E3S Web of Conferences **363**, 02024 (2022) https://doi.org/10.1051/e3sconf/202236302024
INTERAGROMASH 2022

Mathematical modeling of hydrodynamic processes in shallow waters in the presence of pollutants of various origin, as well as areas covered with plastic waste

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Abstract. The paper covers the modeling of hydrodynamic processes in shallow waters in the presence of pollutants of various types, as well as areas covered with plastic waste, including nano- and microplastics. The simulation performed using new and effective mathematical instruments, including assimilation methods of measurement data, restoration of the state function, diagnostics of quality of the developed models, the research the sensitivity of models to variations in input data, the integration of models with various scales. Interrelated non-stationary, spatially inhomogeneous mathematical models of hydrodynamics and biological kinetics of shallow waters were developed and numerically implemented. They describe non-linear processes of hydrophysics, biogeochemical cycles, transport and transformation of suspensions and sediments with microplastic particles and other pollutants, absorption of it by zooplankton and fish, movement of plastic particles through food, the forecast of their impact on the main hydrobionts of shallow waters of the Azov-Black Sea basin, including the Azov Sea, Taganrog Bay, Gelendzhik Bay. The models take into account the heat and salt transport; the complex, dynamically changing water geometry; friction on the bottom and wind stresses; turbulent and advective heat and mass exchange in three coordinate directions; the Coriolis force; river flows; evaporation, temperature and oxygen regimes. They make it possible to improve the accuracy of hydrophysical processes modeling in shallow waters, to detect vortex structures of currents that can be a natural pollution traps, including microplastic. Based on a supercomputer, a complex of application has been designed and adapted for solving predictive problems of water ecology and water resources management.

1 Introduction

The research of hydrodynamic processes in shallow waters, the species and quantitative diversity of biological communities, the circulation of matter and energy balance, the identification of cause-and-effect relationships and mechanisms of individual processes in

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ecological systems is one of the fundamental problems of ecology and hydrobiology [1]. Today, there is an acute problem of maintaining the conditions for the sustainable development of water ecosystems, preserving the biodiversity of commercial resources, developing schemes for optimal nature management, especially in the case of natural and anthropogenic pollution, which is increasing every year.

One of the modern global environmental problems is the pollution of the water environment with microplastics – microparticles of polymers that are formed during the destruction of plastic debris as a result of mechanical abrasion and chemical decomposition. Being in the water environment and remaining practically invisible, they pose a threat to the life of aquatic organisms, birds, and mammals [2, 3].

Russian and foreign scientists are researching the distribution and content of microplastics in the water, determine the most methods for isolating and analyzing polymer particles from the water environment, determining the scale and influence degree on the water hydrobiocenosis. To obtain detailed and accurate hydrobiological information about the water conditions, especially in the case of climatic and industrial challenges, as well as to analyze and predict the ecological situation in the region, new, effective software and algorithmic tools and forecasting instruments are necessary to get a detailed picture of ongoing events.

In view of the increasing incidence of hazardous and large-scale pollution entering waters, it is necessary to develop new methods and tools for mathematical modeling, approbation and application of promising methods for researching the water system conditions. Due to it, we can effectively predict the volumes and types of pollutants that have fallen into water, the dynamics of hydrodynamic processes, the picture of the distribution of pollutant concentrations in the research area and their impact on the water basin as a whole.

This paper covers the development, research and numerical implementation of interrelated non-stationary, spatially inhomogeneous mathematical models of hydrodynamics and biological kinetics of shallow waters that describe nonlinear processes of hydrophysics, biogeochemical cycles, transport and transformation of suspensions and sediments containing particles of microplastics and other pollutants, the absorption of it by zooplankton and fish, the movement of microplastic particles along the food chain, the prediction of their impact on the main hydrobionts of coastal systems like the Azov Sea. In this paper, parallel algorithms and programs were created for predictive modeling of these processes on high-performance computer systems. The developed hydrophysical models take into account the heat and salt transport, complex, dynamically changing water geometry, bottom friction and wind stresses, turbulent and advective heat and mass exchange in three coordinate directions, Coriolis force, river flows, evaporation, temperature and oxygen regimes. These models will improve the simulation accuracy of hydrophysical processes in shallow waters, such as the Azov Sea, Taganrog Bay, Gelendzhik Bay; detect vortex structures of currents that can act as natural pollution traps, including microplastics.

