RF), with south and south-easterly winds. With these wind directions, the dust of the tailings dump is carried by air currents in the north direction, towards Alagir. The aim of the study is to obtain a forecast for the surface concentration of dust with an increased content of lead, zinc and other elements near densely populated areas of the flat part of RNO-Alania.
Materials and Methods. The model takes into account the terrain, surface wind roses and dust deposition processes. The calculations were carried out for the case of neutral stratification and without taking into account the influence of seasonal factors using a mathematical model previously published by the authors.
Results. The model prediction of the dust concentration distribution obtained from calculations is shown. The frequencies and amplitudes of oscillations of unsteady jet streams in the cross section of the Alagir gorge are analyzed. Based on the data of satellite sensing of the Earth's atmosphere, the frequency of winds leading to the transfer of dust in the direction of densely populated areas is estimated.
Discussion and Conclusion. The Unal tailings dump is a source of pollutants and over many years of its existence, soil contamination can be significant. Field studies of the soil in the Alagir area and, possibly, measures for its reclamation are necessary.

Keywords: mountain ravine, dust, mine tailings, mathematical model, complex terrain

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Научная статья

Математическое моделирование распространения пыли от хвостохранилища в Алагирском ущелье РСО-Алания

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Аннотация

Введение. Математическое моделирование аэродинамики горных ущелий и возможных техногенных выбросов в различных метеорологических условиях, особенно увеличивающих перенос загрязняющих веществ в направлении густонаселенных районов, является актуальным средством исследования этих процессов. Аэродинамика и климатические условия уникальны для различных горных ущелий, что требует проведения отдельного исследования для каждого конкретного случая. В работе рассматривается распространение пылевого аэрозоля от Унальского хвостохранилища, расположенного вблизи поселка Верхний Унал (Алагирское ущелье, РСО-Алания, РФ), в случае возникновения южных и юго-восточных ветров. При этих направлениях ветра пыль хвостохранилища переносится течениями воздуха в северном направлении, в сторону Алагира. Целью исследования является получение прогноза для приземной концентрации пыли с повышенным содержанием свинца, цинка и других элементов вблизи густонаселенных районов равнинной части РСО-Алания.

Материалы и методы. Модель учитывает ландшафт местности, приземные розы ветров и процессы осаждения пыли. Вычисления проводились для случая нейтральной стратификации и без учета влияния сезонных факторов с использованием математической модели, ранее опубликованной авторами.

Результаты исследования. Выполнен модельный прогноз распределения концентрации пыли. Проанализированы частоты и амплитуды осцилляций нестационарных струйных течений в поперечном сечении Алагирского ущелья. На основе данных спутникового зондирования земной атмосферы оценена повторяемость ветров, приводящих к переносу пыли в направлении густонаселенных районов.

Обсуждение и заключение. Унальское хвостохранилище является источником загрязняющих веществ и за годы его существования загрязнение почвы может быть значительным. Авторами сделан вывод о необходимости полевых исследований почвы в районе Алагира и, возможно, принятия мер по ее рекультивации.

Ключевые слова: горное ущелье, пыль, хвостохранилище, математическая модель, сложный рельеф

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Introduction. Tailings contain fine-dispersed waste from mining and processing plants, which, as a rule, are stored in an open manner and enter the atmosphere of mountain gorges in the form of a dust aerosol. Often, meteorological measurements are not carried out in full in mountain gorges or are not available at all, and the available data are insufficient to predict the distribution of pollutants (SV). This disadvantage can be partially eliminated by using mathematical modeling and data from weather satellites. The experience of using mathematical modeling taking into account the data of remote sensing of the Earth is given in [1–4].

The study of the atmosphere of mountainous territories using mathematical modeling is carried out for a wide range of tasks [3–11]. In [5–7; 11–13] modern mathematical models, solution methods and basic laws of aerodynamics of mountain gorges are presented. Due to the multifactorial nature of aerodynamics [7], idealized gorges are often modeled and simplified synoptic conditions are considered [5–6; 8].

The dispersion of dust aerosol in mountain gorges and in flat areas differs [12–13]. In addition, each mountain gorge has a unique climate and aerodynamics, for the study of which a detailed mathematical model must include many arrays of initial data, boundary conditions and weather conditions, which is extremely resource-intensive and often faces a lack of necessary data.

In [3–4], a mathematical model of a mountain gorge is used, which does not require detailed input data, but takes into account the main factors: the mountain landscape of the area, surface wind roses, dust deposition processes, atmospheric turbulence. Standardized algorithms for solving hydrodynamic equations of the OpenFOAM computational package implementing the finite volume method are used.

The authors consider the removal of SV from the bowl of the Unal tailings pond of the Sadon lead-zinc combine, located in the bend of the Ardon River near the village of Unal (Alagirsky district, RNO-Alania, RF), in the Alagir gorge, the Northern part of the Caucasian ridge, at 42.862 s. w. and 44.145 v. d., at an altitude of about 1700 meters above sea level. The width of the gorge near the tailings dump reaches 3000 m, the height of the slopes is 2570 m. The tailings dump was created more than 50 years ago and contains about 2.6 million tons of tailings, which contain 0.21 % wt. Pb, 0.32 % wt. Zn, as well as other elements. Reclamation measures significantly reduce dusting processes, however, a significant amount of dust is contained on the slopes of the gorge and in the soils near the tailings dump. The results of field studies of tailings content on the slopes of the gorge from the Unal tailings dump are devoted to works [14–16].

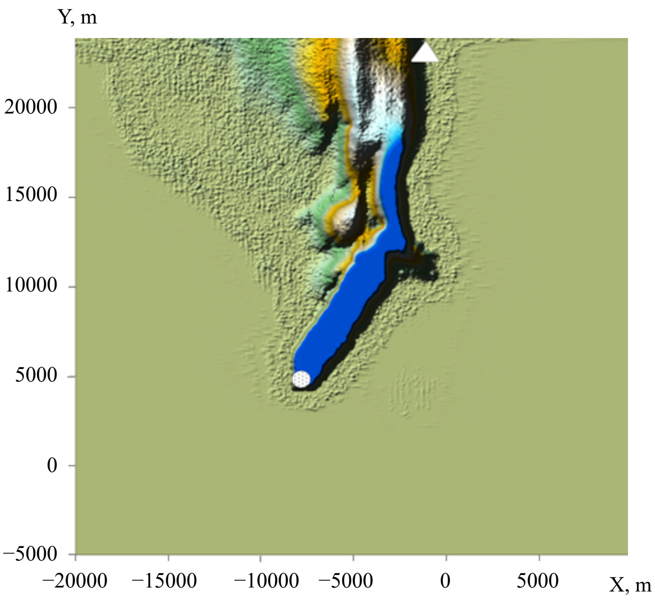
The conditions of separation of dust aerosol particles from the surface obtained in experiments are presented in [17–18]. The determining factors are the strength of the wind and the turbulence of the atmosphere, and the distribution of dust deposited on the slopes is determined by the topography and the wind rose. In [8–9; 19–23], mathematical modeling of aerodynamics and dust propagation is used for real problems.

In this paper, synoptic situations associated with easterly and southeasterly winds over the Alagir gorge are considered, in which dust from the tailings dump spreads in a northerly direction, towards Alagir (RNO-Alania). The occurrence of unsteady jet streams that carry dust in a northerly direction is discussed.

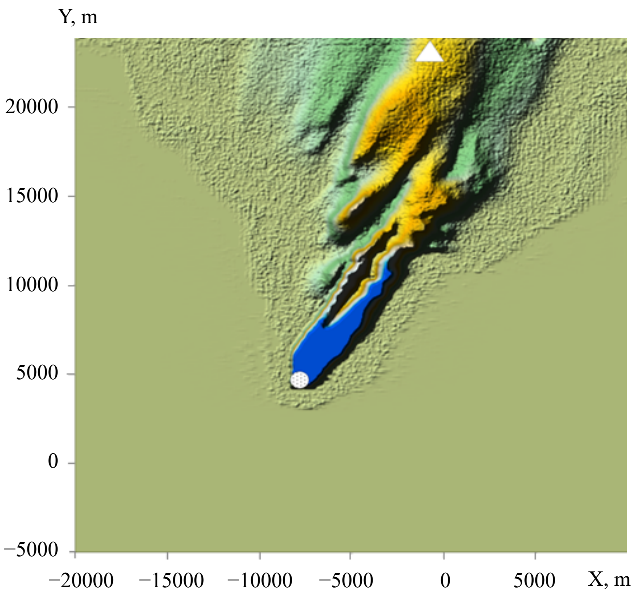
Materials and methods. The mathematical model used, presented in [3–4], is a fairly simple and workable tool useful for estimating the concentration of polluting substance (PS) in the mountain atmosphere. The comparison of forecast values and field measurement data showed satisfactory accuracy sufficient for practical applications.

Research results. Sixteen calculations were carried out with different boundary conditions for wind at the upper boundary of the calculated area with a step of 22.5°: north, north-north-west, north-west, etc. In each calculation, the aerodynamic fields and the concentration of PS from the model source located in the bowl of the Alagirsky Gorge tailings pond were calculated. As a result of averaging and rationing of these calculations, the average concentration of PS is obtained, given in [3]. The normalized PS concentration fields obtained for the south-east, south-south-east and south directions of the external wind are shown here. In other calculated cases, the SV is moved not towards Alagir, but in the direction of sparsely populated areas, reaching which the concentration of PS decreases below the MPC (indicated according to the Federal Law of the Russian Federation "On Sanitary and Epidemiological Welfare of the population" No. 52-FZ of March 30, 1999).

Figure 1 *a* shows the concentration of SV obtained by calculating the south-easterly wind direction; Figure 1 *b* shows the south-south-easterly wind; Figure 1 *c* shows the south wind; Figure 1 *d* shows a topographic map of the calculated area exported from the computational grid. The location of the source is marked with a white circle; the values $0 < C < 0.1C_{max}$ are shown, where C_{max} is the concentration near the source. The triangle marks the southern suburbs of Alagir. The normalization used in [3] was applied. In the areas marked in blue, the concentration exceeds the value of $0.1C_{max}$.



a)



b)

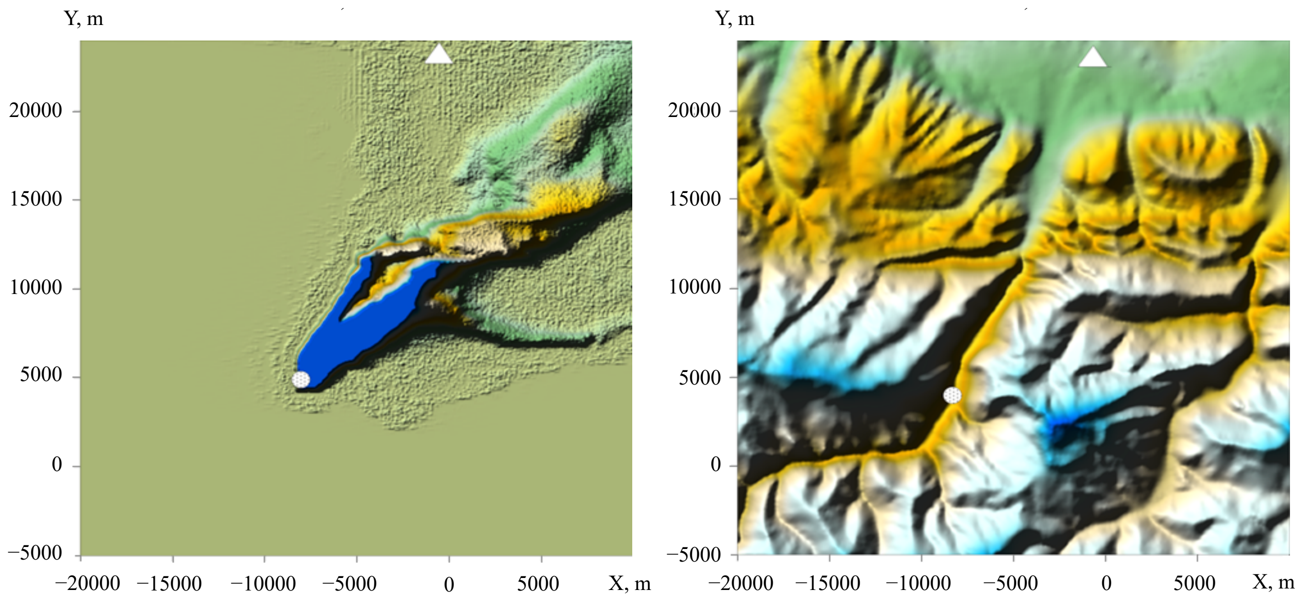


Fig. 1. Forecast maps of the concentration of polluting substance (PS): *a* — south-easterly wind; *b* — south-south-easterly wind; *c* — south wind; *d* — heights.
The *x*-axis is directed to the east, *y* — to the north; the reference point is chosen on the topographic map arbitrarily, near the tailings dump

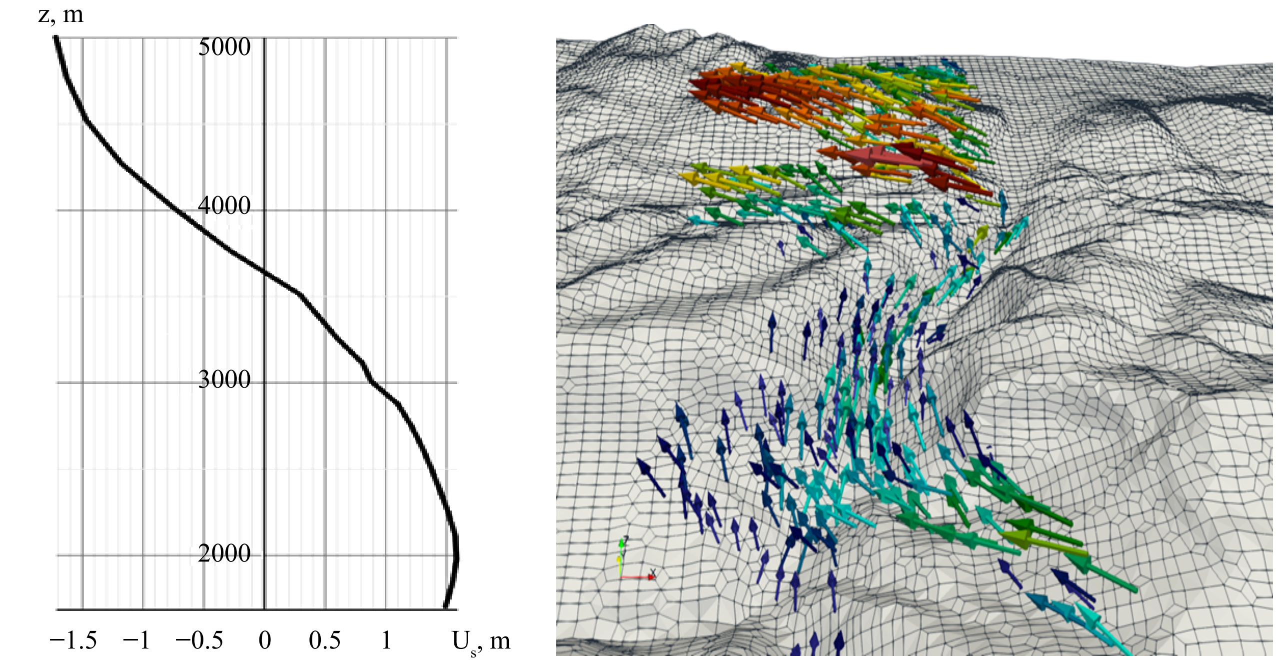
Fig. 1 shows the predicted value of the concentration of PS on the slopes of the Alagir gorge and in the area of the gorge›s exit to the plain near Alagir for synoptic situations in which the concentration of PS will be maximum. The concentration of PS $0.1C_{max}$, shown in Fig. 1, exceeds the MPC (for lead and zinc) by 2–3 times.

