Development and numerical implementation of an algorithm for simulation the pollutant transport in water environment taking into account their destruction and deposition

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Abstract. The paper covers the development of an algorithm for modeling the pollutant distribution dynamics in shallow water and its implementation on a high-performance computer system in a limited time. A mathematical model of the pollutant transport, including oil and petroleum products, in the water environment has been developed taking into account a number of determining hydrodynamic and hydrophysical factors, including destruction and deposition, affecting the nature of their flow. Methods of its numerical implementation have been developed for prediction the pollution spread in shallow waters in limited time on a high-performance computer system. The main advantage of it in predictive modeling of environment processes and phenomena is taking into account the multidisciplinary nature of real processes, the complex geometry of simulated domain, ensuring high accuracy of calculations, performing a large number of calculations in a short time. Simulation of the pollutant transport of various etiologies was performed taking into account a number of determining factors, including their structure and deposition on the bottom surface, on the basis of the developed software and algorithmic tools. It used a scenario approach that meets the basic principles of effective predictive modeling in water systems. The simulation results are the foundation for planning and conducting measures to prevent and eliminate the consequences of technogenic hazards.

1 Introduction

Modeling of hydrobiological processes in water environment today special economic significance for today in view of the active increase of rapid industrialization. To maintain the effective functioning of water system, it is necessary to monitor ecological systems to analyze and predict the ecological situation in waters [1, 2]. At events with natural and/or technogenic challenges (pollution by substances of various origins, acid rain, industrial and agricultural emissions, oil spills, etc.), especially at emergency, it is necessary to implement

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prompt and accurate forecasts of the water system conditions for further measures to eliminate possible negative consequences. Pollutants, arising as a result of human activities, and their impact on the marine environment are quite diverse. These include: compounds of carbon, sulfur, nitrogen, heavy metals, various organic substances, artificially created materials, polymers, radioactive elements, etc. Note that recently the release into the marine environment of domestic and industrial wastewater containing such dangerous pollutants as lead, mercury, arsenic, alkanes (paraffins) and cycloalkanes (naphthenes), aromatic hydrocarbons or more complex chemicals that have a strong toxic effect on all living things. Background concentrations of such substances in many places have already been exceeded by dozens of times.

The most dangerous type of water pollution is the ingress (spills) of oil and oil products, which is already becoming global. Thus, according to experts, about 10 million tons of oil and oil products enter the ocean annually. This substance forms a thin film (slick) on the water surface, which prevents oxygen and gas exchange between air and water. Settling to the bottom, oil enters bottom sediments, thereby contributing to the disruption of the natural processes of life of bottom animals and microorganisms.

To control the biological resources of water environment, as well as to develop measures in the event of climatic and anthropogenic impact, it is necessary to develop a software and algorithmic toolkit based on modern and effective mathematical methods and tools to predict phenomena of a dangerous nature for the possibility of maintaining conditions for the optimal functioning of the marine environment in a limited time.

The pollutant spreading process of various origins was researched in this paper. The oil spills has a special importance as a particularly dangerous type of pollution. The paper is devoted to the construction, research and numerical implementation of a mathematical model of pollutant transport, including oil products, in water environment taking into account a number of determining hydrodynamic and hydrophysical factors, including destruction and sedimentation, which affect the nature of their flow, and methods for its numerical implementation, which allow performing predictive simulation of the pollution spread in shallow water systems in limited time on a high-performance computer system. Note that the main advantage of using high-performance computer systems in predictive modeling of processes and environmental phenomena is taking into account the multidisciplinary nature of real processes, the complex geometry of the simulated area, ensuring high accuracy of calculations, performing a large number of calculations in a short time.

Modeling of hydrobiological processes in shallow water is based on the scenario approach, which makes it possible to analyze and identify relationships between external influence factors and ongoing hydrobiological processes. To calibrate and verify the used mathematical models of hydrobiology, satellite monitoring data were used, which are in the public domain. Due to it, we can identify the effectiveness of the developed software and algorithmic tools at a qualitative and quantitative level.