In further, we plan conduct research and experiments on calculation based on a complex of interrelated mathematical models being developed, which will be implemented on the basis of computationally stable models and algorithms with significant depth differences and significant changes in salinity and temperature, which is typical for shallow waters. The developed program complex will allow numerically solving the model problems of water ecology, performing numerical experiments in various hydrological and meteorological situations, assessing the ingress and accumulation of pollution particles of various origins, etc. to identify trends and patterns of changes in water ecosystem conditions under the influence of natural and anthropogenic factors.

2 Analysis and research of the problem

According to numerous scientific researches for conditions of sustainable development of water environment, both oceanic and shallow water systems, conducted today around the world, microplastic pollution in water is one of the global environmental problems of the world.

The natural complexes of the South of Russia have been researched for a long time by representatives of all areas of the natural sciences. However, today a detailed analysis of obtained data, determination of the vector of properties and mechanisms of the functioning of marine and coastal ecosystems is required, taking into account climatic and anthropogenic impact factors.

Almost 80% of ever created plastic is not recycled in any way and continues to pollute the environment, where it breaks down into smaller particles. Most of the current research is focused on the presence of pollution plastic particles in water and their impact on aquatic life (Fig. 1a). Up to 8 million tons of plastic enters the World Ocean annually, most of it is microscopic particles floating on the water surface or buried in bottom sediments. Since the time of complete plastic decomposition in nature is several hundred years, it accumulates more and more in the water of the planet. Examples of plastic getting into large and small waters are plastic garbage carried as a result of bad weather, illegal dumping of waste into the ocean and washing away of products containing plastic, etc. Plastic undergoes inevitable destruction, forming particles of various sizes and shapes, which then penetrate into the environment and human body. Microplastics are a consequence of the global consumption of plastics causing such pollution. Microplastics are tiny plastic particles ranging in size from 1 μm to 5 mm. The smallest plastic particles are able to penetrate into all corners of the environment – soil, water, air and, as a result, into the human body. Current research proves that microplastics decompose into smaller, nanosized particles (“nanoplastics”) ranging in size from 1 to 1000 nm.

The investigation and detailed research of this problem were performed in this paper. Numerous works of Russian and foreign scientists were researched [4, 5]. The growing desire to research the impact of nano- and microplastics is due to the lack of expert knowledge about the consequences of such pollution for human health and the environment. Moreover, today there is little accurate information about the consequences of pollution with nano- and microplastics. Due to the size of their particles and the ability to penetrate much deeper into the ecosystem, its presence potentially becomes a much more dangerous type of pollution of ecological systems. Pollution by almost invisible plastic particles is a growing problem on a global scale, therefore, government agencies, together with scientific institutions, are paying more and more attention to it.

a) b)

Fig. 1. Water environment pollution by plastic (a); microplastic particles (b).

 https://doi.org/10.1051/e3sconf/202236302024

Nanoplastics and microplastics are ubiquitous components of most water environments, and their increasing prevalence endangers aquatic life each year. Due to the increase in plastic production by an average of 4 – 5% annually, there is an almost exponential increase in the volume of plastic waste entering aquatic ecosystems. Recent studies have documented the entanglement of marine and freshwater biota with plastic debris, especially ghost fishing gear, leading to suffocation, drowning or starvation.