Fig. 1 *a* shows that the concentration of PS on the slopes of the gorges tracks the topography of the surface: the dust aerosol spreads along the axis of the gorge, and is also captured by areas of increased turbulence and carried by the wind. Fig. 1 illustrates the spread of PS to the northeast with a southerly wind, with only a small number of them falling into the suburbs of Alagir. For the south-eastern and south-south-eastern cases near Alagir, the number of PS is reached, exceeding the MPC by 2–3 times for both lead and zinc.

1. Jet streams. The propagation of PS along the gorge is determined not only by the external wind, but also by the jet stream, which occurs in a direction perpendicular to the cross-section of the gorge. In all calculations, a geostrophic approximation is used, in which a balance is maintained in the free atmosphere between the pressure drop and the Coriolis force, which makes it possible to calculate stationary air flows over a flat surface. Inside the cross-section of the gorge, this balance is disturbed, as a result, an air flow is formed inside the gorge with a power depending on the baric gradient.

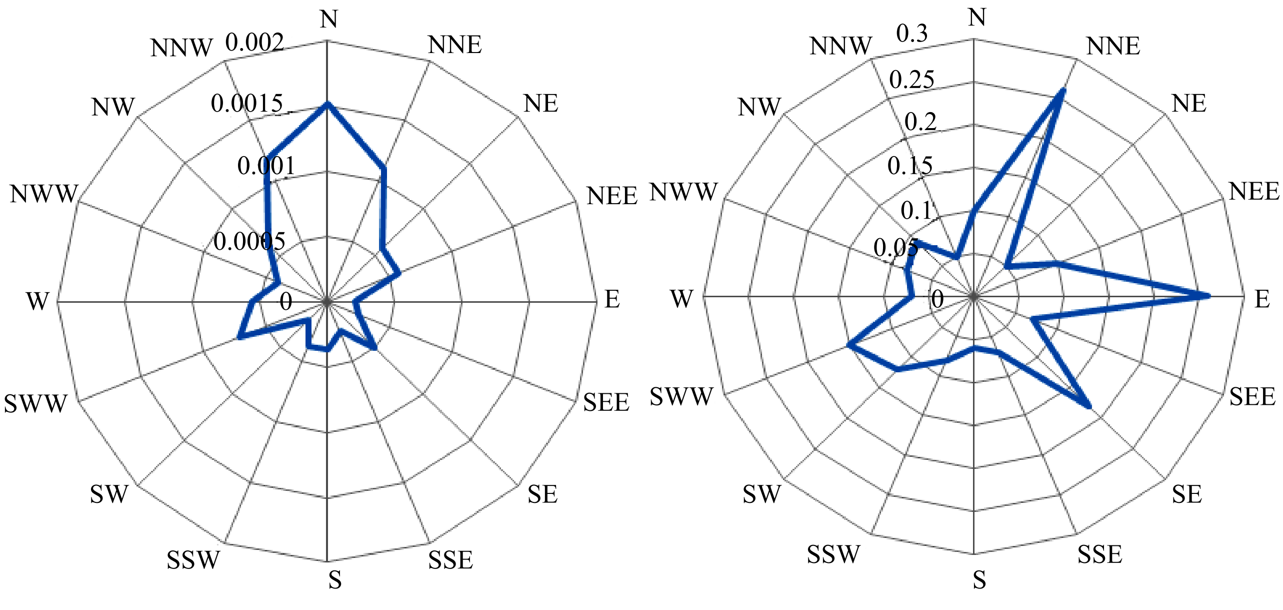
For example, in Fig. 2 and the profile of the northern component of the wind speed (perpendicular to the external wind) above the tailings dump for the case of an easterly wind is given. The northern component of the wind speed directed along the gorge reaches a value of 1.5 m/s, while the wind over the gorge does not have a northern component. In Fig. 2 *b* for the same case, the spatial distribution of the northern component of wind speed is presented. At the exit of the gorge, the jet stream turns to the west under the influence of an external wind. In almost all calculated cases, a similar jet stream occurs, inside of which the source PS is located, which changes the pattern of their scattering, which spreads mainly to the north or south along the gorge.

2. Pulsation frequencies of jet streams. At the point of the computational grid located above the tailings dump, all calculated fields were recorded after each time step. The analysis of these data showed that the flow over the tailings dump in most calculations is non-stationary under constant boundary conditions. For the southeast wind, the frequency is 0.0005 Hz and the pulsation amplitude is ≈0.18 m/s; for the southeast — 0.00024 Hz and ≈0.07 m/s, respectively; for the south wind — 0.00037 Hz and ≈ 0.06 m/s.



a) *b)*

Fig. 2. Jet stream in the Alagir gorge: *a* — profile of the northern component of the wind speed over the tailings dump; *b* — spatial behavior of the jet stream (view from the south of the Alagir gorge in the area of the tailings)



a) *b)*

Fig. 3. Frequencies and amplitudes of oscillations at a point located above the tailings dump at a height of about 20 meters: *a* — frequencies and *b* — amplitudes of oscillations

Fig. 3 shows the frequencies (Fig. 3 *a*) and oscillation amplitudes (Fig. 3 *b*) obtained as a result of 16 calculations for different wind directions at the upper boundary, at a point located above the tailings storage at an altitude of about 20 meters. It can be seen that the frequencies (Fig. 3 *a*) are elongated along the northern direction close to the direction of the gorge axis, and the largest pulsation amplitudes (Fig. 3 *b*) are located in the north-northeast direction coinciding with the gorge axis, as well as in the east and south-east directions when jet currents arise.

Probably, such slow and small changes in wind speed inside the gorge do not lead to noticeable changes in the transfer of PS. In the case of a north-northeast wind, the oscillation occurs in 15 minutes at 0.25 m/s, which leads to the appearance of dust clouds, increased turbulence and increased air removal from the gorge.

3. Wind rose. Wind roses and wind strength by direction, based on satellite measurements of atmospheric characteristics provided by the European Copernicus Global Monitoring System (EuMetSAT and Sentinel weather satellites) [24–25] and measurements provided by the NASA weather satellite system (GEOS, Terra, Aqua) [26] for 20 years of measurements, are given in [4] (Fig. 2). The differences observed there can be attributed to the discrepancy of the areas (about 10×10 km or more for different weather satellites) for which measurements are provided, as well as the averaging time of these measurements.

Based on the available data, it is possible to draw conclusions about the repeatability of the synoptic situations considered in this paper: the repeatability of the south wind is 15.0 % according to Copernicus (ERA-5 reanalysis model) and 10.1 % according to NASA (MERRA2 reanalysis model); south-east — 10.4 % and 3.3 %, respectively; south-south-eastern — 20.9 % and 5.2 %. Thus, the synoptic situations under consideration occur quite often, their total repeatability is 46.3 % according to Copernicus and 18.6 % according to NASA, and their consequences need to be analyzed and monitored.

The accuracy of the wind rose obtained from 16 computational experiments for 16 directions of the external wind and the wind rose measured by a weather station located in the Alagir gorge near the Unal tailings dam was compared. This comparison is described in [4] (Fig. 3) and shows satisfactory agreement with the exception of southern winds, which are more winds in the model rose. Both the shape of the wind rose and the repeatability of the other wind directions practically coincide.

Discussion and Conclusion. The results obtained show that the Unal tailing dump is a source of dust containing soil pollutants. During the existence of the tailing dump, pollution can become very large-scale, as a result of which field studies of the soil in the Alagir area are required, as well as measures for its reclamation.

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MATHEMATICAL MODELLING
МАТЕМАТИЧЕСКОЕ МОДЕЛИРОВАНИЕ

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Stationary and Non-Stationary Periodic Flows Mathematical Modelling using Various Vortex Viscosity Models

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Abstract

Introduction. Mathematical modelling of currents is an urgent research topic in the field of hydrodynamics and oceanography. Despite ongoing research in the field of developing accurate and efficient numerical methods for solving Navier-Stokes equations that take into account vortex viscosity, the problems of accurate prediction and control of turbulence remain unresolved. The influence of nonlinear effects in vortex viscosity models on the accuracy of forecasts and their applicability to various flow conditions also remains relevant. The aim of the study is to study the influence of linearized and quadratic bottom friction and two turbulence models on the numerical solution of stationary and non-stationary periodic flows. Special emphasis is placed on comparing numerical results with analytical solutions within the framework of using various models of bottom friction.

Materials and Methods. The computational models used in this study are based on a simplified two-dimensional wave model and full three-dimensional Navier-Stokes equations. The classical model of shallow water motion and the 2D model without taking into account dynamic changes in the geometry of the reservoir surface are derived from a system of equations for a spatially inhomogeneous three-dimensional mathematical model of wave hydrodynamics of a shallow reservoir. Analytical solutions were found by linearization of the equations, which obviously has its limitations. A distinction is made between two types of nonlinear effects — nonlinearities caused by higher-order terms in the equations of motion, i. e. terms of advective acceleration and friction, and nonlinear effects caused by geometric nonlinearities, this is due, for example, to different water depths and reservoir widths, which will be important when modelling a real sea.

Results. The results of modelling stationary and non-stationary periodic flows in a schematized rectangular basin using linearized bottom friction are presented. The influence of linearization on the numerical solution is investigated in comparison with analytical profiles using models calculating bottom friction in a quadratic formulation. In combination with quadratic bottom friction, two turbulence models are studied: the constant vortex viscosity and the Prandtl mixing length model. The results obtained as a result of three-dimensional modeling are compared with the results of two-dimensional modelling and analytical solutions averaged in depth.

Discussion and Conclusion. New approaches to modelling and studying flows with variable vortex viscosity are proposed, including analysis of the influence of linearization and the use of various turbulence models. For the linearized and quadratic formulations of bottom friction, it is proved that the numerical results for the case of stationary flow show great similarity with analytical solutions, since the surface height is much less than the water depth and advection can be neglected. The numerical results for the unsteady flow also show a good agreement with the theory. Unlike analytical solutions, numerical modeling has minor deviations in the long run. The study of flows, within the framework of using various turbulence models, will make it possible to take into account the influence of nonlinear effects in vortex viscosity models on the accuracy of forecasts and their applicability to various flow conditions. The results obtained make it possible to better understand and describe the physical processes occurring in shallow waters. This opens up new possibilities for applying mathematical modeling to predict and analyze the impact of human activities on the marine environment and to solve other problems in the field of oceanology and geophysics.

Keywords: hydrodynamics, shallow water reservoir, wave motion, numerical modelling

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Научная статья

Математическое моделирование стационарных и нестационарных периодических течений с использованием различных моделей вихревой вязкости

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Аннотация

Введение. Математическое моделирование течений является актуальной исследовательской темой в области гидродинамики и океанографии. Несмотря на непрекращающиеся исследования в области разработки точных и эффективных численных методов для решения уравнений Навье-Стокса, учитывающих вихревую вязкость, задачи точного предсказания и контроля турбулентности остаются нерешенными. Также актуальными остаются вопросы влияния нелинейных эффектов в моделях вихревой вязкости на точность прогнозов и их применимость к различным условиям течения. Целью исследования является изучение влияния линеаризованного и квадратичного донного трения и двух моделей турбулентности на численное решение стационарных и нестационарных периодических течений. Особый акцент сделан на сравнении численных результатов с аналитическими решениями в рамках использования различных моделей донного трения.

Материалы и методы. Вычислительные модели, применяемые в этом исследовании, основаны на упрощенной двумерной волновой модели и полных трехмерных уравнениях Навье-Стокса. Классическая модель движения мелкой воды и 2D-модель без учета динамического изменения геометрии поверхности водоема получены из системы уравнений для пространственно-неоднородной трехмерной математической модели волновой гидродинамики мелководного водоема. Аналитические решения были найдены путем линеаризации уравнений, что, очевидно, имеет свои ограничения. Проводится различие между нелинейностями, вызванными членами более высокого порядка в уравнениях движения (т. е. членами адвективного ускорения и трения), и геометрическими нелинейностями, связанными, например, с различной глубиной воды и шириной водоема, что будет важно при моделировании реального моря.