The regulatory documents were used at developing simulation algorithms. They describe a set of priority measures aimed at eliminating the consequences of pollution and other negative impacts on the environment as a result of natural and/or technogenic challenges [3, 4]: Federal Law No.7 on January 10, 2002 “About Environmental Protection”; Water Code of the Russian Federation; Decree of the Russian Federation Government on May 3, 1994 No.420 “About the protection of life and health of the population of the Russian Federation in the event of the occurrence and elimination of the consequences of emergency situations caused by natural disasters, accidents and catastrophes”; Art. 67 Requirements for the prevention of emergencies at POO and life support facilities, introduced by the order of the Ministry of Emergency Situations of the Russian Federation dated February 26, 2003 No.105 “On approval of requirements for the prevention of emergencies at potentially dangerous objects and life support facilities”; Decree of the Russian Federation Government on

December 30, 2003 No.794 “On the Unified State Emergency Prevention System”. According to Federal Law No.7-FZ on January 10, 2002 (as amended on January 1, 2017) “On Environmental Protection”; Water Code of the Russian Federation (as amended on October 31, 2016 No.384-FZ); Decree of the Russian Federation Government on December 30, 2003 No.794 (as amended on January 26, 2017) “On the unified state system for preventing emergencies”, the time for decisions and eliminating emergencies should be from several hours to 2 – 3 days [5]. According to Decree of the Russian Federation Government No.240 on April 15, 2002 “When a message is received about oil and oil product spill, the spill localization time should not exceed 4 hours in case of a spill in water area, and 6 hours in case of a spill on the soil from the moment the oil and oil product spill is detected or from the moment information about the spill is received”. Thus, the prediction time of water ecosystem situation in the event of the occurrence of natural and technogenic phenomena should be tens to hundreds of times less than the standard time. It requires predictive modeling of hydrobiological processes on high-performance computer systems in the accelerated time.

Therefore, the solution of water ecology problem, especially in the event of natural and technogenic phenomena, is an urgent and necessary condition for further supporting the sustainable development of marine system hydrobiocenoses.

2 Analysis and research of the problem of pollution transport processes modeling in water environment

The development of industry and technological production, especially in recent decades, leads to a significant deterioration of water ecological situation, which are most susceptible to various household, agricultural, and industrial pollution. Thousands of chemicals with unpredictable effects enter watersheds every year, many of which are new chemical compounds.

The necessary to predict hazardous natural and/or technogenic phenomena in water environment is due to the necessary to obtain and systematize data about occurrence process and further hazardous phenomena based on an analysis of the causes and sources of their occurrence. The necessary problems that must be solved at researching the pollution spread processes in water environment are: the assessment of the probability of occurrence of each sources of technogenic accidents, their scale, the size of their zones; possible consequences (both short-term and the prospect of their development) at hazardous phenomena; the need for forces and means to eliminate predicted hazardous phenomena [6].

High requirements are imposed on modern mathematical models of hydrobiology: the model must be of a simulation level to see the detailed evolution of the simulated object and visually analyze its features; the model must comprehensively describe the object or process, have high detail, spatial and temporal resolution [7, 8]. In other words, the developed mathematical model should provide many opportunities for its research and the possibility of modeling not only a given object, but also its various variants and objects similar in physical nature.

The use of operational global space information makes it possible to successfully monitor both fast and slow processes covering large areas. Satellite images of the TERRA, MODIS, NOAA (AVHRR) satellites, the of Earth satellite monitoring results obtained by the Research Center "Planeta", "ESIMO", etc. are used to control the simulation quality (Fig. 1).

The operational use of space information is especially relevant for the territory of the Russian Federation with vast expanses [9].

