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Development of algorithms for assessing risks and vulnerability to anthropogenic impacts

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Abstract. The paper presents currently used approaches to the assessment of water pollution by various types of pollutants. Based on the existing criteria, an algorithm for assessing risks and vulnerability to anthropogenic impacts is proposed. The software package obtained on their basis makes it possible to model the processes of the spread of pollutants in the studied water area, to detect and evaluate the power of sources of pollutants and manage them, to assess risks and vulnerabilities in relation to anthropogenic impacts, to carry out zoning of the water area of a shallow water body in accordance with the levels of anthropogenic loads, to carry out environmental design from the standpoint of sustainable development.

1 Introduction

The report "Managing the risks of extreme events and disasters to promote adaptation to climate change" by the Intergovernmental Panel on Climate Change [1] noted an increase in economic losses caused by natural disasters, as well as the impact of extreme events on the social sphere, agriculture and food security. If we consider the south of Russia, then over the past 10-15 years there have been a number of adverse events, largely due to anthropogenic influence, which have made a significant contribution to the change in the ecosystems of water bodies. Oil spills can serve as an example of such emergencies, which cause pollution of the coastline and bottom sediments with oil products and other harmful substances. For example, compounds of oil products in the form of bitumen and resins were found on the coast of the Black and Azov Seas, with a length of more than 200 km in 2008–2011. decades.

Another example of anthropogenic impact on aquatic ecosystems can be the ingress of pollutants into river systems. For example, in the fall of 2022, due to an accident at a collector in Volgograd, wastewater entered the river. Volga. Also, dredging works on water bodies require a preliminary forecast of the impact of sedimentation of suspended particles and further movement of bottom materials on the ecosystem of the reservoir [2] . For a long period of time, there has been an unfavorable movement of bottom sediments from the estuarine areas of the Don River in a westerly direction, leading to the displacement of traditional species of flora and fauna from the eastern part of the Taganrog Bay, intensive

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blooming of the waters of the bay and the reproduction of the ringing mosquito in the vast areas of the Taganrog Bay.

An actual comprehensive assessment of the level of impact on the aquatic ecosystem is impossible without the use of the most modern mathematical models that allow predicting both the spread of plumes of suspended matter and pollutants in the aquatic environment, and changes in the bottom topography due to the precipitation of suspended soil particles. For an adequate assessment of the scale and intensity of impacts on the aquatic environment and its inhabitants, models for calculating the volumes and areas of pollution zones should take into account wind currents, river flows, complex geometry of the coastline and bottom, surge phenomena, friction on the bottom and wind stresses, and multi-scale turbulence , which determines the mixing parameters for various phases of the process, the settling rate of each suspension component, jet effects, including the accelerated initial immersion of a "heavy" jet or a burst of soil discharge. Also, these models can be supplemented with models of eutrophication of the reservoir, reflecting the impact of certain biogenic substances on the productivity of the reservoir.

For short-term, and even more so long-term, forecasting of the ecological situation of a reservoir, it is necessary to develop a software package that includes not only the models described above, but also allows you to detect and evaluate the power of pollutant sources, assess risks and vulnerabilities in relation to anthropogenic impacts, and carry out water area zoning shallow water reservoir in accordance with the levels of anthropogenic loads, to carry out environmental design from the standpoint of sustainable development.

2 Mathematical model of pollutant transport

2.1 Model of hydrodynamics

The developed model for calculating three-dimensional fields of the velocity vector of the aquatic environment is based on a mathematical model of the hydrodynamics of shallow water bodies [3] :

– equation of motion (Navier – Stokes)

$$
\begin{gathered}
u_t' + uu_x' + vu_y' + wu_z' = -\frac{1}{\rho}P_x' + \left(\mu u_x'\right)_x' + \left(\mu u_y'\right)_y' + \left(\nu u_z'\right)_z', \\
v_t' + uv_x' + vv_y' + wv_z' = -\frac{1}{\rho}P_y' + \left(\mu v_x'\right)_x' + \left(\mu v_y'\right)_y' + \left(\nu v_z'\right)_z', \qquad (1) \\
w_t' + uw_x' + vw_y' + ww_z' = -\frac{1}{\rho}P_z' + \left(\mu w_x'\right)_x' + \left(\mu w_y'\right)_y' + \left(\nu w_z'\right)_z' + g,
\end{gathered}
$$

is the continuity equation in the case of variable density

$$\rho_t' + (\rho u)_x' + (\rho v)_y' + (\rho w)_z' = 0, \qquad (2)$$

where $\mathbf{V} = \{u, v, w\}$ are the velocity vector components [m/s]; P – pressure [Pa], ρ – density [kg/m 3], μ, ν– horizontal and vertical components of the turbulent exchange coefficient [m2/s], g – gravitational acceleration [m/s 2].