Результаты исследования. Представлены результаты моделирования стационарных и нестационарных периодических течений в схематизированном прямоугольном бассейне с использованием линеаризованного донного трения. Исследовано влияние линеаризации на численное решение в сравнении с аналитическими профилями, использующими модели, рассчитывающие донное трение в квадратичной формулировке. В сочетании с квадратичным трением о дно изучаются две модели турбулентности: постоянная вихревая вязкость и модель длины перемешивания Прандтля. Результаты, полученные в результате трехмерного моделирования, сравниваются с результатами двумерного моделирования и аналитическими решениями, усредненными по глубине.

Обсуждение и заключение. Предложены новые подходы к моделированию и исследованию течений с переменной вихревой вязкостью, включая анализ влияния линеаризации и использование различных моделей турбулентности. Для линеаризованной и квадратичной формулировок донного трения доказано, что численные результаты для случая стационарного течения демонстрируют большое сходство с аналитическими решениями, поскольку высота поверхности намного меньше глубины воды и адвекцией можно пренебречь. Численные результаты для нестационарного течения также показывают хорошее соответствие теории. В отличие от аналитических решений численное моделирование имеет незначительные отклонения в долгосрочной перспективе. Исследование течений, в рамках использования различных моделей турбулентности, позволит осуществить учет влияния нелинейных эффектов в моделях вихревой вязкости на точность прогнозов и их применимость к различным условиям течения. Полученные результаты позволяют лучше понять и описать физические процессы, происходящие в мелководных водоемах. Это открывает новые возможности применения математического моделирования для прогнозирования и анализа воздействия человеческой деятельности на морскую среду и для решения других задач в области океанологии и геофизики.

Ключевые слова: гидродинамика, мелководный водоем, волновое движение, численное моделирование

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Introduction. Mathematical modelling of flows is an important and relevant tool for scientific and engineering research, allowing to identify possible risks, optimize processes and investigate complex physical phenomena that are difficult or impossible to study experimentally. The application of the mathematical modeling method makes it possible to study the main characteristics of currents: velocity, pressure, concentration, temperature, which cannot be measured directly. For example, modeling can help predict the spread of pollution in water systems or determine the optimal flood control strategy.

Many scientists are engaged in flow research using various models of vortex viscosity. The analysis of studies [1−10] related to the development of numerical methods aimed at solving the Navier-Stokes equations for complex periodic flows in the field of turbulence and fluid dynamics suggests that modeling stationary and nonstationary periodic flows remains an important scientific and applied problem.

Despite the successes in this direction — the development of more accurate and efficient numerical methods for solving Navier-Stokes equations that take into account vortex viscosity (these methods allow for more accurate modeling of complex flows, such as the flow around bodies with a high degree of vortex activity), there are also unsolved problems. This includes, for example, accurate prediction and control of turbulence. The influence of nonlinear effects in vortex viscosity models on the accuracy of forecasts and their applicability to various flow conditions also remains relevant. Such models make it possible to obtain a more accurate and realistic description of the behavior of the fluid flow. This is especially important when studying turbulent flows, where vortex viscosity is one of the key factors influencing the nature of fluid movement. Modelling of such flows makes it possible to refine the parameters of vortices, determine their effect on other physical processes and develop methods for controlling or controlling the flow.

The use of various vortex viscosity models makes it possible to take into account flow features such as flow geometry, the presence of obstacles, changes in density or viscosity. Each vortex viscosity model has its limitations and its choice depends on specific factors and modeling goals. Comparing the results obtained using different models allows them to be refined and verified, as well as to draw more accurate conclusions about the behavior of the flow.

Materials and Methods. The computational models used in this study are based on a simplified two-dimensional wave model and full three-dimensional Navier-Stokes equations.

A spatially inhomogeneous three-dimensional mathematical model of wave hydrodynamics of a shallow reservoir includes [1]:

– Navier-Stokes equations of motion:

$$\begin{gathered} u'_t + uu'_x + vu'_y + wu'_z = -\frac{1}{\rho} P'_x + \left(\mu u'_x\right)'_x + \left(\mu u'_y\right)'_y + \left(\nu u'_z\right)'_z, \\ v'_t + uv'_x + vv'_y + wv'_z = -\frac{1}{\rho} P'_y + \left(\mu v'_x\right)'_x + \left(\mu v'_y\right)'_y + \left(\nu v'_z\right)'_z, \\ w'_t + uw'_x + vw'_y + ww'_z = -\frac{1}{\rho} P'_z + \left(\mu w'_x\right)'_x + \left(\mu w'_y\right)'_y + \left(\nu w'_z\right)'_z + g; \end{gathered} \tag{1}$$

– continuity equation:

$$\rho'_t + \left(\rho u\right)'_x + \left(\rho v\right)'_y + \left(\rho w\right)'_z = 0, \tag{2}$$

where $\mathbf{V} = \{u, v, w\}$ is the water flow velocity vector; ρ is the density of the aquatic environment; P is the hydrodynamic pressure; g is the acceleration of gravity; μ, ν are the coefficients of turbulent exchange in horizontal and vertical directions; $\mathbf{n}$ is the vector of the normal to the surface describing the boundary of the computational domain.

2D mathematical model of the motion of the aquatic environment is based on 3D model and includes:

– Navier-Stokes equations:

$$u'_t + uu'_x + vu'_y + wu'_z = -\frac{1}{\rho}P'_x + \left(\mu u'_x\right)'_x + \left(\mu u'_y\right)'_y + \left(\eta u'_z\right)'_z,$$

$$v'_t + uv'_x + vv'_y + wv'_z = -\frac{1}{\rho}P'_y + \left(\mu v'_x\right)'_x + \left(\mu v'_y\right)'_y + \left(\eta v'_z\right)'_z;$$

– continuity equation (for incompressible fluid): $u'_x + v'_y + w'_z = 0$;

– equation of hydrostatics: $P = \rho g\,(z + \xi)$.

In the hydrostatic case, the continuity equation has the form [11, 12]:

$$\theta'_t + \left(Hu\right)'_x + \left(Hv\right)'_y = 0,$$

where $\theta = \min(\chi, \xi)$; $H = h + \theta$, h is the depth of the reservoir.

From the developed system of equations, it is possible to obtain a classical model of shallow water movement and a 2D model without taking into account the dynamic change in the geometry of the reservoir surface.

Analytical solutions for a depth-averaged model and a model that contains vertical information are:

$$U = \widetilde{A}\cdot\left(\frac{1}{1 - i\sigma_1}\right)e^{i\omega t},$$

$$\overline{u} = \widetilde{A}\cdot\left(1 - \frac{\widetilde{\gamma}}{bd}\tanh(bd)\right)e^{i\omega t},$$

where $\widetilde{\gamma}$ is a function only of σ_2 and bd.

Thus, the depth-averaged velocities in both models look very similar and can be described by a function of dimensionless parameters σ_1, σ_2 and bd respectively, where:

$$\sigma_1 = \frac{8}{3\pi}c_{f_1}\frac{\widehat{U}}{\omega d}, \quad \sigma_2 = \frac{8}{3\pi}c_{f_2}\frac{\widetilde{u}_b}{\omega d}, \quad bd = \sqrt{\frac{i\omega d^2}{\nu_t}}.$$

Analytical solutions were found by linearization of equations, which has its limitations. A distinction is made between two types of nonlinear effects:

1. Non-linearities caused by higher-order terms in the equations of motion, i.e. the terms of advective acceleration and friction. kU friction linearization is based on optimal reproduction of the prevailing singular progressive wave. Although such linearization is effective for the purposes of this study, it distorts the propagation and generation of other components of the motion of the aquatic environment.

2. Nonlinear effects caused by geometric nonlinearities that result from the dependence of the cross section on the height of the surface. This is due, for example, to the different water depth and width of the reservoir, which will be important when modelling a real sea.

Turbulence modelling. Turbulent viscosity expresses momentum transfer in a turbulent flow. Several models of turbulent viscosity are available:

− constant vortex viscosity model;

− Prandtl length mixing model;

− k–ε model;

− Large eddy simulation (LES) [4, 7–8].

The constant vortex viscosity model is a simple model describing vortex viscosity as the product of velocity and length scale:

$$\nu_e = \frac{1}{6}\kappa d u_*.$$

The Prandtl mixing length model uses the mixing length hypothesis, in which the velocity characterizing turbulent fluctuations is proportional to the velocity difference in the average flow at a distance l_m, at which mixing or momentum transfer occurs, and is determined as $l_m \cdot \frac{\partial \overline{u}}{\partial x}\cdot$ when reused l_m as a control length scale, the vortex viscosity can be written as the product of this scale squared by the local velocity gradient [13–15].

The model k–ε relates the turbulence viscosity to the kinetic energy of turbulence k and the velocity of turbulence dispersion. The evolution of k and ϵ in time is described by the transfer equations.

When working with large coherent turbulent structures, the method of Large eddy simulation (LES) should be used. In LES models, large turbulence scales are directly resolved on the computational grid, while smaller scales are accounted for using the closure formulation.

The simulation is performed using the following boundary conditions:

− losed boundaries on the bottom, embankment or wall (with or without wall friction);

− free surface boundary;

− constant water level at open borders;

− harmoniously changing water level.

The coefficient of friction in the depth-averaged model (c_{f1}), differed from the coefficient of friction in the vertical information model (c_{f2}), while a constant vertical vortex viscosity was used. In practice, numerical modelling usually uses a viscosity that varies vertically in accordance with the turbulent mixing model along the length. Using this definition of vortex viscosity and integrating over water depth provides a logarithmic velocity profile:

$$u(z)=\frac{u_*}{\kappa}\ln\left(\frac{z+d}{z_0}\right), \tag{3}$$

where u_* is the shear stress velocity; κ is the von Karman constant (not to be confused with the bottom friction coefficients κ_1, κ_2). The parameter z_0 may be related to the actual roughness:

$$z_0=\frac{\kappa_N}{30},$$

where κ_N is the empirically determined roughness height.

For the depth-averaged model, the shear stress of the formation can be related to the depth-averaged velocity, through $\tau_b=c_{f_1}|U|U=u_*^2$. in combination with the logarithmic profile of equation (3), an expression for the coefficient of friction is found c_{f1}:

$$\frac{1}{\sqrt{c_{f_1}}}=\frac{1}{\kappa}\ln\left(e^{-1}\frac{d}{z_0}\right). \tag{4}$$

For a 3D model with a vertical dimension, the shear stress of the layer can be related to the coefficient of friction (c_{f2}) through $\tau_b=c_{f2}\,|u_b|\,u_b$. The bottom voltage is defined as:

$$\tau_b=|u_*|u_*\Rightarrow u_b=\frac{u_*}{\sqrt{c_{f_2}}}.$$

As a result, an expression for the coefficient of friction will be obtained:

$$\frac{1}{\sqrt{c_{f_2}}}=\frac{1}{\kappa}\ln\left(e^{-2}\frac{\Delta z_b}{z_0}\right). \tag{5}$$

The ratio between and is found by equating (4) and (5):

$$\frac{1}{\sqrt{c_{f_1}}}=\frac{1}{\sqrt{c_{f_2}}}-\frac{1}{\kappa}\ln\left(e^{-1}\frac{\Delta z_b}{d}\right).$$

Results. Calculations are performed for stationary and non-stationary (periodic flow) flows. In the stationary case, the gradient of the water level is constant over time. In the non-stationary case, a periodically changing flow is investigated. In both cases, numerical modelling is performed using linearized bottom friction corresponding to the analytical approach. The numerical response of horizontal (depth-averaged) velocities should correspond to analytical velocity profiles averaged over depth. The observed difference can only be caused by numerical approximations, i. e. time integration and (horizontal) discretization.

For both flow cases, the geometry of the computational domain is represented as a rectangular basin with two open borders on the short sides and a water depth of 12 m. The width of the pools is small (40 m) compared to the length. For the case of steady flow, the basin is extended by 20.000 m in length. A pool of this length is necessary for the full development of the water level gradient.

The boundary conditions for the stationary case determine the water level of 20 cm at the inflow boundary (left), the water level of 0 m at the outflow boundary (right) and zero normal velocity on the side walls and surface (upper boundary). Thus, the water level is fixed with a slope $i_w=10^{-5}$ (Fig. 1).

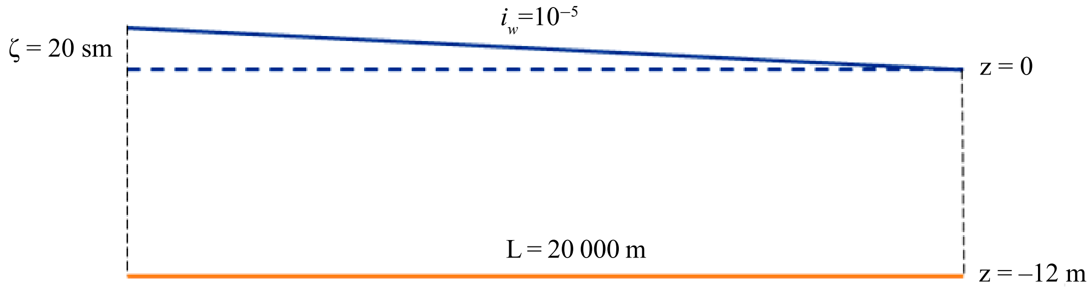

Fig. 1. Steady flow in a long channel

When the 3D results are averaged in depth (3D-DA), they can be directly compared with the corresponding results of the 2D model. The same values were selected for the roughness coefficient κ_N in both models, c_{f1} was chosen to be 0.002, κ_N should be 0.086 m, therefore, c_{f2} will be equal to 0.0042. This is the input data for a linearized bottom friction model.

Thus, the simulation with quadratic bottom friction was actually performed before the linearized case. This allows comparison between all models (2D and 3D, linear and quadratic).

In combination with quadratic bottom friction, two turbulence models are studied: the constant vortex viscosity and the Prandtl mixing length model. Ultimately, both calculations will result in the same velocity averaged over depth, provided that a certain value is selected for the viscosity of the vertical vortex corresponding to the selected specific bottom friction coefficients, resulting v_t = 0.22 m^2/s (Table 1).