To model the spatial distribution of pollutants, including plastic particles, in shallow water, the physical impact of plastic particles entering the water column was researched. The microplastic n water acts like a magnet, attracting and transferring bacteria and various pollutants. Zooplankton and sediment-eating animals such as sea worms and mussels mistake tiny plastic particles for food. Floating on the water surface, debris prevents sunlight from entering, which is dangerous for the life of plankton and algae, which play a critical biological role in the food chain and maintaining the ecosystem by producing essential nutrients. Being food for other sea creatures, the disappearance of plankton and algae will lead to the disappearance of other species, including those that a person consumes. The small size of plastic granules and fibers contributes to their easy penetration into plankton – the basis of food chains and further into the human body. In addition, plastic is dangerous because it does not disintegrate in water for a long time, as it cools and becomes covered with algae. Marine debris becomes dangerous food for local inhabitants (gets stuck in the stomach, as a result of which the animal can no longer eat, dying of hunger), and also often causes physical damage (entanglement in nets, packaging materials, etc.). Scientists predict that by 2050, 99.8% of seabirds will eat plastic. Taking small plastic granules for eggs, birds feed their cubs with them, which leads to their imminent death. The small size of plastic granules and fibers contributes to their easy penetration into plankton – the basis of food chains and further into the human body. In addition, plastic is dangerous because it does not disintegrate in water for a long time, as it cools and becomes covered with algae. Marine debris becomes dangerous food for local inhabitants (gets stuck in the stomach, as a result of which the animal can no longer eat, dying of hunger), and also often causes physical damage (entanglement in nets, packaging materials, etc.).

Plastics adsorb persistent organic pollutants and heavy metals, which are carcinogens, on their surfaces. At the same time, their sorption capacity increases with their aging and destruction. During photodegradation, dyes and chemicals (bisphenol A) are released from plastic, which enter the water. Plastic has the property of accumulating toxins in its granules, which are transferred to marine life when consumed instead of food, which can cause genetic problems, poisoning and accumulation in the bodies. Thus, along the food chain, it is transmitted to other animals, and also reaches humans.

The geographical position and relatively small size of shallow water determine the high spatial and temporal variability of the main abiotic factors of the water ecosystem, including salinity, which is determined by river runoff, water exchange with other water areas, and fluctuations in the total moisture content of the basin. Violation of the natural habitat conditions of hydrobionts in water bodies entails changes in their production indicators and structural changes.

One of the most important groups in the community of aquatic animals is zooplankton, which in the ecosystem performs the function of an energy transformer in the food chain from producers to secondary consumers, in particular, fish. Zooplankton constitutes the food base of planktophage fish and juveniles of other valuable commercial species, which is one of the most important factors determining the fish productivity of water bodies. Zooplankton populations are very sensitive to microplastic content in water. Therefore, the assessment of the impact and the construction of forecasts for the dynamics of zooplankton populations in the presence of nano- and microplastics is an urgent task that can be solved by effective means of mathematical modeling.

When performing this work, the features and principles of the emergence and spread of such a dangerous type of pollutants as garbage islands, which subsequently affect the hydrodynamics of a reservoir, were researched.

Garbage islands are large concentrations of anthropogenic (i.e., human-made) debris that float on the surface of the water. These spots are formed due to the convergence of water currents and wind at one point, which twist the garbage into a whirlwind and drag it to the center.

Many waters in different parts of the world have been turned into landfills: household waste, soil, gravel, etc. are dumped into them. Such physical pollution of water not only changes its composition, but also prevents sunlight from entering. Human activities and natural processes have a detrimental effect on the hydrosphere, causing pollution of natural waters due to the entry into streams, rivers, lakes, seas and oceans of various chemicals, solid waste or the reproduction of microscopic living organisms (bacteria, fungi, algae) in them. Violation of the ecological balance in the existing ecosystems of deltas and coastal systems leads to negative changes in them and in the region as a whole.

Existing methods of pollution control, including mechanical, physico-chemical and biological methods, should be used in combination. At the same time, using the power of modern computational methods, technical and software tools, computational experiments with object models make it possible to research objects in detail in sufficient completeness, inaccessible to purely theoretical approaches. It is necessary to predict changes in the ecological situation of shallow waters due to the occurrence of natural and technogenic phenomena based on the methods and tools of mathematical modeling in coastal systems with different spatial resolutions from tens of meters to several kilometers. In accordance with the regulations, the time for decision to eliminate an emergency of a natural or technogenic nature should be from several hours to 2 – 3 days, i.e. the time for forecasting of the ecological situation of water ecosystems in the event of emergency events and catastrophic natural and technogenic phenomena occurring in them is limited. Therefore, to operational forecast of the impact of microparticles of natural and technogenic origin on the hydrobiology of the coastal systems of the South of Russia, it becomes necessary to use high-performance computing systems, parallel algorithms and programs that allow three orders of magnitude or more to accelerate the time of prognostic calculations.