The system of equations (1)–(2) is considered under the initial condition $\mathbf{V} = \mathbf{V}_0$ and under the following boundary conditions:

– at the input: $u = u_0$, $v = v_0$, $P_{\mathbf{n}}' = 0$, $V_{\mathbf{n}}' = 0$;

– lateral boundary (shore and bottom): $\rho\mu u_{\mathbf{n}}' = -\tau_x$, $\rho\mu v_{\mathbf{n}}' = -\tau_y$, $V_{\mathbf{n}} = 0$, $P_{\mathbf{n}}' = 0$;

– upper bound: $\rho\mu u_{\mathbf{n}}' = -\tau_x$, $\rho\mu v_{\mathbf{n}}' = -\tau_y$, $w = -\omega - P_t' / \rho g$, $P_{\mathbf{n}}' = 0$;

where ω is the intensity of liquid evaporation, τ_x, τ_y are the components of the tangential stress.

The components of the tangential stress for the free surface $\{\tau_x, \tau_y\} = \rho_a Cd_s |\mathbf{w}| \{w_x, w_y\}$, $Cd_s = 0.0026$, where $\mathbf{w}$ is the vector of wind velocity relative to water, ρ_a is the density of the atmosphere, Cd_s is the dimensionless coefficient of surface resistance, which depends on the wind speed, is considered in the range of 0.0016–0.0032 [4] .

The components of the tangential stress for the bottom, taking into account the movement of water, can be written as follows $\{\tau_x, \tau_y\} = \rho Cd_b |\mathbf{V}| \{u, v\}$, $Cd_b = gn^2 / h^{1/3}$, where $n = 0.04$ the group coefficient of roughness in the Manning formula is 0.025–0.2; h is the depth of the water area, [m].

2.2 Particulate transport model

To describe the transport of suspended particles, we use the diffusion-convection equation, which can be written in the following form:

$$\frac{\partial c_r}{\partial t} + \frac{\partial (uc_r)}{\partial x} + \frac{\partial (vc_r)}{\partial y} + \frac{\partial \left((w + w_{s,r}) c_r \right)}{\partial z} = \\ = \frac{\partial}{\partial x}\left(\mu \frac{\partial c_r}{\partial x} \right) + \frac{\partial}{\partial y}\left(\mu \frac{\partial c_r}{\partial y} \right) + \frac{\partial}{\partial z}\left(\nu \frac{\partial c_r}{\partial z} \right) + F_r, \tag{3}$$

where c_r is the concentration of the r-th fraction of suspension [mg/l]; $w_{s,r}$ – settling speed of the r-th fraction of suspension [m/s]; F_r is a function describing the distribution intensity of the sources of the r-th fraction of suspended matter [mg/(l s)].

Expression (3) is considered under the following boundary conditions:

– on the free surface: $(c_r)_z' = 0$;

– near the bottom surface: $D_v (c_r)_z' = w_s c_r$;

– there is no flow on the lateral surface $(c_r)_{\mathbf{n}}' = 0$ if $(\mathbf{V}, \mathbf{n}) \geq 0$, and the suspension goes beyond the boundary of the computational domain $D_h (c_r)_{\mathbf{n}}' = \mathbf{V}_{\mathbf{n}} c_r$, if $(\mathbf{V}, \mathbf{n}) < 0$, where $\mathbf{V}_{\mathbf{n}}$ is the normal component of the velocity vector, $\mathbf{n}$ is the normal vector directed inside the computational domain.

Mathematical models of the transport of suspended particles make it possible to predict the spread of suspended plumes in the aquatic environment and the change in the bottom topography due to the precipitation of suspended particles of soil. On the basis of model (1)–(3), the processes of movement and settling of suspended particles during dredging operations can be considered, as well as the possibility of optimizing the areas of existing soil dumps can be considered. Optimizing the size of spoil heap areas minimizes damage to biotopes.