Table 1

Input parameters for the case of steady flow

Parameter	The calculated value of the parameter
c_{f1}	0.002
c_{f2}	0.004
κ_1	$2.9 \cdot 10^{-5}$
κ_2	$8.3 \cdot 10^{-5}$
v_t	0.22 m^2/s

The simulation was performed for a long channel with linearized bottom friction. The values of the input parameters used for this simulation are summarized in Table 2. Theoretical velocity profiles for steady-state flow with linearized bottom friction are used to compare numerical results with analytical ones. Unlike analytical solutions, numerical modelling has minor deviations in the long run.

Table 2

Input parameters for stationary flow with linearized bottom friction

Fundamental parameters	Derived parameters
$i_\omega = 10^{-5}$	$\Delta z_b = d/nz = 2$ m
$d = 12$ m	0.004
$\kappa_N = 0.086$ m	$\kappa_1 = 5.7 \cdot 10^{-5}$
$nz = 6$	$\kappa_2 = 8.3 \cdot 10^{-5}$
v_t	$v_t = 0.22$ m^2/s

In both 2D and 3D, numerical results are consistent with analytical solutions. When constructing the velocity profile $u(z)$ in AZOV3D, an ideal correspondence to the theoretical parabolic profile was demonstrated (Fig. 2, green shows the result of AZOV3D, black shows the analytical solution).

The following is an example that examines the effect of linearization on the numerical solution in comparison with analytical profiles for the same long channel. For this example, AZOV3D models are used that calculate bottom friction in a quadratic formulation.

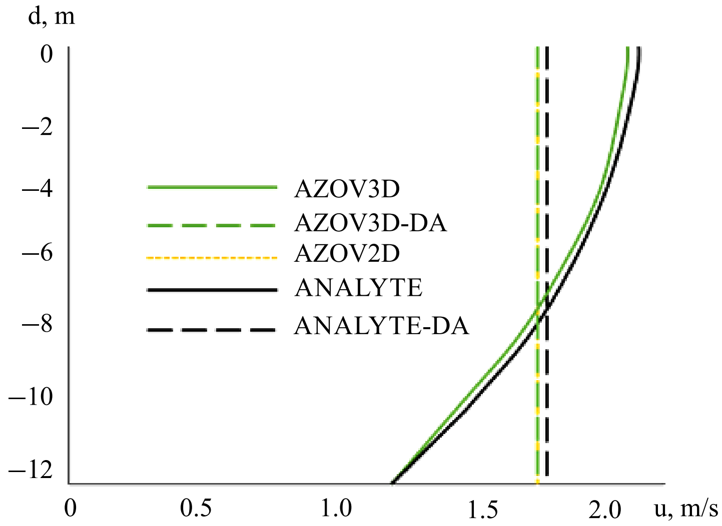

Fig. 2. Parabolic velocity profiles for steady flow with linearized bottom friction and constant vertical vortex viscosity

First, a simulation with a constant vortex viscosity is performed, and then another turbulence model is tested — the mixing length model. Table 3 shows the values of the input parameters used for this simulation.

Table 3

Input parameters for the stationary case with quadratic lower friction

Fundamental parameters	Derived parameters
$i_{\omega} = 10^{-5}$ $d = 12$ m $\kappa_N = 0.086$ m $nz = 6$ $\kappa = 0.4$	$\Delta z_b = d/nz = 2$ m $c_{f1} = 0.002$ $c_{f2} = 0.0042$ $v_t = 0.22$ m²/s $u_* = 0.077$ m/s

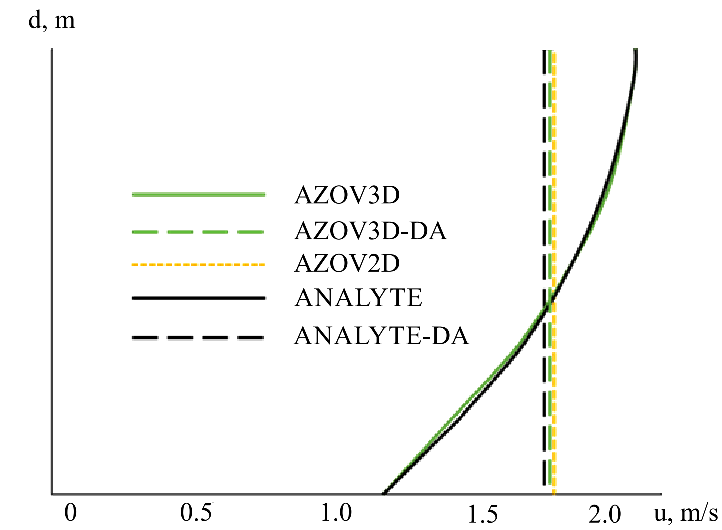

Fig. 3. Parabolic velocity profiles for steady-state flow with quadratic bottom friction and constant vertical vortex viscosity

The numerical results are compared with the theoretical velocity profile in a similar way to the linearized case and are completely consistent with the analytical solution, as shown in Fig. 3 for the case with constant vortex viscosity and in Fig. 4 for the case with the mixing length model. The velocity profiles are reproduced correctly: in the case of a constant vortex viscosity, a parabolic velocity profile, and in the case of a mixing length model, a logarithmic profile. Both 2D and 3D modeling correspond to the theory.

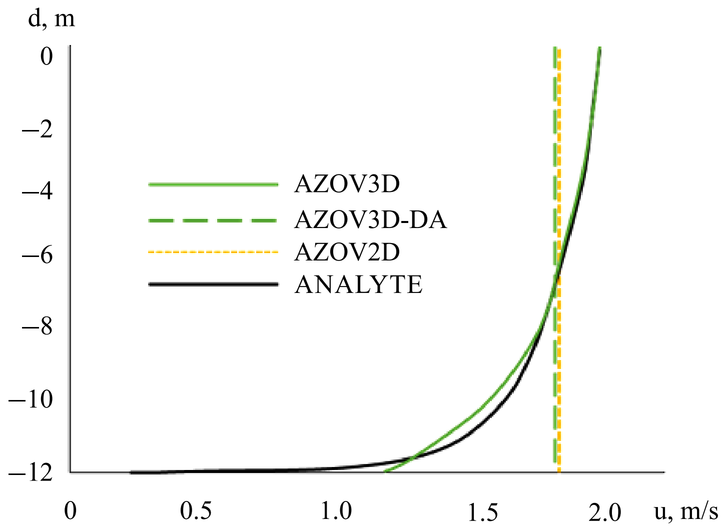

Fig. 4. Logarithmic velocity profiles for steady-state flow with quadratic bottom friction and viscosity determined by the mixing length model

For both the linearized formulation of bottom friction and the quadratic one, it is proved that the numerical results for stationary flow, as expected, show great similarity with analytical solutions. Since the surface height is much less than the depth of the water, advection can be neglected, so that the numerical characteristic is reproduced in full accordance with the theory, providing a good starting point for unsteady flow.

The numerical results for the unsteady flow show a good agreement with the theory. In addition, the analytical approach showed that the speed calculated using a 2D model is more likely to be greater than the 3D speed than vice versa. This behavior is certainly reflected in the numerical examples above, since all calculated ratios are greater than one.

Discussion and Conclusion. Calculations have been performed for stationary and non-stationary (periodic flow) currents using linearized bottom friction. In both 2D and 3D, numerical results are consistent with analytical solutions. When constructing the velocity profile in AZOV3D, an ideal correspondence to the theoretical parabolic profile is shown.

The effect of linearization on the numerical solution is studied in comparison with analytical profiles using models calculating bottom friction in a quadratic formulation. In combination with quadratic bottom friction, two turbulence models are studied: the constant vortex viscosity and the Prandtl mixing length model. The numerical results are compared with the theoretical velocity profile in a similar way to the linearized case and are consistent with the analytical solution, but unlike analytical solutions, numerical modelling has minor deviations in the long run. A parabolic velocity profile is obtained in the case of a constant vortex viscosity, and a logarithmic one in the case of a mixing length model.

For the linearized and quadratic formulations of bottom friction, it is proved that the numerical results for the case of stationary flow show great similarity with analytical solutions, since the surface height is much less than the water depth and advection can be neglected. The numerical results for the unsteady flow also show a good agreement with the theory. The analytical approach showed that the speed calculated using a 2D model is highly likely to be higher than the 3D speed, which is confirmed by numerical data. The study of flows in various turbulence models makes it possible to determine the influence of nonlinear effects on the accuracy of forecasts in vortex viscosity models and their applicability to various flow conditions.

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Mathematical Model of Spreading Oil Pollution in Coastal Marine Systems

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Abstract
Introduction. The negative consequences that may arise due to an accidental oil spill are difficult to account for, since they disrupt many natural processes and relationships within the ecosystem of the reservoir. After an oil spill, a dense layer of oil film forms on the water surface quite quickly, preventing access to air and light (after a spill of one ton of oil, an oil slick about 10 mm thick forms on the surface of the reservoir after 10 minutes). As a result, the fauna and flora of the reservoir suffer. If the accident occurred in the coastal zone near a populated area, then the toxic effect is enhanced, because petroleum products in combination with various pollutants of human origin can form dangerous compounds. For high-risk areas (the main routes of transportation of petroleum products, places of their bunkering and unloading, etc.), it is necessary to predict various scenarios for the spread and transformation of oil pollution, taking into account their multifractional composition, turbulent diffusion and advective transport, destruction under the influence of natural factors. The aim of the work is to build a linearized non-stationary spatially heterogeneous mathematical model of transport and transformation of oil pollution, taking into account the above factors.
Materials and Methods. The oil that has entered the aquatic environment is represented as a surface and suspended substance in the water column. Oil is subject to a variety of transformation processes: advection, gravitational spreading, emulsification, dispersion, dissolution, biodegradation, etc. The study of these processes and their forecasting, as a rule, requires the development of mathematical and software. In mathematical and numerical modeling, one should start from the system of Navier-Stokes equations and continuity equations, as well as introduce additional physical tolerances of the flow geometry, acceptable and justified in each case, as shown by world experience and objective analysis of the physical picture of processes. Mathematical modeling of the oil distribution process in coastal marine systems has been performed.
Results. Mathematical oil distribution model has been created, taking into account its multifractional composition. It is assumed that oil fractions can be in water in dissolved or undissolved states. The modeling takes into account such physical characteristics of particles as density, acceleration of gravity, molar mass, etc. After the linearization of the problem under consideration, difference schemes using extended uniform grids were constructed.
Discussion and Conclusion. Pollution caused by an oil spill in the aquatic environment occurs very quickly and is often very destructive. An important factor will be prompt response, which plays a crucial role in minimizing its negative consequences. Modeling of the oil spill process can be useful for determining the location and condition of oil at sea, conducting a risk analysis of the spread of the substance and developing measures to localize and eliminate pollution.

Keywords: coastal marine systems, emergency oil spill, oil slick, multi-fraction composition of oil, concentration of oil particles, mathematical modelling, continuous model approximation

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Научная статья

Математическая модель процесса распространения нефтяных загрязнений в прибрежных морских системах

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Аннотация

Введение. Негативные последствия, которые могут возникнуть по причине аварийного разлива нефти, носят, как правило, трудно учитываемый характер, поскольку нарушают многие естественные процессы и взаимосвязи внутри экосистемы водоёма. После разлива нефти на водной поверхности довольно быстро образуется плотный слой нефтяной пленки, препятствующий доступу воздуха и света (после разлива одной тонны нефти через 10 минут на поверхности водоёма образуется нефтяное пятно толщиной около 10 мм). Вследствие этого страдает животный и растительный мир водоема. Если авария произошла в прибрежной зоне неподалеку от населенного пункта, то токсический эффект усиливается, потому что нефть/нефтепродукты в сочетании с различными загрязнителями человеческого происхождения могут образовывать опасные соединения. Для территорий повышенного риска (основных маршрутов транспортировки нефтепродуктов, мест их бункеровки и выгрузки и др.) необходимо прогнозировать различные сценарии распространения и трансформации нефтяных загрязнений с учетом их многофракционного состава, турбулентной диффузии и адвективного переноса, деструкции под воздействием природных факторов и т. д. Целью работы является построение линеаризованной нестационарной пространственно-неоднородной математической модели транспорта и трансформации нефтяных загрязнений с учетом перечисленных выше факторов.

Материалы и методы. Попавшая в водную среду нефть представляется в виде поверхностной и взвешенной в водной толще субстанции. Нефть подвержена множеству трансформационных процессов: адвекции, гравитационному растеканию, эмульгированию, диспергированию, растворению, биодеградации и др. Исследование данных процессов и их прогнозирование, как правило, требует разработки математического и программного обеспечения. Как показывает мировой опыт и объективный анализ физической картины процессов, при математическом и численном моделировании следует отталкиваться от системы уравнений Навье-Стокса и уравнений неразрывности, а также вводить дополнительные физические допуски геометрии потока, приемлемые и обоснованные в каждом конкретном случае. С учетом данных соображений выполнено математическое моделирование процесса распространения нефти в прибрежных морских системах.

Результаты исследования. Создана математическая модель процесса распространения нефти, учитывающая её многофракционный состав. Предполагается, что фракции нефти могут находиться в воде в растворенном или нерастворенном состояниях. При моделировании учитываются такие физические характеристики частиц как плотность, ускорение свободного падения, молярная масса и др. После линеаризации рассматриваемой задачи были построены разностные схемы, использующие расширенные равномерные сетки.

Обсуждение и заключение. Загрязнение, вызванное разливом нефти в водной среде, происходит очень быстро и нередко является весьма разрушительным. В данной ситуации важным фактором будет оперативное реагирование, играющее решающую роль для минимизации его негативных последствий. Моделирование процесса разлива нефти может быть полезным для определения местоположения и состояния нефти в море, проведения риск-анализа распространения субстанции и разработке мер по локализации и ликвидации загрязнения.