The researched hydrobiological processes are represented by complex systems with a significant number of parameters: they are three-dimensional in space, non-stationary and characterized by essentially non-linear dependencies [6].

In addition, the complexity in the physical description of the transfer of microplastic particles is, firstly, the variety of particle properties and, secondly, the variability of these properties over the life time of the plastic in the environment. Indeed, already the initial density of plastics varies over a wide range from 0.01 – 0.05 kg/m3 (for foamed forms) to almost 3 kg/m3, the microplastic particle sizes in water environment are characterized by distributions and the forms are extremely diverse [7]. At the same time, the integral particle density changes with time as a result of aging of the material, biofouling and/or aggregation with particles of organic matter or sediment, particle sizes decrease as they fragment due to mechanical loads and UV radiation. The description of object behavior of this kind is a difficult problem. Especially in the natural conditions of the coastal sea zone.

In numerical modeling problems, global problems of plastic pollution transport have been solved for today in the oceans and seas. However, to develop more reliable predictive models, it is necessary to accumulate data on the concentrations and variability of the microplastic concentration in the water column and on the coast, as well as parameterization sources of microplastics and exchange processes with the shore [8]. Most field researches provide data on instantaneous microplastic concentrations in water, regardless of the current hydrometeorological situation, prevailing currents and without indicating possible temporal variability.

3 Development and numerical implementation of an algorithm for modeling the pollution transport in water environment

Currently, there are no well-established approaches for modeling the processes of entry into a reservoir, movement, flooding, sedimentation, absorption of microplastic particles by living organisms. Therefore, a separate problem is the development of mathematical models for description the listed processes.

To solve the hydrodynamics problem, as well as the pollutant transport of various origins, including micro- and nanoparticles of plastic, the conditions for applicability and efficiency of the developed solution algorithm were investigated. The hydrodynamics changes in the case of pollution with plastic waste were researched on the example of modeling the concentration changes of zooplankton populations in shallow water (the Azov Sea as an example) in case of pollution with plastic particles (Fig. 2).

a) b)

Fig. 2. Satellite image of the Azov Sea (a); plastic particles in the marine environment (b).

Scenario approach was used to research the effect of plastic pollution in shallow water on the number of zooplankton populations in the Azov-Black Sea region based on mathematical modeling methods and tools. The mathematical model of the pollutant distribution, including nano- and microplastic particles, the basic types of plankton, in shallow water, has the form [9, 10]:

$$\frac{\partial S_i}{\partial t} + u\frac{\partial S_i}{\partial x} + v\frac{\partial S_i}{\partial y} + (w - w_{gi})\frac{\partial S_i}{\partial z} + \sigma S_i = \mu_i\left(\frac{\partial^2 S_i}{\partial x^2} + \frac{\partial^2 S_i}{\partial y^2}\right) + \frac{\partial}{\partial z}\left(\upsilon_i(z)\frac{\partial S_i}{\partial z}\right) + f(x,y,z,t), \quad (1)$$

where $\boldsymbol{U} = (u, v, w)$ is the water flow velocity vector; w_{gi} is the rate of gravitational sedimentation of the i-th component, if it is in a suspended state; σ_i is the decomposition coefficient of the i-th impurity; f is the chemical and biological source (drain); μ_i, υ_i are diffusion coefficients in horizontal and vertical directions; S_i is the concentration of the i-th impurity, $i = \overline{1,10}$: 1 is the mercury(Hg); 2 is the lead (Pb); 3 is the manganese(Mn); 4 is the iron (Fe^{+2}); 5 is the oxygen; 6 is the phytoplankton (Aphanizomenon flos-aquae blue-green algae); 7 is the zooplankton (Copepoda); 8 is the biogenic substance; 9 is the nanoplastic; 10 is the microplastic .

The computational domain G is a closed pool bounded by a cylindrical side surface σ , undisturbed water surface Σ_0, bottom $\Sigma_H = \Sigma_H(x,y)$. $\sum$ is a piecewise smooth boundary of the domain G, $\sum = \sum_0 \cup \sum_H \cup \sigma$, $0 < t \le T_0$. Let's $\boldsymbol{n}$ is the external normal vector to the Σ, $\boldsymbol{U_n}$ is the normal component of the vector U.