2.3 Water eutrophication model

On the basis of the diffusion-convection equation (3) already considered above, a model of water eutrophication can be built, that is, the process of saturation of water bodies with biogenic elements, accompanied by an increase in the biological productivity of the water area, is described. Eutrophication can be the result of both natural changes in the water body and anthropogenic impacts. The model is a set of equations for each S_i - the value of the concentration of the *i*-th impurity [5, 6] :

$$\frac{\partial S_i}{\partial t}+\frac{\partial (uS_i)}{\partial x}+\frac{\partial (vS_i)}{\partial y}+\frac{\partial \left((w+w_{s,\mathrm{i}})S_i\right)}{\partial z}=$$
$$=\frac{\partial}{\partial x}\left(\mu\frac{\partial S_i}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu\frac{\partial S_i}{\partial y}\right)+\frac{\partial}{\partial z}\left(\nu\frac{\partial S_i}{\partial z}\right)+\psi_i, \quad (4)$$

where $w_{s,\mathrm{i}}$ is the gravitational settling of the i-th component, if it is in suspension; ψ_i - a chemical and biological source (drain) or a term describing aggregation (sticking-spreading), if the corresponding component is a suspension, the index i indicates the type of substance, $i=\overline{1,15}$: 1 - hydrogen sulfide (H_2S); 2 - elemental sulfur (S); 3 - sulfates (SO_4); 4 - thiosulfates (and sulfites); 5 - total organic nitrogen (N); 6 - ammonium (NH_4) (ammonium nitrogen); 7 - nitrites (NO_2); 8 - nitrates (NO_3); 9 - phytoplankton; 10 - zooplankton; 11 - dissolved oxygen (O_2); 12 – silicates (SiO_3 – metasilicate; SiO_4 – orthosilicate); 13 - phosphates (PO_4); 14 - iron (Fe^{2+}); 15 - silicic acid (H_2SiO_3 - metasilicic; H_2SiO_4 - orthosilicic).

The computational domain G is a closed basin bounded by the undisturbed surface of the reservoir Σ_0, the bottom $\Sigma_H=\Sigma_H(x,y)$ and the cylindrical surface σ for the time interval $0<t\le T_0$. $\Sigma=\Sigma_0\cup\Sigma_H\cup\sigma$ is the piecewise-smooth boundary of the domain G. Let be $\mathbf{n}$ the vector of the outer normal to the surface Σ, be the $\mathbf{u_n}$ component of the water flow velocity vector that is normal with respect to . Σ

Initial conditions for model (4): $S_i\big|_{t=0}=S_{i0}(x,y,z),\quad i=\overline{1,15}.$

Boundary conditions for model (4):

– on the surface σ : $S_i=0$ if $\mathbf{u_n}<0$; $\frac{\partial S_i}{\partial \mathbf{n}}=0$, if $\mathbf{u_n}\ge 0$, $i=\overline{1,15}$;

– on Σ_0: $\frac{\partial S_i}{\partial z}=\varphi(S_i)$, $i=\overline{1,15}$;

– at the bottom Σ_H : $\frac{\partial S_i}{\partial z}=-\varepsilon_{S_i}S_i$, $i=\overline{1,15}$,

where ε_{S_i} is the coefficient of absorption of the i th impurity by bottom sediments.

With calms and wind situations close to them, anaerobic conditions arise in the bottom layers of shallow water bodies (for example, the Sea of Azov). Restoration of surface water-saturated sludge entails the release into solution (except for hydrogen sulfide) of sulfates, divalent manganese and iron, organic compounds, ammonium, silicates and phosphates. Using the model (1)–(2) and (4), the processes of ammonification, nitrification, nitrate reduction (denitrification), assimilation NH_4, oxidation H_2S, sulfate reduction, oxidation and reduction of manganese can be described, and it is also possible to study the mechanism of conditions for the formation of kills as a result of anthropogenic eutrophication , predict changes in oxygen and biogenic regimes.

3 Algorithm for assessing risks and vulnerability to anthropogenic impacts

3.1. Vulnerability of water areas

Under the vulnerability of the water area we mean the ability of the aquatic ecosystem to change its parameters as a result of external influences, leading to disruption of the functioning and structure of its community [7]. There are various methods for assessing the vulnerability of natural objects. Most of these approaches are characterized by the calculation of some total vulnerability index, depending on a different set of factors [8-10].

For example, the level of pollution of a reservoir is estimated by the "water pollution index" (WPI), which is a generalized indicator of water pollution and is used for comparative assessments of the level of pollution, determining priority pollutants and their sources:

$$k_S = \sum_{i=1}^{k} \left(\overline{S}_i / Sp_i \right) / k \tag{5}$$

where k_S is WPI; $\overline{S}_i$ – yearly average value of the actual concentration of the i -th pollutant (pollutant) in the water body [mg/l]; Sp_i – maximum permissible concentration of the same i pollutant [mg/l]; k - a strictly specified number of indicators taken for calculation, including, without fail, dissolved oxygen and BOD 5.