Ключевые слова: прибрежные морские системы, аварийный разлив нефти, нефтяной слик, многофракционный состав нефти, концентрация частиц нефти, математическое моделирование, аппроксимация непрерывной модели

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Introduction. There is an increase in the volume of trade in oil and petroleum products all over the world, with a significant share in their transportation being occupied by maritime shipping. To ensure the environmental safety of waterways and nearby infrastructure, certain restrictions and measures are observed throughout the entire transportation of goods. Despite this, over the past 50 years, 5.86 million tons of oil spilled into the sea have been recorded in the world. Moreover, about 80 % of this oil is spilled at a distance of no more than 10 nautical miles from the coast [1]. The negative consequences of oil pollution of reservoirs can be significantly reduced with timely localization and elimination of pollution. For these purposes, a developed set of measures is needed for their use by rapid response services. This set of measures, among other things, should contain some apparatus that allows forecasting the distribution of oil pollution. These forecasts require the use of mathematical and numerical modelling methods [2–4].

Scientific research in this area is carried out in Russia and abroad by such scientific centers as the P.P. Shirshov Institute of Oceanology of the Russian Academy of Sciences (Russia), the Institute of Water Problems of the Russian Academy of Sciences (Russia), the State Hydrological Institute (Russia), the Chinese Petroleum University and the Institute of Oceanology of the Chinese Academy of Sciences in Qingdao (China), the universities of Tasmania and Macquarie (Australia), Memorial University of Newfoundland (Canada)In Russia and abroad, etc. [5–9]. The accumulation of new knowledge and experimental data encourages us to obtain new results on the problem we are interested in.

This paper presents a mathematical model of the distribution of oil pollution, taking into account the following physical parameters and processes: the multifractional composition of oil, turbulent diffusion and advective transfer, evaporation, destruction under the influence of microorganisms, etc. This mathematical model is integrated with the hydrodynamic model described, for example, in [10, 11]. For the initial boundary value problem modeling the processes under consideration, difference schemes on grids with uneven steps in boundary cells (near the boundary) are constructed.

Materials and Methods

Problem statement. We will use a rectangular Cartesian coordinate system *Oxyz*. Let $\Omega \subset R^3$ be the calculated area, $\Omega = \{0 < x < L_x, 0 < y < L_y, 0 < z < L_z\}$. We consider the case of an oil release within a short time interval (a single-stage release) into the area under consideration. The oil that has entered the area Ω forms a spot on the free surface Ω_0. The area of coverage of the initial unexploded oil slick is indicated by σ.

Note that in the initial boundary value problem modelling the spread of oil pollution, a number of processes are considered on the surface of a reservoir and therefore a two-dimensional formulation is used here. The process of oil distribution and transformation in the coastal zone is described by the following equations [12]:

– equations for the concentration of the fraction of the oil number α ocated in the surface layer:

$$\frac{\partial c_\alpha}{\partial t} + u\frac{\partial c_\alpha}{\partial x} + v\frac{\partial c_\alpha}{\partial y} = \frac{\partial}{\partial x}\left(\mu_h^*\frac{\partial c_\alpha}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu_h^*\frac{\partial c_\alpha}{\partial y}\right) - \left(\frac{K_E P_\alpha}{R\theta} + K_D S_\alpha\right) X_\alpha m_\alpha - \frac{\omega_\alpha c_\alpha}{q\left(c_\alpha + K_s\right)} M, \tag{1}$$

$$c_\alpha\big|_{t=0} = \begin{cases} 0, & (x,y) \notin \sigma, \\ c_{\alpha 0}, & (x,y) \in \sigma; \end{cases} \quad \frac{\partial c_\alpha}{\partial \vec{n}} = 0, \ (x,y) \in \gamma; \tag{2}$$

– equations for the concentration of microorganisms — destructors of oil:

$$\frac{\partial M}{\partial t} + u\frac{\partial M}{\partial x} + v\frac{\partial M}{\partial y} = \frac{\partial}{\partial x}\left(\mu_h\frac{\partial M}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu_h\frac{\partial M}{\partial y}\right) + \frac{\omega_\alpha c_\alpha}{c_\alpha + K_s} M - \lambda M, \tag{3}$$

$$M\big|_{t=0} = M_0, \quad \frac{\partial M}{\partial \vec{n}} = 0, \quad (x,y) \in \gamma; \tag{4}$$

– equations for the concentration of the fraction of the number α of oil in the dissolved state:

$$\frac{\partial \varphi_\alpha}{\partial t} + u\frac{\partial \varphi_\alpha}{\partial x} + v\frac{\partial \varphi_\alpha}{\partial y} + w\frac{\partial \varphi_\alpha}{\partial z} = \frac{\partial}{\partial x}\left(\mu_h\frac{\partial \varphi_\alpha}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu_h\frac{\partial \varphi_\alpha}{\partial y}\right) + \frac{\partial}{\partial z}\left(\mu_v\frac{\partial \varphi_\alpha}{\partial z}\right), \tag{5}$$

$$\frac{\partial \varphi_\alpha}{\partial z} = K_D S_\alpha X_\alpha m_\alpha, \ (x,y,z) \in \Omega_0, \tag{6}$$

$$\frac{\partial \varphi_\alpha}{\partial \vec{n}} = 0, \quad (x,y,z) \in \Omega \setminus \Omega_0. \tag{7}$$

The following designations are used in equations (1)–(7): *u*, *v*, *w* are the components of the aqueous medium velocity vector; c_α is the concentration of the fraction of the oil number α located in the surface layer, $\alpha = \overline{1, A'}$; $\mu_h^* = \mu_h + (\rho_\alpha - \rho_w) g h^3 / \mu_h$ (μ_h is the coefficient of horizontal diffusion of particles, *g* is the acceleration of gravity, $\rho_\alpha \rho_w$ are the particle densities of the fraction α and water, respectively, *h* is the thickness of the oil film); K_E is the mass transfer coefficient for hydrocarbon, $K_E = 2{,}5 \cdot 10^{-3} U^{0.78}$ (*U* is the wind speed relative to water); P_α is the vapor pressure of the fraction particles α; *R* is the universal gas constant, *R* = 8.314; θ is the ambient temperature above the surface of the spot; K_D is the coefficient of mass transfer of dissolution; S_α is the solubility in water of the particles of the fraction α, $\alpha = \overline{A'+1, A}$; X_α is the molar fraction of fraction particles α; m_α is the value of the molar mass of the fraction particles α; q is the value of the proportionality coefficient between the number of microorganisms and the absorbed substrate; M is the concentration of microorganisms; ω_α is the value of the maximum growth rate of microorganisms when feeding on fraction particles α; K_S is the saturation coefficient value; λ is the rate of death of microorganisms; φ_α is the concentration of the fraction α of oil in the dissolved state; $\alpha = \overline{A'+1, A}$; μ_v is the coefficient of vertical diffusion; $\vec{n}$ is the vector of the external normal to the surface describing the boundary of the computational domain; γ is the area describing the surface layers of the reservoir.

Mathematical model of the spread of oil pollution is obtained using a superposition of the results of solving the problem (1)–(7) for each fraction.

Results

Linearization of the problem. A uniform grid with a step τ: $\omega_\tau = \{t_n = n\tau, n = 1,..., N; N\tau \equiv T\}$ is built on the time interval $0 < t \le T$. The linearization of the tasks under consideration has been performed on the time grid ω_τ. The linearization was performed in such a way that in equation (1), which determines the concentration of the fraction on a given time layer, the concentrations of microorganisms on the previous time layer were used.

At each time step $n = 1,2,...,N$, $t_{n-1} < t \le t_n$ let the solutions of equations (1)–(3) be the functions $\tilde{c}_\alpha^n$, $\tilde{M}^n$, $\tilde{\varphi}_\alpha^n$, $n = 1,2,..., N+1$ respectively. In this case, the linearized analogue of the problem under consideration for all intervals $t_{n-1} < t \le t_n$, $n = 1,2,...,N$ will be written as:

$$\frac{\partial \tilde{c}_\alpha^n}{\partial t} + u^n \frac{\partial \tilde{c}_\alpha^n}{\partial x} + v^n \frac{\partial \tilde{c}_\alpha^n}{\partial y} = \frac{\partial}{\partial x}\left(\mu_h^* \frac{\partial \tilde{c}_\alpha^n}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu_h^* \frac{\partial \tilde{c}_\alpha^n}{\partial y}\right) - \left(\frac{K_E P_\alpha}{R\theta} + K_D S_\alpha\right) X_\alpha m_\alpha - \frac{\mu_\alpha \tilde{c}_\alpha^n}{q\left(\tilde{c}_\alpha^n + K_s\right)} \tilde{M}^{n-1}, \tag{8}$$

$$\left.\tilde{c}_\alpha^1\right|_{t=0} = \begin{cases} 0, & (x,y) \notin \sigma, \\ c_{\alpha 0}, & (x,y) \in \sigma, \end{cases}$$
$$\tilde{c}_\alpha^n(x,y,t_{n-1}) = \tilde{c}_\alpha^{n-1}(x,y,t_{n-1}),\ n = 2,...,N,\ (x,y) \in \gamma, \tag{9}$$

$$\frac{\partial \tilde{c}_\alpha^n}{\partial \vec{n}} = 0,\ (x,y) \in \gamma; \tag{10}$$

$$\frac{\partial \tilde{M}^n}{\partial t} + u^n \frac{\partial \tilde{M}^n}{\partial x} + v^n \frac{\partial \tilde{M}^n}{\partial y} = \frac{\partial}{\partial x}\left(\mu_h \frac{\partial \tilde{M}^n}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu_h \frac{\partial \tilde{M}^n}{\partial y}\right) + \frac{\mu_\alpha \tilde{c}_\alpha^{n-1}}{\tilde{c}_\alpha^{n-1} + K_s} \tilde{M}^n - \lambda \tilde{M}^n, \tag{11}$$

$$\left.\tilde{M}^1\right|_{t=0} = M_0,$$
$$\tilde{M}^n(x,y,t_{n-1}) = \tilde{M}^n(x,y,t_{n-1}),\ n = 2,...,N,\ (x,y) \in \gamma, \tag{12}$$

$$\frac{\partial \tilde{M}^n}{\partial \vec{n}} = 0,\ (x,y) \in \gamma; \tag{13}$$

$$\frac{\partial \tilde{\varphi}_\alpha^n}{\partial t} + u^n \frac{\partial \tilde{\varphi}_\alpha^n}{\partial x} + v^n \frac{\partial \tilde{\varphi}_\alpha^n}{\partial y} + w^n \frac{\partial \tilde{\varphi}_\alpha^n}{\partial z} = \frac{\partial}{\partial x}\left(\mu_h \frac{\partial \tilde{\varphi}_\alpha^n}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu_h \frac{\partial \tilde{\varphi}_\alpha^n}{\partial y}\right) + \frac{\partial}{\partial z}\left(\mu_v \frac{\partial \tilde{\varphi}_\alpha^n}{\partial z}\right), \tag{14}$$

$$\frac{\partial \tilde{\varphi}_\alpha^n}{\partial z} = K_D S_\alpha X_\alpha m_\alpha,\ (x,y,z) \in \Omega_0, \tag{15}$$

$$\frac{\partial \tilde{\varphi}_\alpha^n}{\partial \vec{n}} = 0,\ (x,y,z) \in \Omega \setminus \Omega_0. \tag{16}$$

If $n = 1$, then it is sufficient to take the functions of the initial conditions from formulas (9) as $\tilde{c}_\alpha^1(x,y,0)$. If $n = 2$, then the function of the initial condition is taken from formulas (12) $\tilde{M}^1(x,y,0)$, it is substituted into equation (8) and then the solution of problems (8)–(10) and (14)–(16) is carried out in the interval $t_1 < t \le t_2$, in the course of which the concentration values are found $\tilde{c}_\alpha^2(x,y,t_1)$, $\tilde{\varphi}_\alpha^2(x,y,t_1)$. In turn, equation (11), which contains a function $\tilde{c}_\alpha^1(x,y,0)$, in the right part, has a solution $\tilde{M}^2(x,y,t_1)$. When continuing this process for cases $n = 3,...,N$ we will adhere to the described logic. Functions $\tilde{c}_\alpha^n(x,y,t_{n-1}) = \tilde{c}_\alpha^{n-1}(x,y,t_{n-1})$ and $\tilde{\varphi}_\alpha^n(x,y,z,t_{n-1}) = \tilde{\varphi}_\alpha^{n-1}(x,y,z,t_{n-1})$ are determined when solving problems (8)–(10) and (14)–(16) in the interval $t_{n-1} < t \le t_{n-2}$, $n = 3,...,N$ assuming that the known functions are $\tilde{M}^{n-1}(x,y,t_{n-1})$ for the previous time period $t_{n-2} < t \le t_{n-1}$.

Difference scheme for linearized problem. The terms describing the convective transport of particles from equations (8), (11) and (14) have the form in symmetric form [13]:

$$\frac{1}{2}\left[u\frac{\partial \tilde{c}_\alpha^n}{\partial x}+v\frac{\partial \tilde{c}_\alpha^n}{\partial y}+\frac{\partial\left(u\tilde{c}_\alpha^n\right)}{\partial x}+\frac{\partial\left(v\tilde{c}_\alpha^n\right)}{\partial y}\right],$$

$$\frac{1}{2}\left[u\frac{\partial \tilde{M}^{n-1}}{\partial x}+v\frac{\partial \tilde{M}^{n-1}}{\partial y}+\frac{\partial\left(u\tilde{M}^{n-1}\right)}{\partial x}+\frac{\partial\left(v\tilde{M}^{n-1}\right)}{\partial y}\right],$$

$$\frac{1}{2}\left[u\frac{\partial \tilde{\varphi}_\alpha^n}{\partial x}+v\frac{\partial \tilde{\varphi}_\alpha^n}{\partial y}+w\frac{\partial \tilde{\varphi}_\alpha^n}{\partial z}+\frac{\partial\left(u\tilde{\varphi}_\alpha^n\right)}{\partial x}+\frac{\partial\left(v\tilde{\varphi}_\alpha^n\right)}{\partial y}+\frac{\partial\left(w\tilde{\varphi}_\alpha^n\right)}{\partial z}\right],$$

this makes it possible, as a result of discretization, to construct a difference advective transfer operator with the property of skew symmetry [14, 15].