Let us add the initial conditions to the system (1):

$$S_i|_{t=0} = S_{i0}(x,y,z),\ i = \overline{1,10}. \quad (2)$$

The boundary conditions have the form:

$$S_i = 0 \ \ on\ \sigma,\ if\ U_n < 0;\ \frac{\partial S_i}{\partial n} = 0\ on\ \sigma,\ if\ U_n \geq 0\ ;$$
$$\frac{\partial S_i}{\partial z} = -\varepsilon_i S_i\ on\ \Sigma_H, \frac{\partial S_i}{\partial z} = \varphi(S_i)\ on\ \Sigma_0, \varphi(S_i) = \begin{cases} \xi_i(S_i), i \neq 5; \\ \frac{a_0}{\nu_i}(K_i - S_i), i = 5; \end{cases} \quad (3)$$

where a_0 is the aeration coefficient; K_{10} is the oxygen dissolved concentration at saturation; ε_i is the absorption coefficient of the i -th substance by bottom sediments; ξ_i are given functions;$i = \overline{1,10}$.

The detailed structure of the biotic cycle processes in water environment including nano- and microplastics transport is given in Fig. 3.

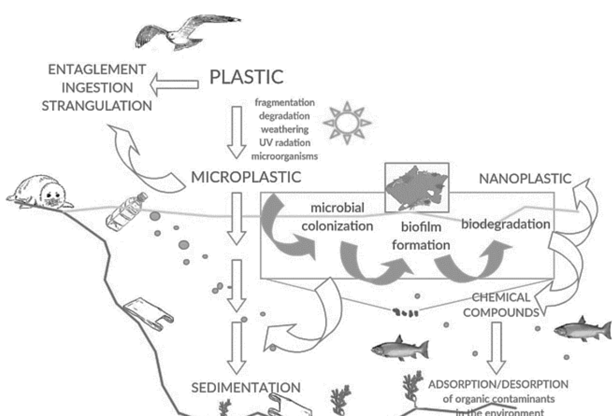


Fig. 3. Nano- and microplastics circulation in water environment.

The developed model is more accurate than existing models, takes into account a number of determining factors that have a significant impact on calculation results (advective transport, parametrized microturbulent diffusion, including in the vertical direction, gravitational sedimentation of pollutant microparticles, including plastic and plankton particles; non-linear interaction of plankton populations; biogenic, temperature and oxygen regimes; influence of salinity, illumination, temperature, etc.).

The model for the pollutant transport, including particles of nano- and microplastics, in shallow water is based on three-dimensional mathematical model of hydrodynamics, including three Navier-Stokes motion equations and the continuity equation [10-12].

The developed model problem of water ecology (1) – (3) is included in software complex. To reduce the error in solving it, in the computational domain of a complex shape, its discretization was performed on the basis ofa linear combination of the "cabaret" and "cross" schemes, taking into account partial filling of the calculation cells [13] with weight coefficients obtained as a result of minimizing the approximation error, which makes it possible to more accurately describe small-sized eddies that arise in the coastal part of shallow water bodies. The use of schemes of a higher order of accuracy, taking into account the partial occupancy of the computational cells when discretizing models, made it possible to significantly increase the accuracy of modeling and reduce the computation time [14].

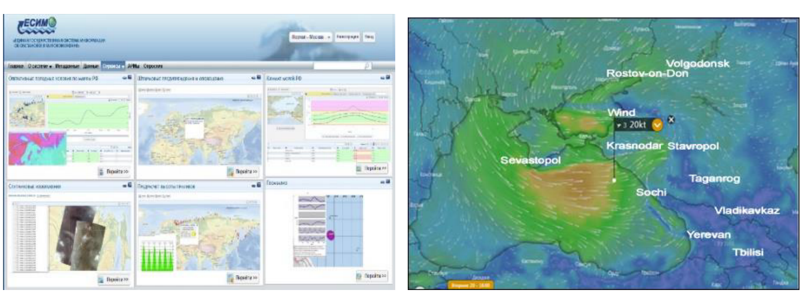
To solve the obtained grid equations, an adaptive modified alternating-triangular method of variational type was used, which has a better rate of convergence when the asymptotic stability of difference schemes is satisfied [15, 16].