The maximum allowable concentration (MPC) is understood as the maximum concentration of a harmful substance, which leaves water, when used indefinitely for a long time, as harmless as in the complete absence of this substance [11] . In the course of substantiating the MPC for each substance, a hazard class is preliminarily determined, which characterizes the following properties of xenobiotics:

- the ability to accumulate in the body and cumulate the effect of a harmful action;
- the likelihood of causing long-term effects (i.e. the degree of danger of chronic poisoning);
- the rate of resorption of a substance by the tissues of a living organism.

The traditional approach to determining the level of pollution of a water body is most often based on a comparison of the actual concentrations of individual elements and substances to their MPC. Actual concentrations should be obtained from regular measurements and analysis of the water body. It should be noted that by now quite a lot of complaints have been accumulated against the MPC system itself, related, among other things, to the complexity of applying this approach with a significant number of evaluated compounds and their impact on the environmental situation.

Under the biological oxygen demand or biochemical oxygen demand (BOD) is understood the amount of oxygen consumed for aerobic biochemical oxidation under the action of microorganisms and the decomposition of unstable organic compounds contained in the test water. BOD is one of the most important criteria for the level of pollution of the reservoir with organic substances, it determines the amount of easily oxidized organic pollutants in the water. The analysis determines the amount of oxygen that has gone for a set time, usually 5 days - BOD $_5$, without access to light at 20 ° C for the oxidation of pollutants contained in a unit volume of water). The k ingredients involved in the calculation include those that have the highest relative concentrations (ratio $\overline{S}_i / Sp_i$). For oxygen, the ratio was found Sp_i to $\overline{S}_i$.

3.2. The risk of pollution of the water area

Under the risk [12] we will understand the probability of the realization of the danger, or the expected amount of damage associated with the entry of pollutants into the water. The risk can be determined by the formula:

$$risk = exposure \times toxicity\,, \tag{6}$$

where "exposure" is the amount of pollutants per one biological target, " toxicity" is the potential hazard of the pollutant, its ability to cause harm.

In Russia, according to regulatory documents [13] , all harmful substances are divided into four groups according to the nature of their impact, depending on the degree of impact on organisms. Each group combines substances of the same level of exposure. The substance is assigned to that hazard class and is produced according to the indicator, the value of which corresponds to the highest hazard class and in which its effect is manifested in the minimum concentration, although this does not mean that this substance does not exhibit other harmful effects. It should be noted that making a decision on the admissibility of using a particular pollutant, the need to limit or completely prohibit its production (i.e., determining an acceptable level of risk), along with the development of control measures and the preparation of relevant regulatory documentation - all this falls within the scope of risk management.

The risk factor R for the aquatic ecosystem was determined by the formula:

$$R = Ef_S \cdot E_S\,, \tag{7}$$

where E_S is the exposure factor, Ef_S is the pollutant impact efficiency factor. The exposure factor for water was calculated using the formula:

$$E_S = S \cdot P_S \cdot k_{BA} / U\,, \tag{8}$$

where S is the concentration of pollutants in water; U – how the chemical is used ($U = 5$ when "closed", i.e. indoors, use, $U = 1$ with the "open" method); P_S – hydrolysis rate characteristic (equal to 1 for fast hydrolysis and 2 for slow hydrolysis); k_{BA} - bioaccumulation factor.

Exposure factors for water can take values of 0.4–25 S. For a general assessment of the toxicity of pollutants (chemicals) Ef_S in the EU countries, it is customary to use a set of standard tests that provide the necessary minimum information on the toxicity of pollutants [14, 15] . There are several quantitative measures of toxicity [14]:

– NOEC (No Observed Effect Concentration) - maximum concentration substances, which not causes negative effects at tested organisms; (is the highest tested concentration for which there are no statistically significant difference of effect ($p<0.05$) when compared to the control group in long-term ecotoxicity studies)

– LOEC (Lowest Observed Effect Concentration) - the smallest concentration substances,which causes reciprocal reaction at tested organisms ; (is the highest tested concentration for which there are no statistically significant difference of effect ($p<0.05$) when compared to the control group in long-term ecotoxicity studies.)

– EC_{50} (Median Effective Concentration) - concentration substances, which causes sublethal Effect 50% of those tested organisms; (is the effect concentration at which 50% effect (mortality, inhibition of growth, reproduction, etc.) is observed compared to the control group)

– LC_{50} (Median Lethal Concentration) - the concentration of a substance that causes a sublethal effect in 50% of the tested organisms.

Of the possible test sets [15], three related to water were selected: LC 50 for 96 hours for fish; LC 50 within 48 hours for daphnia (zooplankton); LC 50 growth inhibition of microalgae.