In the domain $\overline{G}$ we will construct a connected grid $\overline{\omega}_h$, $\overline{\omega}_h=\overline{\omega}_x\times\overline{\omega}_y\times\overline{\omega}_z$ where $\overline{\omega}_x=\{x_i: x_i=ih_x;\ i=0,1,...,N_x; N_xh_x\equiv L_x\}$, $\overline{\omega}_y=\{y_j: y_j=jh_x; j=0,1,...,N_y; N_yh_y\equiv L_y\}$, $\overline{\omega}_z=\{z_k: z_k=kh_x;\ \ k=0,1,...,N_y; N_zh_z\equiv L\}$. The set of internal nodes of the grids $\overline{\omega}_h,\overline{\omega}_x,\overline{\omega}_y,\overline{\omega}_z$ will be denoted, respectively, as $\omega_h\omega_x\omega_y\omega_z$. On the space-time grid $\omega_{\tau h}=\omega_\tau\times\omega_h$ we approximate the problem (8)–(16) with the task in nodes shifted by half the grid step speeds and in the corresponding coordinate direction.

Next, the "–" symbol is above the functions c_α^n, c_α^{n-1}, φ_α^n, φ_α^{n-1} and M^n, M^{n-1} will indicate that they belong to the class of grid functions. The functions $\tilde{c}_\alpha^n$, $\tilde{\varphi}_\alpha^n$, $\tilde{M}^n$ are considered as sufficiently smooth functions of continuous variables.

After approximation in the inner nodes of the grid $\overline{\omega}_h$ the equations (8), (11) and (14) will take the form:

$$\begin{gathered}
\frac{\overline{c}_\alpha^n-\overline{c}_\alpha^{n-1}}{\tau}+\frac{1}{2h_x}\left(u^n\left(x_i+0.5h_x,y_j\right)\overline{c}_\alpha^n\left(x_i+h_x,y_j\right)-u^n\left(x_i-0.5h_x,y_j\right)\overline{c}_\alpha^n\left(x_i-h_x,y_j\right)\right)+\\
+\frac{1}{2h_y}\left(v^n\left(x_i,y_j+0.5h_y\right)\overline{c}_\alpha^n\left(x_i,y_j+h_y\right)-v^n\left(x_i,y_j-0.5h_y\right)\overline{c}_\alpha^n\left(x_i,y_j-h_y\right)\right)=\\
=\frac{1}{h_x^2}\left(\mu_h^*\left(x_i+0.5h_x,y_j\right)\left(\overline{c}_\alpha^n\left(x_i+h_x,y_j\right)-\overline{c}_\alpha^n\left(x_i,y_j\right)\right)-\mu_h^*\left(x_i-0.5h_x,y_j\right)\left(\overline{c}_\alpha^n\left(x_i,y_j\right)-\overline{c}_\alpha^n\left(x_i+h_x,y_j\right)\right)\right)+\\
+\frac{1}{h_y^2}\left(\mu_h^*\left(x_i,y_j+0.5h_y\right)\left(\overline{c}_\alpha^n\left(x_i,y_j+h_y\right)-\overline{c}_\alpha^n\left(x_i,y_j\right)\right)-\mu_h^*\left(x_i,y_j-0.5h_y\right)\left(\overline{c}_\alpha^n\left(x_i,y_j\right)-\overline{c}_\alpha^n\left(x_i,y_j-h_y\right)\right)\right)-\\
-\left(\frac{K_EP_\alpha}{R\theta}+K_DS_\alpha\right)X_\alpha m_\alpha-\frac{\omega_\alpha\overline{c}_\alpha^n\left(x_i,y_j\right)}{q\left(\overline{c}_\alpha^n\left(x_i,y_j\right)+K_s\right)}\overline{M}^{n-1}\left(x_i,y_j\right);
\end{gathered}\tag{17}$$

$$\begin{gathered}
\frac{\overline{M}^n-\overline{M}^{n-1}}{\tau}+\frac{1}{2h_x}\left(u^n\left(x_i+0.5h_x,y_j\right)\overline{M}^n\left(x_i+h_x,y_j\right)-u^n\left(x_i-0.5h_x,y_j\right)\overline{M}^n\left(x_i-h_x,y_j\right)\right)+\\
+\frac{1}{2h_y}\left(v^n\left(x_i,y_j+0.5h_y\right)\overline{M}^n\left(x_i,y_j+h_y\right)-v^n\left(x_i,y_j-0.5h_y\right)\overline{M}^n\left(x_i,y_j-h_y\right)\right)=\frac{1}{h_x^2}\left(\mu_h^*\left(x_i+0.5h_x,y_j\right)\cdot\right.\\
\left.\cdot\left(\overline{M}^n\left(x_i+h_x,y_j\right)-\overline{M}^n\left(x_i,y_j\right)\right)-\mu_h^*\left(x_i-0.5h_x,y_j\right)\left(\overline{M}^n\left(x_i,y_j\right)-\overline{M}^n\left(x_i+h_x,y_j\right)\right)\right)+\\
+\frac{1}{h_y^2}\left(\mu_h^*\left(x_i,y_j+0.5h_y\right)\left(\overline{M}^n\left(x_i,y_j+h_y\right)-\overline{M}^n\left(x_i,y_j\right)\right)-\mu_h^*\left(x_i,y_j-0.5h_y\right)\cdot\right.\\
\left.\cdot\left(\overline{M}^n\left(x_i,y_j,0\right)-\overline{M}^n\left(x_i,y_j-h_y\right)\right)\right)+\frac{\omega_\alpha\overline{c}_\alpha^{n-1}\left(x_i,y_j\right)}{\overline{c}_\alpha^{n-1}\left(x_i,y_j\right)+K_s}\overline{M}^n\left(x_i,y_j\right)-\lambda\overline{M}^n\left(x_i,y_j\right);
\end{gathered}\tag{18}$$

$$\begin{gathered}
\frac{\overline{\varphi}_\alpha^n-\overline{\varphi}_\alpha^{n-1}}{\tau}+\frac{1}{2h_x}\left(u^n\left(x_i+0.5h_x,y_j,z_k\right)\overline{\varphi}_\alpha^n\left(x_i+h_x,y_j,z_k\right)-u^n\left(x_i-0.5h_x,y_j,z_k\right)\overline{\varphi}_\alpha^n\left(x_i-h_x,y_j,z_k\right)\right)+\\
+\frac{1}{2h_y}\left(v^n\left(x_i,y_j+0.5h_y,z_k\right)\overline{\varphi}_\alpha^n\left(x_i,y_j+h_y,z_k\right)-v^n\left(x_i,y_j-0.5h_y,z_k\right)\overline{\varphi}_\alpha^n\left(x_i,y_j-h_y,z_k\right)\right)+\\
+\frac{1}{2h_z}\left(w^n\left(x_i,y_j,z_k+0.5h_z\right)\overline{\varphi}_\alpha^n\left(x_i,y_j,z_k+h_z\right)-w^n\left(x_i,y_j,z_k-0.5h_z\right)\overline{\varphi}_\alpha^n\left(x_i,y_j,z_k-h_z\right)=\right.
\end{gathered}$$

$$= \frac{1}{h_x^2}\Big(\mu_h \left(x_i + 0.5h_x, y_j, z_k\right)\Big(\overline{\varphi}_\alpha^n\left(x_i + h_x, y_j, z_k\right) - \overline{\varphi}_\alpha^n\left(x_i, y_j, z_k\right)\Big) - \mu_h \left(x_i - 0.5h_x, y_j, z_k\right)\cdot \tag{19}$$

$$\left(x_i, y_j, z_k\right) - \overline{\varphi}_\alpha^n\left(x_i + h_x, y_j, z_k\right)\Big)\Big) + \frac{1}{h_y^2}\Big(\mu_h \left(x_i, y_j + 0.5h_y, z_k\right)\Big(\overline{\varphi}_\alpha^n\left(x_i, y_j + h_y, z_k\right) - \overline{\varphi}_\alpha^n\left(x_i, y_j, z_k\right)\Big) -$$

$$, y_j - 0.5h_y, z_k\right)\Big(\overline{\varphi}_\alpha^n\left(x_i, y_j, z_k\right) - \overline{\varphi}_\alpha^n\left(x_i, y_j - h_y, z_k\right)\Big)\Big) + \frac{1}{h_z^2}\Big(\mu_v\left(x_i, y_j, z_k + 0.5h_z\right)\Big(\overline{\varphi}_\alpha^n\left(x_i, y_j, z_k + h_z\right) -$$

$$- \overline{\varphi}_\alpha^n\left(x_i, y_j, z_k\right)\Big) - \mu_v\left(x_i, y_j, z_k - 0.5h_z\right)\Big(\overline{\varphi}_\alpha^n\left(x_i, y_j, z_k\right) - \overline{\varphi}_\alpha^n\left(x_i, y_j, z_k - h_z\right)\Big)\Big).$$

To the difference equations (17)–(19), it is necessary to add the initial conditions for $(x, y, z) \in \omega_h$ as well as the approximation of the boundary conditions.

To set the boundary conditions, it is convenient to introduce an extended grid:

$$\overline{\omega}^* = \Big\{\left(x_i, y_j, z_k\right), i = -1, 0, ..., N_x + 1;\ j = -1, 0, ..., N_y + 1; k = -1, 0, ..., N_z + 1;$$

$$x_i = ih_x; y_j = jh_j; z_k = kh_z; N_x h_x = L_x; N_y h_y = L_y; N_z h_z = L_z\Big\}.$$

We will consider the known values of the components of the velocity vector of the aquatic medium at the nodes of the grid $\overline{\omega}^* \setminus \overline{\omega}_h$ with fractional index values, for example, u^n $(-0{,}5h_x, y_j, z_k)$, u^n $(L_x + 0{,}5h_x, y_j, z_k)$, v^n $(x_i, -0{,}5\ h_y, z_k)$, v^n $(x_i, L_y + 0{,}5\ h_y, z_k)$,$w^n$ $(x_i, y_j, -0{,}5\ h_z)$, w^n $(x_i, y_j, L_z + 0{,}5\ h_z)$, etc.

We will approximate the boundary conditions using the example of condition (15). The arguments for boundary conditions (10), (13) and (16) are carried out in a similar way.

We will assume that $\overline{\varphi}_\alpha^n(x, y, z) = 0$, if $(x, y, z) \in \overline{\omega}^* \setminus \overline{\omega}_h$. For those grid nodes $\overline{\omega}^* \setminus \overline{\omega}_h$, that are outside the calculated area, the value of the components of the velocity vector of the aquatic medium is assumed to be zero.

Let's formally write down the expression:

$$C_z\left(\overline{\varphi}_\alpha^n\right)\Big|_{z=0} = \frac{1}{2h_z}\Big(w^n\left(x_i, y_j, 0.5h_z\right)\overline{\varphi}_\alpha^n\left(x_j, y_j, h_z\right) - w^n\left(x_i, y_j, -0.5h_z\right)\overline{\varphi}_\alpha^n\left(x_j, y_j, -h_z\right)\Big), \tag{17}$$

which can be considered as a difference approximation of the convective term at $z = 0$.

Along with (17), it is possible to write the equality for the boundary condition (15):

$$\frac{\overline{\varphi}_\alpha^n\left(x_j, y_j, h_z\right) - \overline{\varphi}_\alpha^n\left(x_j, y_j, -h_z\right)}{2h_z} = K_D S_\alpha X_\alpha m_\alpha,$$

from which we obtain:

$$\overline{\varphi}_\alpha^n\left(x_j, y_j, h_z\right) = \overline{\varphi}_\alpha^n\left(x_j, y_j, -h_z\right) + 2h_z K_D S_\alpha X_\alpha m_\alpha, \tag{18}$$

From expressions (17) and (18) we obtain:

$$C_z\left(\overline{\varphi}_\alpha^n\right)\Big|_{z=0} \equiv \frac{1}{2h_z}\Big(w^n\left(x_i, y_j, 0.5h_z\right)\Big(\overline{\varphi}_\alpha^n\left(x_i, y_j, -h_z\right) + 2h_z K_D S_\alpha X_\alpha m_\alpha\Big) - w^n\left(x_i, y_j, -0.5h_z\right)\overline{\varphi}_\alpha^n\left(x_j, y_j, -h_z\right)\Big). \tag{19}$$

Next, let us formally consider the equality on an extended grid $\overline{\omega}^*$

$$D_z\left(\overline{\varphi}_\alpha^n\right)\Big|_{z=0} \equiv \frac{1}{h_z}\left(\mu_v\left(x_i, y_j, 0.5h_z\right)\frac{\overline{\varphi}_\alpha^n\left(x_i, y_j, h_z\right) - \overline{\varphi}_\alpha^n\left(x_i, y_j, 0\right)}{h_z} - \mu_v\left(x_i, y_j, -0.5h_z\right)\frac{\overline{\varphi}_\alpha^n\left(x_i, y_j, 0\right) - \overline{\varphi}_\alpha^n\left(x_i, y_j, -h_z\right)}{h_z}\right). \tag{20}$$

Since there is no turbulent diffusion on the free undisturbed surface of the reservoir, we can assume that μ_v $(x_i, y_j, -0{,}5\ h_z) \equiv 0$. With this in mind, from the expression (20) we get

$$D_z\left(\overline{\varphi}_\alpha^n\right)\Big|_{z=0} \equiv \frac{1}{h_z^2}\mu_v\left(x_i, y_j, 0.5h_z\right)\Big(\overline{\varphi}_\alpha^n\left(x_i, y_j, h_z\right) - \overline{\varphi}_\alpha^n\left(x_i, y_j, 0\right)\Big).$$

From (18) and (21) we find

$$\mathrm{D}_z\left(\overline{\varphi}_\alpha^n\right)\Big|_{z=0} \equiv \frac{1}{h_z^2}\mu_v\left(x_i, y_j, 0.5h_z\right)\left(\overline{\varphi}_\alpha^n\left(x_j, y_j, -h_z\right) - \overline{\varphi}_\alpha^n\left(x_i, y_j, 0\right) + 2h_z K_D S_\alpha X_\alpha m_\alpha\right).$$

Discussion and Conclusion. The paper presents a mathematical model of the process of spreading and transformation of oil pollution in coastal marine systems. This model takes into account the multifractional composition of oil pollution, turbulent diffusion and advective transport, destruction of oil particles under the influence of microorganisms, etc. The approximation of the proposed model is performed with the second order of accuracy relative to the steps of the spatial grid. The issues related to the study of the monotony of the constructed difference scheme and its convergence to the solution of the initial initial boundary value problem are the subject of further research by the author.