The research of the main processes that affect the dynamics of pollutant transfer in water ecosystems was performed in this paper. It was found that one of the fundamental factors for adequate forecasts of pollution spread in water systems is the preparation and processing of initial data; research of climatic and geographical features of investigated region; the hydrodynamic features of water area (the presence of underwater hydraulic structures, the shape of the bottom surface, etc.), the investigated pollutant properties.

The main pollutants of water systems and the processes occurring in water directly during the pollution have been researched [10]. Hazardous pollutants of the water environment that have a negative impact on the water hydrobiocenosis include organic substances of various classes and degrees of solubility in water, in the form of a thin film on the water surface or particles and impurities deposited on the bottom. The thin film weakens its ultraviolet irradiation, hinders oxygen exchange between the atmosphere and hydrosphere, and disrupts photosynthesis processes. This contributes to a significant deterioration in the vital activity of biota or leads to their death.

Sinking to the bottom, the pollutants enter the bottom sediments and are involved in the natural substances cycles, distort them or increase the cumulative pollution of natural ecosystems.

The Azov-Black Sea region (Fig. 1, the image of the Russian satellite Meteor-M No.2 dated October 10, 2018), namely the Gelendzhik Bay, was chosen as the simulation object for problem solution, in view of one of the most populated and used territories in southern Russia (Fig. 2).

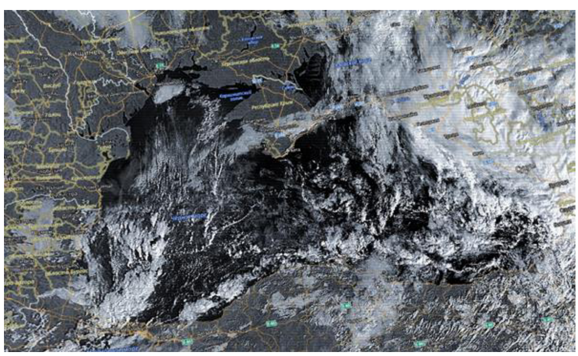

Fig. 1. Satellite image of the Azov-Black Sea region.

Fig. 2. Satellite image of the Gelendzhik Bay.

The features of the investigated region were researched. Gelendzhik Bay is a shallow and non-freezing bay of the Black Sea. The coastal concavity has the shape of an almost symmetrical horseshoe and a relatively shallow depth (from 3 to 11 m). The surface bay area

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is approximately 10 km². The bottom of the bay is mostly rocky and is composed of rocks, erosion products of neighboring mountains and bottom sediments of anthropogenic origin. Various types of phytoplankton inhabit the water area of the bay. Several rivers and streams flow into the bay from the Markoth ridge.

Natural-climatic and hydrochemical features of the Gelendzhik Bay is presented in a wide range by its semi-closedness, difficult water exchange and the active influence of human economic activity. Widespread climatic features typical for this region (storm winds, surges, heavy rainfall, abnormal air temperatures, tornadoes, undercurrents, rise of deep waters to the surface in summer, bora, etc.) cause considerable interest in researching of its ecosystem functioning, which, depending on the severity of the situation of natural and/or technogenic nature, experience a huge load.

The types of main pollutants in the Gelendzhik Bay (2017), the values of which exceed the MPC (maximum permissible concentration) standards in water, were defined (Table 1). Iron is absorbed and accumulated by phytoplankton, which affects the rate of development and change of the dominant species of sea water microflora. Lead belongs to the class of highly hazardous substances. It is toxic to aquatic plants and tends to accumulate in fish biomass, making it dangerous for food consumption. Its maximum concentration in the bay exceeds the MPC by almost 1.5 times. Mercury compounds are highly toxic, have a negative effect on the nervous system, lead to damage to the musculoskeletal system and irritation of the mucous membrane. Its concentration according to the maximum indicator is exceeded by 2.5 times.

Table 1. Ranges of variability and average annual values of pollutants in the Gelendzhik Bay.