For various pollutants, the LC $_{50\ \text{parameter}}$ (absolute toxicity of a substance that causes the death of 50% of fish) varies within: Cu (0.02 - 1); Zn (0.5 - 5); Pb (0.5 - 10); Cd (0.5 - 105); Cr (3.5 - 118); Ni (5 - 100); Fe (1.4 - 133) mg/l depending on the salinity of the water and fish species.

3.3. Description of the algorithm for assessing risks and vulnerability to anthropogenic impacts

The procedure for conducting a risk and vulnerability assessment with respect to anthropogenic impacts can be described as follows:

1. The study of geographical, topological, climatic, geological, hydrological features of a water body.
2. Identification of possible sources of pollutants: river runoff, pollutant discharges from enterprises, shipping, etc. Modeling of possible scenarios for the spread of pollutants based on models (1) – (5).
3. Assessment of the toxic effect of pollutants that may come from the sources identified above. Conducting selected three tests to determine the effectiveness of the impact of pollutants Ef_S based on (8).
4. Calculation of the risk factor R based on (7), which is normalized (S_y is the normalized risk factor) by the formula $\left(S-S_{\min}\right)/\left(S_{\max}-S_{\min}\right)$ if the risk increases with the growth of S. The normalized risk factor is $S_y \in [0,1]$.
5. Based on the obtained risk assessment, preliminary conclusions are made: the risk is considered high at $S_y > 0,55$; potentially significant at $0,3 < S_y < 0,55$; missing at $S_y < 0,3$.

3.4. An example of a water area pollution risk assessment

Cu (copper)) enter the Sea of Azov with the Don River runoff. S Anthropogenic sources of copper: non-ferrous metallurgy enterprises; copper-containing pesticides; galvanic production; burning coal and oil. The toxic effect of copper is a tin poison that causes acute poisoning. If the concentration of copper in water is 80 µg/l, the minimum concentration value recorded in the waters of the Sea of Azov is 0.001 mcg/l, maximum 100 µg/l; $U=1$ (open method); the degree of hydrolysis of the substance $P_S = 1,5$; accumulates in the hydrobiont selected as a biological target to concentrations exceeding the content in water by 20 times. Let's take LC $_{50}$ for pike perch equal to 4 mg/l, for zooplankton 50 mg/l. Let us take the effective dose of microalgae growth inhibition equal to 20 mg/l, $k_{BA} = 2$.

$E_S = S \cdot P_S \cdot k_{BA} / U = 80 \cdot 1{,}5 \cdot 2 = 240$. We normalize the risk R: $S_y \approx 0{,}52$. Because $0{,}3 < 0{,}52 < 0{,}55$, then we get that the risk is potentially significant.

The approach to water quality assessment described above is part of the forecast complex being developed by the team. Data on the location of pollutant sources can be obtained, in particular, by processing satellite images.

4 Simulation results

4.1. Simulation of suspension transport during soil dumping

As a model example, let us consider the simulation of the process of sedimentation of suspension during dredging [2] based on model (1) – (4). Input data for the water area and suspension: the length of the reservoir is 3 km; the width of the reservoir is 1.4 km; the depth of the reservoir is 10 m; flow velocity 0.2 m/s; loading volume 741 m ^{3}; suspension sedimentation rate (according to Stokes) 2.042 mm/s; soil density 1600 kg/ m ^{3} ; the percentage of silt particles (d < 0.05 mm) in sandy soils is 26.83%.

Computational domain parameters: step along horizontal spatial coordinates 20 m; step along the vertical spatial coordinate 1 m; calculation interval 2 hours, time step 1 minute. Figure 1 shows the dynamics of changes in the concentration of suspended particles (mg/l) over time. The values of the suspended matter concentration field in the section of the computational domain by a plane passing through the unloading point and formed by vectors directed: vertically and along the flow are given. The currents are directed from left to right. Based on the materials obtained, we calculate the total amount of polluted water during the dumping of soil (Table 1).

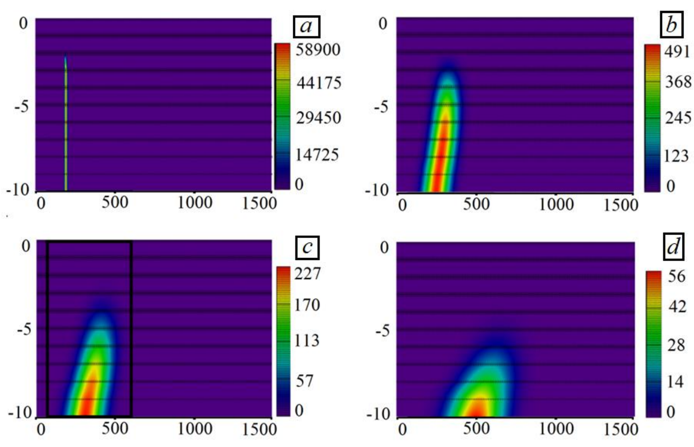

Fig. 1. The field of concentration of suspended particles at different points in time: (a) the initial moment; (b) after 15 min; (c) after 30 min; (d) 45 minutes after unloading.