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Pollutions Spreading Process Modelling in an Aquatic Ecosystem

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Abstract

Introduction. Pollution of shallow waters is becoming an increasingly serious problem. It is important to study the mechanisms of pollution distribution in them to protect and restore such vulnerable ecosystems, it is necessary to develop strategies for the development of sustainable and environmentally friendly use of natural resources, minimizing the negative impact on the environment. Part of this work is the construction of a mathematical model for the spread of pollutants (in particular, phosphates) in shallow reservoirs. The aim of the work is to construct scenarios for changes in the concentration of phosphates at various parameters of the model.

Materials and Methods. The phosphate transport mathematical model in a shallow reservoir is described, implemented using a modified alternating triangular iterative method to solving grid equations.

Results. The developed mathematical model is numerically implemented in the form of a software module. This model is an important tool for assessing and predicting the various pollution sources impact to the water quality of ecosystems such as lakes and reservoirs.

Discussion and Conclusion. The resulting model can be used to analyze various pollution scenarios, for example, to determine optimal waste management strategies and prevent pollution of water resources. In addition, the software module developed by the authors allows you to simulate the process of the phosphates concentration changing and can be useful for conducting scientific and engineering research in the aquatic ecology field and developing effective methods for adapting hydrobiocenosis to changes in the aquatic ecosystem.

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

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Научная статья

Моделирование процесса распространения загрязнения водной экосистемы фосфатами

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Аннотация

Введение. Загрязнение мелководных водоемов является очень серьезной проблемой. Для защиты и восстановления таких уязвимых экосистем крайне важно изучить механизмы распространения в них загрязнений, разработать стратегии по развитию устойчивого и экологически чистого использования природных ресурсов, минимизации негативного влияния на окружающую среду. Частью этой работы является построение математической модели распространения загрязнений (в частности, фосфатов) в мелких водоемах. Целью работы является построение сценариев изменения концентрации фосфатов при различных параметрах модели.

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

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

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

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

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

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

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

a) *b)* *c)*

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Taking into account the expression

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

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

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

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

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

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

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

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

Taking into account the expressions:

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

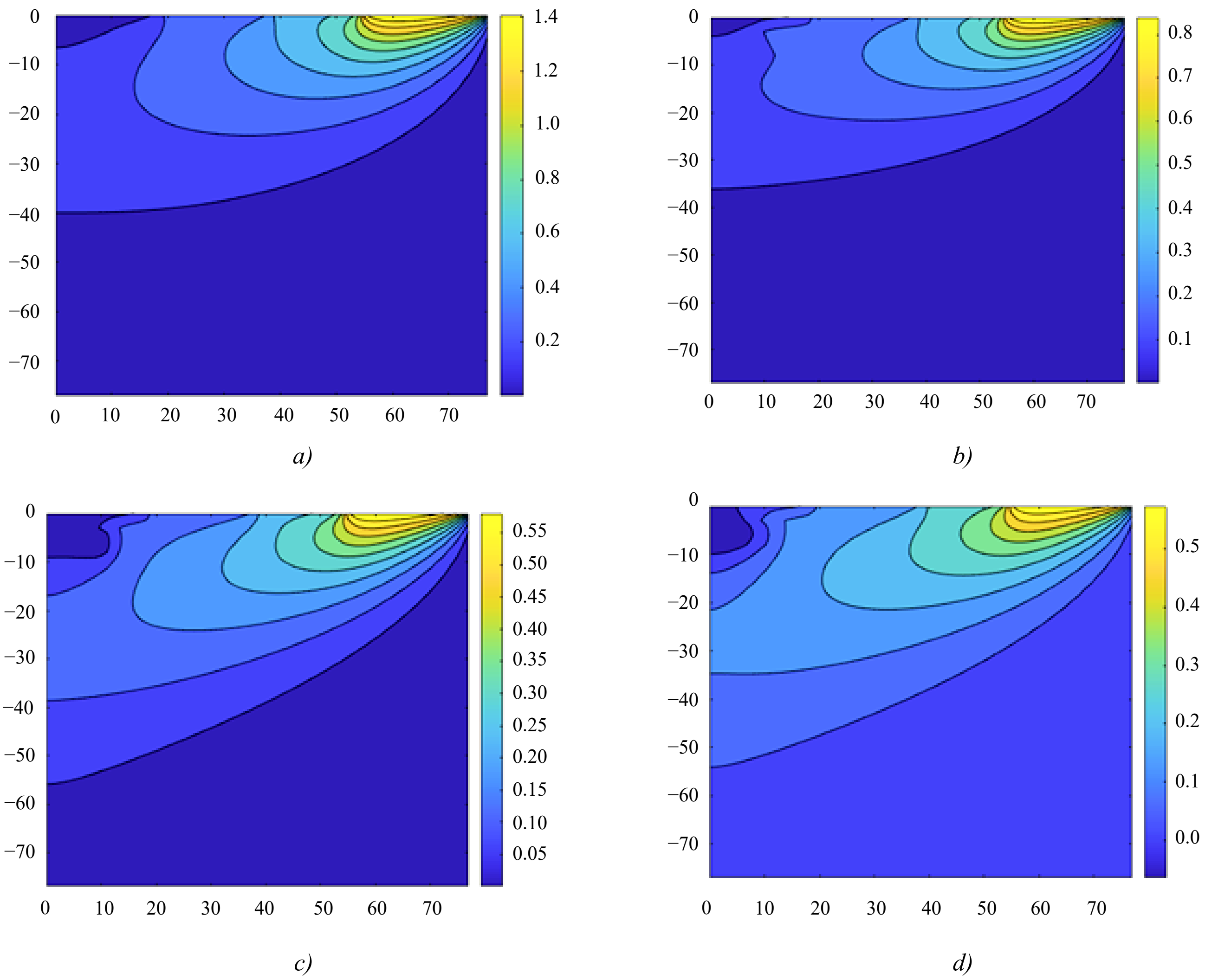
$$\mu_{i+1/2,j}-\mu_{i-1/2,j} = \left(\mu_{i,j}\right)' h_x + O\left(h_x^2\right),$$

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

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

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

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



a) b) c) d)

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

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

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

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

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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 τ. 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

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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 τ. 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

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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.

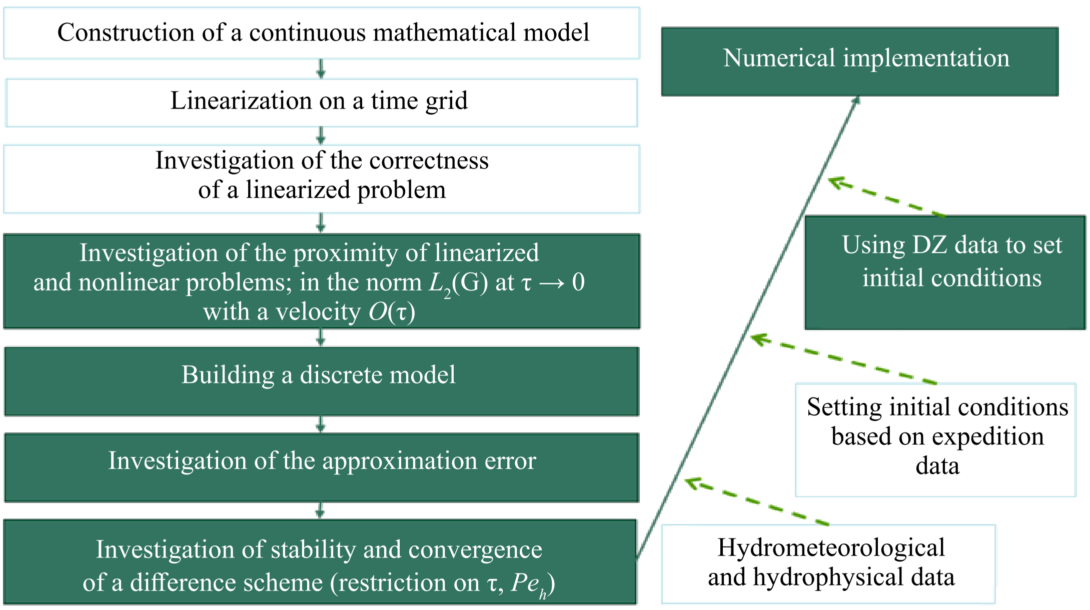

Fig. 1. Research scheme of continuous and discrete mathematical models

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.

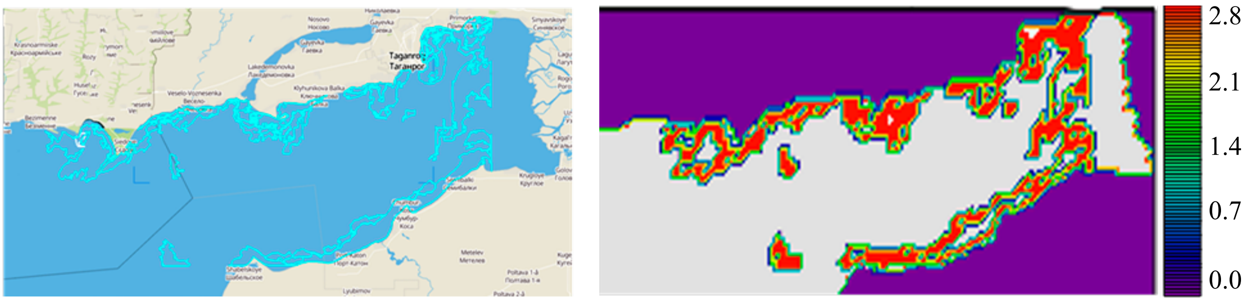

Fig. 2. Determination of the initial modeling of the dynamics of phytoplankton concentrations of RPC "Azov3d"

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]:

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

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 nitrates, 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_{temp}) and its salinity (S) in accordance with the equations (2)–(14) [8]:

$$R_{F_i} = C_{F_i}\left(1 - K_{F_iR}\right)q_{F_i} - K_{F_iD}q_{F_i} - K_{F_iE}q_{F_i}, \quad i = \overline{1,3}, \tag{2}$$

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

$$R_{DOP} = \sum_{i=1}^{3} s_P K_{F_iE} q_{F_i} + K_{PD} q_{POP} - K_{DN} q_{DOP}, \tag{4}$$

$$R_{PO_4} = \sum_{i=1}^{3} s_P C_{F_i}\left(K_{F_iR} - 1\right) q_{F_i} + K_{PN} q_{POP} + K_{DN} q_{DOP}, \tag{5}$$

$$R_{NH_4} = \sum_{i=1}^{3} s_N C_{F_i}\left(K_{F_iR} - 1\right)\frac{f_N^{(2)}\left(q_{NH_4}\right)}{f_N\left(q_{NO_3}, q_{NO_2}, q_{NH_4}\right)} q_{F_i} + \sum_{i=1}^{3} s_N\left(K_{F_iD} + K_{F_iE}\right) q_{F_i} - K_{42} q_{NH_4}, \tag{6}$$

$$R_{NO_2} = \sum_{i=1}^{3} s_N C_{F_i}\left(K_{F_iR} - 1\right)\frac{f_N^{(1)}\left(q_{NO_3}, q_{NO_2}, q_{NH_4}\right)}{f_N\left(q_{NO_3}, q_{NO_2}, q_{NH_4}\right)} \cdot \frac{q_{NO_2}}{q_{NO_2} + q_{NO_3}} q_{F_i} + K_{42} q_{NH_4} - K_{23} q_{NO_2}, \tag{7}$$

$$R_{NO_3} = \sum_{i=1}^{3} s_N C_{F_i}\left(K_{F_iR} - 1\right)\frac{f_N^{(1)}\left(q_{NO_3}, q_{NO_2}, q_{NH_4}\right)}{f_N\left(q_{NO_3}, q_{NO_2}, q_{NH_4}\right)} \cdot \frac{q_{NO_3}}{q_{NO_2} + q_{NO_3}} q_{F_i} + K_{23} q_{NO_2}, \tag{8}$$

$$R_{Si} = s_{Si} C_{F_3}\left(K_{F_3R} - 1\right) q_{F_3} + s_{Si} K_{F_3D} q_{F_3}, \tag{9}$$

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:

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

$$C_{F_3} = K_{NF_3}\, f_{T_{\text{temp}}}\left(T_{\text{temp}}\right) f_S(S) \min\left\{f_P\left(q_{PO_4}\right), f_N\left(q_{NO_3}, q_{NO_2}, q_{NH_4}\right), f_{Si}\left(q_{Si}\right)\right\}, \tag{11}$$

where   is the maximum specific growth rate of phytoplankton.

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

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

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

$$f_S(S) = \begin{cases} k_s, \text{ для } S \le S_{\text{opt}}, \\ \exp\left(-b_1\left\{\left(S - S_{\text{opt}}\right)/S_{\text{opt}}\right\}^2\right), \text{ для } S > S_{\text{opt}}, \end{cases} \tag{14}$$

where $k_s = 1$; T_{opt}, S_{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):

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

$$\frac{\partial q_i}{\partial z} = 0, \text{ at } \textstyle\sum_o \quad \frac{\partial q_i}{\partial z} = -\varepsilon_i q_i \text{ at the bottom } \textstyle\sum_H, \tag{16}$$

$$q_i\,(x, y, z, 0) = q_{0i}\,(x, y, z),\ \vec{V}\ (x, y, z, 0) = \vec{V_0}\ (x, y, z),\ t = 0,\ i \in M, \tag{17}$$
$$T_{\text{temp}}\ (x, y, z, 0) = T_{\text{temp0}}\,(x, y, z),\ S\,(x, y, z, 0) = S_0\ (x, y, z),\ (x, y, z) \in \overline{G}\ ,$$

where ε_i are non-negative constants; $i \in M$; ε_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_{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.