The developed numerical algorithms make it possible to study the mechanisms of transport of suspended and bottom substances, the distribution of pollutant concentrations of various origins, and to describe the dynamics of changes in zones covered with plastic waste in a shallow water body [17].

With parallel implementation, grid domain decomposition methods for computationally laborious diffusion-convection problems were developed, taking into account the architecture and parameters of a high-performance computing system, built on adaptive iterative methods of the variational type for a moderate number of cores, as well as on the basis of explicit regularized schemes with high efficiency and speed for systems with massive parallelism [18].

To improve the efficiency of the algorithm for the numerical implementation of the model problem (1) - (3), the NVIDIA Tesla K80 graphics accelerator with CUDA technology was used, which made it possible to implement solutions to the problem of efficient resource allocation when solving high-dimensional SLAE. The dependence of the SLAE solution time by the alternating-triangular method on the matrix size and the number of non-zero diagonals is obtained. A distinctive feature of the software implementation is the use of a more compact data structure for storing a sparse matrix. To increase the efficiency of calculations of fragments of the computational grid assigned to graphics accelerators, an algorithm and its software implementation in the CUDA C language [19] have been developed.

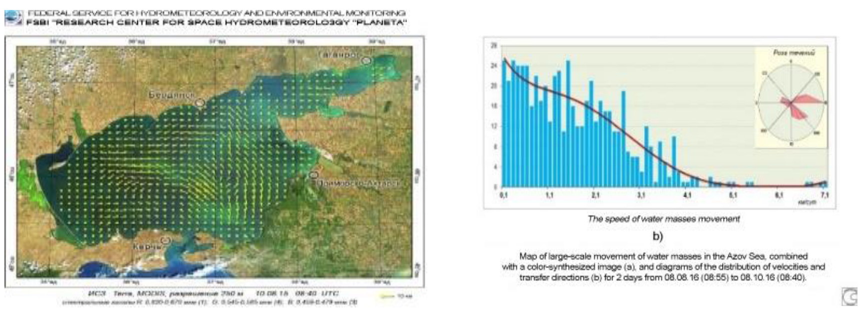
The main calibration method for a three-dimensional mathematical model of biological kinetics used to research the pollutant dynamics in shallow water is the selection of calculation algorithms based on the analysis of the available databases of ecological data on the inland seas of the South of Russia and obtained in the course of studies carried out jointly with the services, including Southern Scientific Center of the Russian Academy of Sciences, FGBNU "AzNIIRH", expeditions, as well as the systems of the portal "Analytical GIS", which presents the Vector-raster GIS GeoProcessor 1.5, Vector-raster GIS GeoTime II, Vector GIS KOMPAS-III and KOMPAS-V, multidisciplinary data on the natural environment for different regions of the world [http://geo.iitp.ru/index.php], data from the portal of the Unified State System of Information on the Situation in the World Ocean "ESIMO", data from NOAA (National Oceanic and Atmospheric Administration);satellite monitoring data of the Research Center "Planeta" (Fig. 4, 5) [20-22].



a)

b)

Fig. 4. Navigation panel of the ESIMO portal (a); Earth satellite sensing data: wind velocity and direction in the Azov-Black Sea basin (taken http://hobitus.com/noaa) (b).



a) b)

Fig. 5. Maps of large-scale movement of water masses in the Azov Sea combined with a color-synthesized image (a); diagrams of the distribution of velocities and directions of transport (b) (data from SRC "Planeta").

The number of computational experiments were performed to research the effect of microparticles of natural and technogenic origin, including particles of nano- and microplastics, on the hydrobiology of water systems in the South of Russia (in this case, the Azov Sea). It was performed using the SC that implements the developed mathematical model and numerical methods. At modeling spatially inhomogeneous processes of interaction between the main hydrobionts of the Azov Sea (1) – (3), external periodicity was taken into account, leading to the complication of the system [23, 24].

Figure 5 shows the dynamics of the distribution of zooplankton concentration at different time. The simulation of biological kinetics processes was performed taking into account the vegetation period of phytoplankton. The maximum values of biogenic substance concentrations are colored in white, the minimum values of phyto- and zooplankton – in black.