Table 1. Volumes of contaminated water when dumping soil.

Lot number	Total volume of polluted water at a single discharge, million m3	Including water with concentrations of pollutants, million m3			Number of resets	Total volume of water with concentrations of pollutants, million m3		
		>0.25 mg/l	>20 mg/l	>100 mg/l		>0.25 mg/l	>20 mg/l	>100 mg/l
1	1.285	0.89	0.245	0.15	124	110.36	30.38	18.6

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2	1.12	0.813	0.202	0.105	50	40.65	10.1	5.25
3	1.279	0.889	0.24	0.15	45	40.005	10.8	6.75

On the basis of the developed software package, which includes modules for calculating hydrodynamic processes, the transport of airborne particles and the biological productivity of phyto- and zooplankton, the volume of water contaminated during dumps of soil was determined, the areas of areas in which the death of bottom vegetation is observed on dumps and in areas of dredging were calculated. works. This software package makes it possible to predict both the distribution of suspended plumes in the aquatic environment and the change in the bottom topography due to the precipitation of suspended particles of soil. On the basis of the developed software package, it was found that reducing the size of the areas of soil dumps allows minimizing the damage caused to biotopes.

4.2. Modeling the transport of suspended particles in the mouth area

Let us consider the results of the software implementation of the mathematical model of water movement in the mouth area (1) – (4) in the presence of a significant density gradient of the aquatic environment caused by the presence of suspended particles.

Input data for the water area and suspended matter: the length of the reservoir is 50 m; reservoir width 50 m; the depth of the reservoir is 2 m; flow velocity 0.2 m/s; suspension sedimentation rate (according to Stokes) 2.042 mm/s; density of fresh water under normal conditions 1000 kg/m^3; suspension density 2700 kg/m^3; the volume fraction of suspension is 1/17.

Computational domain parameters: step along horizontal spatial coordinates 0.5 m; step along the vertical spatial coordinate 0.1 m; calculation interval 5 minutes, time step 0.25 seconds. Figure 2 shows the geometry of the computational domain in the form of a depth map.

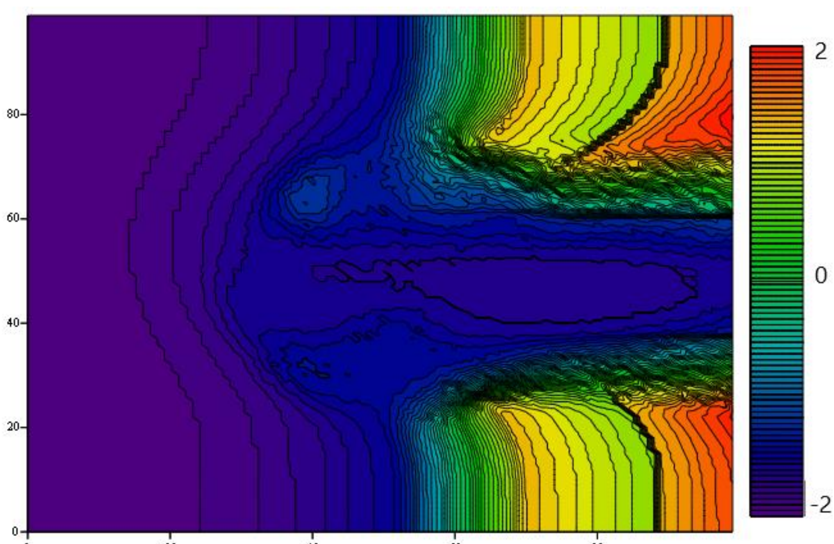

Fig. 2. Map of the depths of the computational area

Figures 3–4 present the results of modeling the process of suspension transport as a result of mixing and movement of water in the mouth area in the presence of a significant density gradient of the aquatic environment (on the left is the average concentration over depth, on the right is the density in the cross section by the xOz plane passing through the center of the computational domain (at y = 25 m)). Figures 3–4 describe the movement of suspended matter in the mouth area; on the vertical sections on the right, one can observe a change in the concentration of suspended matter in stratified layers of the aquatic environment with changing density over time.