Pollutant	Minimum	Maximum	Average	MPC standards
Oil products, mg/l	0.006	0.036	0.019	0.05
Phenol, mcg/l	<0.06	0.4	0.21	1
Iron (Fe^{+2}), mg/l	0.005	0.169	0.036	0.05
Manganese (Mn), mg/l	0.009	0.326	0.075	0.05
Mercury (Hg), mcg/l	0.017	0.250	0.046	0.1
Zinc (Zn), mcg/l	0.22	7.78	1.43	50
Cadmium (Cd), mcg/l	1.28	3.15	2.15	10
Lead (Pb), mcg/l	2.05	14.34	5.08	10
Benz(a)pyrene, ng/dm³	<0.5	<0.5	<0.5	5

The petroleum hydrocarbons were selected as compounds that are especially dangerous for water flora and fauna for simulation the pollutant transport processes in water environment taking into account their destruction and bottom sedimentation. Oil gets into the water as a result of its natural outcrops in the occurrence areas, as well as oil production, oil refining, transportation and use as industrial raw materials and fuel.

To adequately predict the water ecosystem conditions, their main properties and behavioral features entering the water column were researched. Phenols (compounds of oil and oil products) form a fluorescent film (slick) on the water surface. It contributes to the disruption of natural biological processes and the ecosystem balance; changes in the physicochemical water properties, as a result of which the gas exchange process with the atmosphere is disturbed; changes in the qualitative and quantitative composition of water biopopulations (phyto- and zooplankton, fish, algae), etc.

In this paper, the dynamics of changes in oil particles entering the water column, depending on its fractional composition and physicochemical parameters of hydrocarbons, was researched. In the period up to one day after the oil spill, these processes are especially intense, and only the mixing of heavy fractions with a suspension in water and individual components of the bottom (silt, sand, and bottom sediments) occurs over a period of several days to a month or more. Oil and its derivatives are a mixture of hydrocarbons with different physical characteristics: for gasoline, the solubility is about 10 – 500 mg/dm3; for diesel fuel – 10 – 20 mg/dm3; for oil (depending on the chemical composition) – 10 – 50 mg/dm3; for kerosene – 2 – 5 mg/dm3. The degree of petroleum products solubility decreases in the series: paraffinic, cycloparaffinic, aromatic. The soluble oil fraction in water is about 5 – 10-3%. It should be taken into account that oil forms stable emulsions with water, while up to 15% of the volume of all oil passes into the water column; Easily soluble components of oil include its most toxic components. bottom sediments) occur over a period of several days to a month or more.

The main processes that occur with oil after it enters the water were researched, among them the destruction of oil slick pseudo-fractions; evaporation; biodegradation; spreading; dissolution; precipitation (Fig. 3).

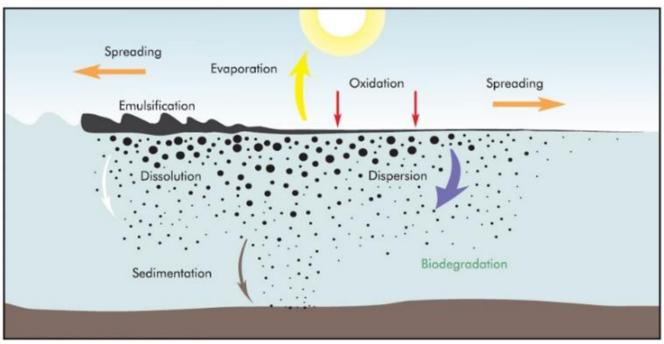

Fig. 3. Diagram of oil distribution and destruction processes in water environment.

After hitting the water surface, the oil slick, like other pollutants, spreads and transports along the surface, undergoing a number of chemical and physical changes. It begin immediately from the moment oil hits the water surface and continue depending on the type of spilled oil, its physical and chemical characteristics and hydrological and meteorological conditions during the period of the substance residence in water.