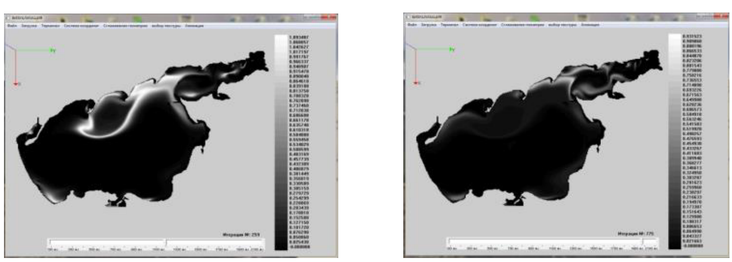


Fig. 6. Distribution of zooplankton concentration at different time.

It was determined that the stable heterogeneity of the spatial distribution of pollution biogenic substance and phytoplankton is also due to diffusion processes and the presence of an ectocrine regulation mechanism in phytoplankton, i.e. regulation of the growth rate by isolating biologically active metabolites into the medium.

4 Conclusion

Conducted on the basis of the developed and numerically implemented problem of modeling the spread of microplastic particles and its effect on the abundance of zooplankton in a shallow water body, software-analytical studies have shown the adequacy and performance of the mathematical model built in this work, integrated into the software package, which allows using it when planning prognostic calculations to determine the quality of water in different periods of time.

Development of optimized mathematical models of pollutant transport in a shallow water body, taking into account a number of determining factors, including micro-turbulent diffusion, water flow movement, gravitational settling of pollutants and plankton, biogenic, temperature and oxygen regimes, coastal abrasion, floods, untreated water runoff by the enterprise, secondary pollution with impurities when they rise from the bottom of the reservoir under the influence of wave processes, eutrophication, "blooming" of algae that cause deadly phenomena, the influence of temperature, salinity and illumination, as well as the study of the conditions for the applicability and effectiveness of the developed algorithms for its numerical implementation will make it possible to carry out an accurate and prompt forecast of changes in the hydrodynamics of a reservoir, the impact on biocenotic communities,assessment and prospects for the spread of pollution in both the short and long term.

The developed model for the distribution of pollutants, including particles of nano- and micro-plastics, basic types of plankton in a complex computational domain, made it possible to study the effect of pollution of a shallow water body by plastic particles on the number of zooplankton populations in the Azov-Black Sea region. With the help of schemes of higher order of accuracy used in discretization, the accuracy of modeling has been significantly increased and the computation time has been reduced. The model and algorithms for its numerical implementation were integrated into the PC, which makes it possible to predict possible scenarios for the development of shallow water bodies in the South of Russia when hazardous natural and man-made phenomena occur in them.

The results of numerical experiments on the NVIDIA Tesla K80 graphics accelerator showed the advantage of the parallel algorithm with a large number of computational nodes. As a result of the research, an algorithm and a software module were developed that implement it for solving SLAE (self-adjoint and non-self-adjoint cases) using NVIDIA CUDA technology.

The software implementation of the proposed model makes it possible to determine the limits and prospects for its use. On the basis of a high-performance computing system, experimental software has been developed for modeling various scenarios for the development of ecosystems in shallow water bodies with pollution of various origins and areas covered with plastic waste. With a parallel implementation, methods have been developed for decomposition of grid domains for computationally labor-intensive problems of diffusion-convection, taking into account the architecture and parameters of the aircraft.

Thus, the developed set of interrelated models of the hydrobiology of a shallow water body, taking into account the main factors affecting the hydrodynamics of the water body and the spatial distribution of pollutants, including micro- and nanoplastics, can be used to assess hydrophysical changes in the geosystem monitoring of marine systems, formation scenarios for optimal nature management of water resources. The PC is planned to be replicated in the future to other shallow water systems in the South of Russia. It is planned that the developed software and algorithmic tools will improve the accuracy of predictive modeling of the state of the ecosystem of a shallow water body by 10–20%.

The study was supported by the Russian Science Foundation grant No. 22-11-00295, https://rscf.ru/en/project/22-11-00295/.

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