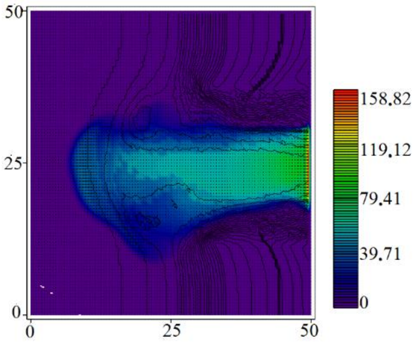

Fig. 3. The movement of water in the mouth area in the presence of a significant gradient in the density of the aquatic environment after 1 minute: a) concentration of suspended matter in water; b) density field of the aquatic environment

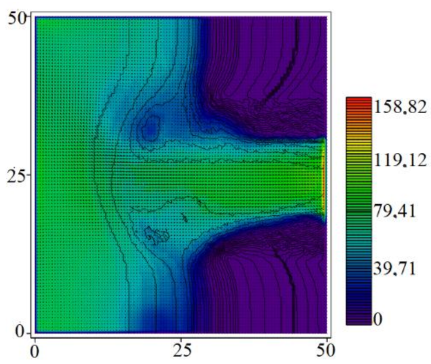

Fig. 4. The movement of water in the mouth area in the presence of a significant gradient in the density of the aquatic environment after 5 minutes: a) concentration of suspended matter in water; b) density field of the aquatic environment

The developed software package can be used to calculate the transfer both for heavy impurities and for impurities that are lighter than water.

4.3. Assessment of the ecological state of the Sea of Azov

When identifying zones of ecological disaster and risk, the "Criteria for assessing the ecological situation of territories to identify zones of ecological emergency and zones of ecological disaster" [16], as well as the work of G.G. Vinberg [17]. The assessment of the ecological state was carried out according to the level of anthropogenic load in accordance with R 52.24.661–2004 [18], the proportion and degree of anthropogenic impact were estimated using the formulas:

$$D = \left(N_1 / N\right) \cdot 100\%, \tag{9}$$

$$C = \left(N_2 / N_1 \right) \cdot 100\%, \tag{10}$$

where D, C is the proportion and degree of anthropogenic impact, respectively; N – total number of standardized priority pollutants; N_1 - the number of ingredients exceeding the MPC; N_2 - the number of ingredients exceeding 10 MPC. The assessment of the ecological state of the Sea of Azov can also be carried out according to system-forming indicators based on the statistical characteristics of the variation series of values for the concentrations of easily oxidizable organic substances (according to biological oxygen demand BOD_5), ammonium nitrogen compounds, and the values of the content of oxygen dissolved in water [19–21].

To assess the quality of sea water, the most informative complex indicators of water quality [22] were used, including the specific combinatorial index of water pollution (SCWPI) and the water quality class (WQC).

Taking into account the main external factors in the models of hydrodynamics and biological kinetics made it possible to reproduce a positive trend in salinity in the Sea of Azov basin [23] . It was revealed that the formation of a stratification of water masses by oxygen content in all seasons of the year was noted throughout the water area. During the period of increasing salinity and reducing the average annual runoff of the Don River in the Taganrog Bay, a decrease in the concentration of biogenic elements was noted, although the high intensity of phytoplankton productivity remains. The concentrations of biogenic elements in the modern period of salinization in the sea itself remain at the level of average annual values, however, an increase in salinity, leading to a change in the taxonomic groups of phytoplankton, reduces the level of primary production of organic matter [23]. The increase in the proportion of the organic form of nitrogen and phosphorus during the period of salinization in the Taganrog Bay is associated with the development of primary production of phytoplankton, and in the sea proper with the supply of allochthonous organic matter with continental runoff. In general, the ecological state of the Sea of Azov is insignificant, but it is improving according to the WPI index, sea water in recent years has been classified as moderately polluted.

5 Conclusion

The paper presents currently used approaches to the assessment of water pollution by various types of pollutants. It should be noted that in order to monitor and assess the risks of anthropogenic impact on water bodies, it is necessary to assess the qualitative and quantitative composition of discharged pollutants, as well as predict adverse events caused by anthropogenic impact.

It is known that more than 60% of pollutants, which have a significant impact on the processes of development and death of biota, enter the reservoir from the atmosphere far from the river runoff. Due to the increase in the anthropogenic load on coastal systems, there is an urgent need to analyze and predict the spread of pollutants in the water area of the reservoir, coming from the river runoff and from the atmosphere [19]. For the studied water area of the Azov-Black Sea basin, it was found that the main atmospheric air pollutants in the Sea of Azov region are chemicals: sulfur dioxide, nitrogen dioxide, benzene, formaldehyde, cadmium and its compounds, the concentration of which today exceeds the maximum permissible concentrations [24].