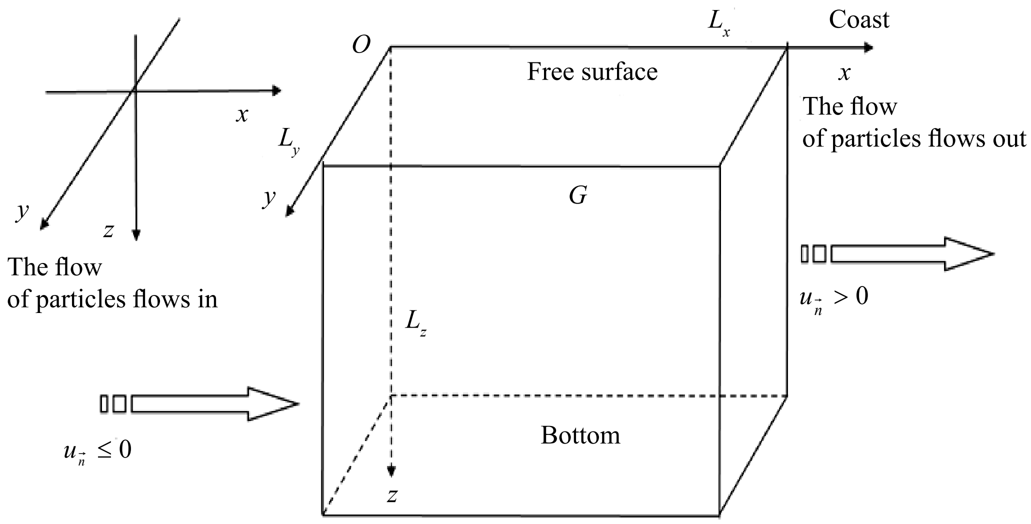

Fig. 3. Schematic representation of the considered area

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).

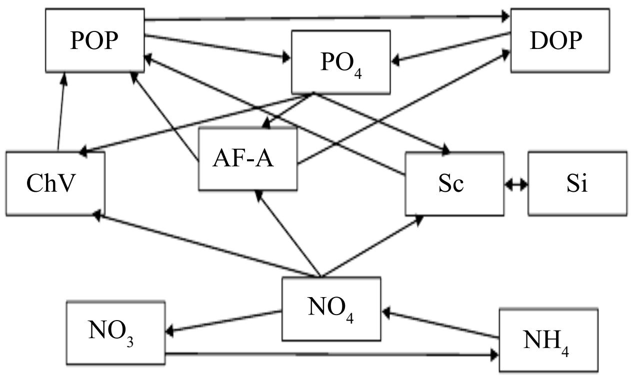

Fig. 4. Structure of the model of biogeochemical transformation of phosphorus, nitrogen and silicon forms

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 ω_τ in time increments τ:

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

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_{qi} ($i \in M$), the solutions of which are functions $\tilde{q}_i^n$ ($n = 1,2,...N$) of the form:

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

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:

$$\frac{\partial z_i^n}{\partial t} + u\frac{\partial z_i^n}{\partial x} + v\frac{\partial z_i^n}{\partial y} + w\frac{\partial z_i^n}{\partial z} - \operatorname{div}\left(\vec{k} \cdot \operatorname{grad} z_i^n\right) = \tilde{R}_{q_i}^n - R_{q_i}^n, \tag{19}$$

$$i = 1,...,10,\ n = 1,...,N,\ (x, y, z) \in G,\ t_{n-1} < t < t_n.$$

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

We will assume that each of the qi 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:

$$\|\xi\|_{L_2(x,y,z)} \equiv (\xi,\xi)^{\frac{1}{2}} \equiv \left(\iiint_G \xi^2(x,y,z)\,dxdydz\right)^{\frac{1}{2}}.$$

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:

$$\int_{t_{n-1}}^{t_n}\left(\iiint_G z_i^n \cdot \frac{\partial z_i^n}{\partial t}\,dG\right)dt + \int_{t_{n-1}}^{t_n}\left(\iiint_G z_i^n \cdot \operatorname{div}\left(\vec{V}\cdot z_i^n\right)dG\right)dt - \int_{t_{n-1}}^{t_n}\left(\iiint_G z_i^n \cdot \operatorname{div}\left(\vec{k}\cdot \operatorname{grad} z_i^n\right)dG\right)dt =$$

$$= \int_{t_{n-1}}^{t_n}\left(\iiint_G \left(\tilde{R}_{q_i}^n - R_{q_i}^n\right)z_i^n\,dG\right)dt.$$

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

$$\left\|z_1^n(x,y,z,t_n)\right\|_{L_2(G)}^2 \le \left\|z_1^{n-1}(x,y,z,t_{n-1})\right\|_{L_2(G)}^2 + \tag{20}$$

$$+2\left[K_{NF_1}\left(1-K_{F_1R}\right) - K_{F_1D} - K_{F_1E} - 4\left[k_h\left(\frac{1}{H_x^2}+\frac{1}{H_y^2}\right) + k_{v_{\min}}\frac{1}{H_z^2}\right]\right]\cdot \int_{t_{n-1}}^{t_n}\left(\iiint_G \left(z_1^n(x,y,z,t)\right)^2 dG\right)dt,$$

guaranteeing the proximity (convergence at $\tau \to 0$) of solutions of a linearized and nonlinear problem. For the substance F_1 (the original function $q_{F1} \equiv q_1$) in $L_2(G)$ on a sequence of grids, if the expression in square brackets is non-negative, we obtain:

$$\omega_\tau(\tau \to 0):\ \left\|z_1^n(x,y,z,t_n)\right\|_{L_2(G)} \underset{C_1 \equiv \text{const}>0}{\le} \underset{n=1,2,\ldots,N}{C_1\tau}.$$

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 τ, 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 ($i = 4,\ldots,10$) 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 $\overline{\omega}_\tau \times \overline{\omega}$, and use the template of the difference scheme (control volume) (Fig. 5).

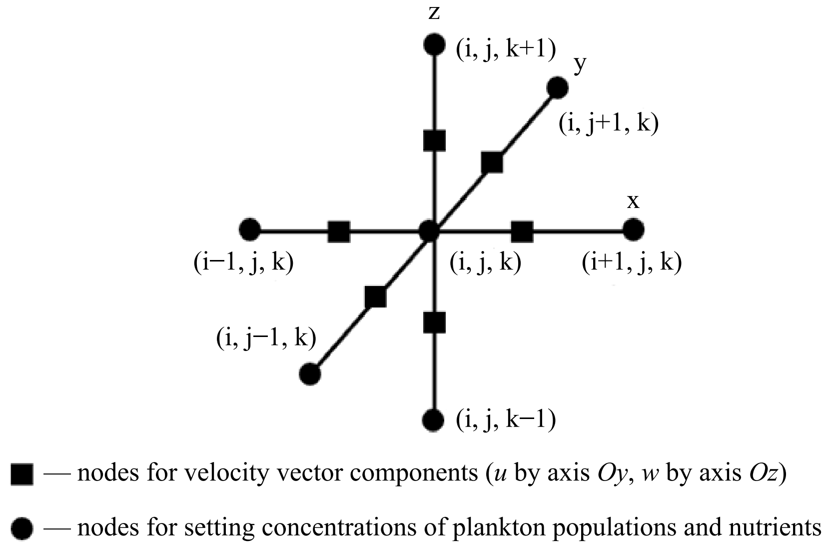

Fig. 5. Schematic designation of the control volume and the scheme template

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: $(x, y, z) \in \omega$, $i = 1,\ldots,10$:

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

And to the type of diffusion transfer operator:

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

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:

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

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 $|h|\to 0$ and $\tau\to 0$ 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.

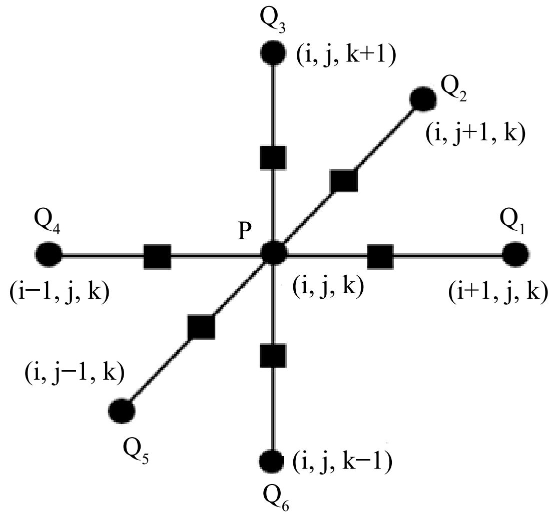

Fig. 6. The template of the difference scheme with the designation of nodes

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

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

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

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:

$$10^{-4}\le\frac{\left|u^n(x_i\pm 0{,}5h_x,y_j,z_k)\right|h_x}{k_h(x_i\pm 0{,}5h_x,y_j,z_k)}\le 1,\ \ \tau\le\frac{10^2}{6\cdot 1\,\text{м}/\text{с}}\cong 16{,}6\ [\text{с}], \quad (25)$$

$$10^{-4}\le\frac{\left|v^n(x_i,y_j\pm 0{,}5h_y,z_k)\right|h_y}{k_h(x_i,y_j\pm 0{,}5h_y,z_k)}\le 1,\ \ \tau\sim 16{,}6\ [\text{с}], \quad (26)$$

$$10^{-4}\le\frac{\left|w^n(x_i,y_j,z_k\pm 0{,}5h_z)\right|h_y}{k_v(x_i,y_j,z_k\pm 0{,}5h_z)}\le 1,\ \ \tau\le\frac{10^{-1}}{6\cdot 10^{-3}\,\text{м}/\text{с}}\cong 16{,}6\ [\text{с}]. \quad (27)$$

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:

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

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

The theorem. If:

$$D(P) \equiv A(P) - \sum_{\substack{Q_m \in Ш'(P) \\ m=1,2,\ldots,6}} B(P,Q_m) > 0, B(P,Q_m) \geq 0, m = 1,2,\ldots,6,$$

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

$$A(P)z^n(P) - \sum_{\substack{Q_m \in Ш'(P) \\ m=1,2,\ldots,6}} B(P,Q_m)z^n(Q_m) = F(P), - P \in \overline{\omega}, z^n(P) = 0, P \in \Upsilon_n^* \equiv \overline{\omega}^* \setminus \overline{\omega},$$

is fair assessment:

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

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:

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

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

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:

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

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

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

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

where the initial approximations on each time layer n =1, 2,…, 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 $n = 0, n+1 = 1, \overline{q}_i^{1,0}$ 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:

$$\left\| z_i^{n+1,S+1} \right\|_{C(\overline{\omega})} \leq \rho \left\| z_i^{n+1,S} \right\|_{C(\overline{\omega})}.$$

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).

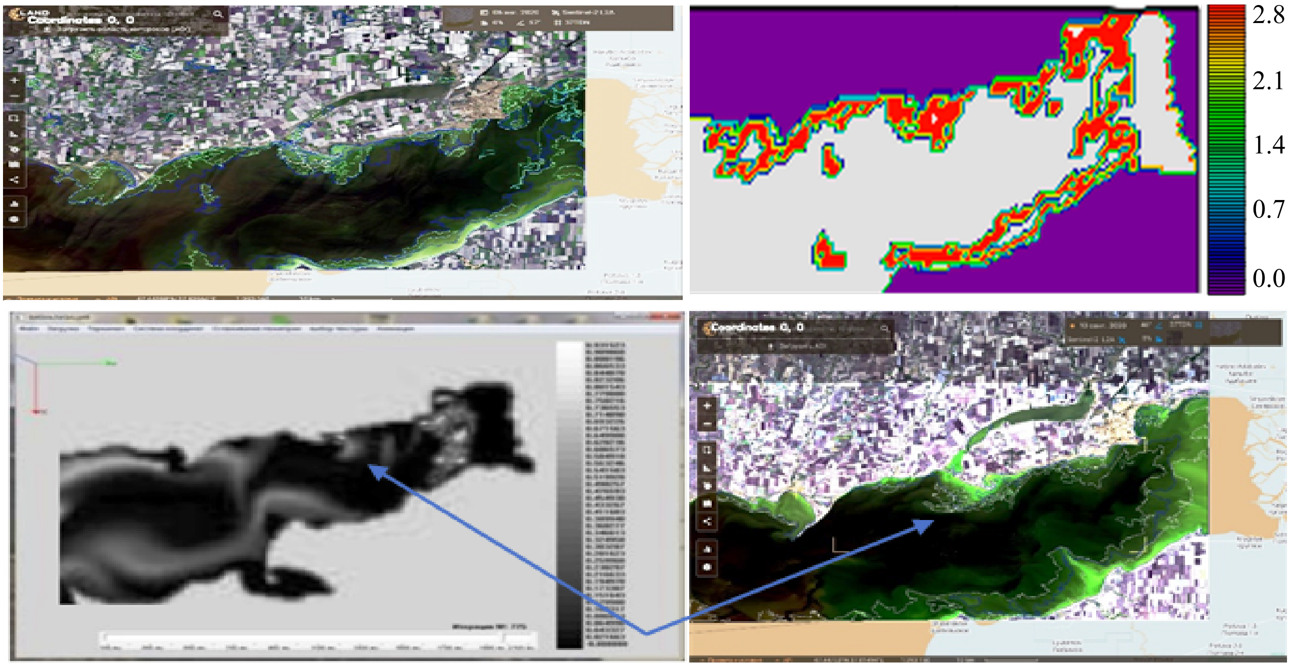

Fig. 7. Modelling the dynamics of phytoplankton concentrations of RPC "Azov3d"

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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