The developed software package takes into account such important parameters for modeling the situation in a reservoir as the characteristics of water pollution in terms of the proportion and degree of anthropogenic impact, risk factors, etc. The developed algorithm allows modeling the dynamics of the propagation of pollutants entering the Sea of Azov with river runoff and from the surface layer of the atmosphere, taking into account meteorological conditions, processes of interaction and settling of pollutants. The software package allows you to simulate the conditions for the development of the ecological situation of a shallow reservoir on an accelerated time scale to further prevent negative consequences associated with material damage and a threat to human health and life.

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References

1. IPCC, 2012 https://www.ipcc.ch/report/managing-the-risks-of-extreme-events-and-disasters-to-advance-climate-change-adaptation
2. I. Kovtun, E. Protsenko, A. Sukhinov, A. Chistyakov, Fundamental and Applied Hydrophysics, **9(2)**, 27-38 (2016)
3. Belotserkovsky, O. Turbulence, New Approaches, pp 1-286s (Nauka, Moskva, 2003)
4. E. Alekseenko, B. Roux, and etc., Coastal hydrodynamics in a windy lagoon, Computers and Fluids, **77**, 24–35 (2013)
5. A. Sukhinov, A. Chistyakov, A. Semenyakina, A. Nikitina, ComputerResearch and Modeling, **8(1)**, 151-168 (2016)
6. A. Nikitina, A. Sukhinov, and etc., Mathematical Modeling, **28(7)**, 96-106 (2016)
7. I. Kesoretskikh, S. Zotov, Bulletinof the I. Kant Baltic Federal University. Kant, **1**, 51-57 (2012)
8. E. Gundlash, M. Hayes, Marine technology society journal, **12(4)**, 18–27 (1978)
9. D. Amaro Medina, V. Dmitriev, Vestnik of Saint Petersburg University. Earth Sciences, **64(2)**, 162-184 (2019)
10. I. Kesoretskikh, S. Zotov, N. Lazareva, Springer Proceedings in Earth and Environmental Sciences, 153-161 (2020)
11. I. Rodziller, Forecast Forecast of water quality in reservoirs - wastewater receivers, pp 1-263, (Stroyizdat, Moskva, 1984)
12. GOST R 55059-2012 Safety in emergencies. Emergency risk management. Terms and definitions
13. GOST 12.1.007-76 Occupational safety standards system. Noxious substances. Classification and general safety requirements
14. Guidance on information requirements and chemical safety assessment. Chapter R.10: Characterisation of dose [concentration]-response for environment. – European Chemicals Agency, 2008. 65 p. URL: https://echa.europa.eu/guidance-documents/guidance-on-information-requirements-and-chemical-safety-assessment
15. Soil and Sediment Risk Assessment of Organic Chemicals. Technical Report No. 92. – European Centre for Ecotoxicology and Toxicology of Chemicals. Brussels, December, pp 1-145 (2004)
16. Criteria for assessing the ecological situation of territories for identifying zones of an environmental emergencyand zones of ecological disaster, http://docs.cntd.ru/document/901797511

17. G.G. Vinberg, Journal of General Biology, **61(5)**, 549–560 (2000)
18. Methodological guidelines RD 52.24.643-2002. Method of integrated assessment of the degree of contamination of land surface waters by hydrochemical indicators, pp.1-49, St. Petersburg, Gidrometeoizdat, (2003)
19. Methodological guidelines RD 52.24.661-2004. Recommendations. Assessment of the risk of anthropogenic impact of priority pollutants on land surface waters, pp.1-26,. Moskva, publishing House of the Meteorological Agency of Roshydromet, (2006)
20. V. Danilov-Danilyan, A. Gotovtsev, A. Nikanorov, Vodnye resursy, **39(58)**, 510-520 (2012)
21. R. Jamalov, K. Myagkova, and etc., Water and ecology: problems and solutions, **4(72)**, 26-39 (2017)
22. A. Nikanorov, V. Bryzgalo, O. Reshetnyak, Voda: khimiya i ekologiya, **12**, 15-21 (2013)
23. A. Sukhinov, V. Tishkin, Experience in modeling hydrophysical processes in the Sea of Azov Supercomputer technologies in science, education and industry, 156-164 (2012)
24. G. Matishov, O. Stepanyan, and etc., Bulletin of the Southern Scientific Center, **11(2)**, 36-44 (2015)