Thus, for high-quality and operational prediction of water system conditions at its pollution, it is necessary to comprehensively analyze the features and properties of the pollutant, which can affect the simulation quality.

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

The simulation of pollutant transport processes by various origins, including oil and oil products, taking into account the hydrophysical and biological parameters of the water, the complex geometry of computational domain, climatic environmental factors, destruction and bottom sedimentation, was performed on the basis of the developed mathematical model. The model is a complete 3D system distribution equations for pollutants, including oil and oil products [11, 12]:

$$\frac{\partial S_i}{\partial t} + u\frac{\partial S_i}{\partial x} + v\frac{\partial S_i}{\partial y} + (w - w_{gi})\frac{\partial S_i}{\partial z} + \sigma S_i =$$

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$$= \mu_i \left(\frac{\partial^2 S_i}{\partial x^2} + \frac{\partial^2 S_i}{\partial y^2} \right) + \frac{\partial}{\partial z} \left(\upsilon_i(z) \frac{\partial S_i}{\partial z} \right) + f(x, y, z, t), \quad (1)$$

where u, v, w are components of the water flow velocity vector; w_{gi} is the rate of gravitational sedimentation of the i-th component, if it is in suspension; σ_i is the expansion coefficient of the i-th impurity; f is the chemical-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, $i = \overline{1,6}$: 1 is the mercury(Hg); 2 is the lead (Pb); 3 is the manganese (Mn); 4 is the iron (Fe^{+2}); 5 is the phytoplankton (Aphanizomenon flos-aquae blue-green algae); 6 are oil and oil products.

The model includes pollutants whose concentration in the Gelendzhik Bay, according to the analysis of scientific publications and environmental databases, exceeds the MPC. This model takes into account the water flow movement; microturbulent diffusion; interaction and gravitational sedimentation of pollutants and plankton; biogenic, temperature and oxygen regimes; salinity. The input data for this model are the velocity vector components of water environment, which are described by the hydrodynamic model by Sukhinov A.I., Chistyakov A.E. [13].

Calculations were performed in a complex computational domain – Gelendzhik Bay – with a lateral surface σ, undisturbed water surface Σ_0, the bottom Σ_H, variable depth H in the Cartesian coordinate system at the axes Oz, Oy, Ox, directed vertically downward, to the north and east, respectively.

The initial conditions for system (1) have the form:

$$S_i(x, y, z, 0) = S_{0i}(x, y, z) \quad (2)$$

The computational domain G (Gelendzhik Bay) is a closed area bounded by the undisturbed water surfaceΣ_0, bottom $\Sigma_H = \Sigma_H(x, y)$ and cylindrical surface σ for $0 < t \leq T_0$. $\Sigma = \Sigma_0 \cup \Sigma_H \cup \sigma$ is a piecewise-smooth boundary of the domain G (Fig. 4).

Let U_n is the component of the water flow velocity vector, normal with respect to the boundary Σ, $\boldsymbol{n}$ is the outer normal vector to Σ.

Then the boundary conditions for model (1) have the form:

$$S_i = 0 on \sigma, \text{if} U_n < 0; \frac{\partial S_i}{\partial \boldsymbol{n}} = 0 \text{ on } \sigma, \text{if } U_n \geq 0;$$
$$\frac{\partial S_i}{\partial z} = \varphi(S_i) \text{on } \Sigma_0; \frac{\partial S_i}{\partial z} = -\varepsilon_i S_i \text{ on } \Sigma_H, \quad (3)$$

where ε_i is the absorption coefficient of the *i*-th component by the bottom material, φ is a given function.

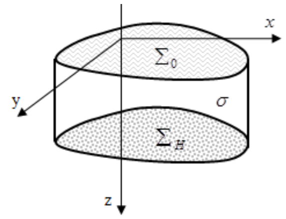

Fig. 4. The computational domain G.

The calculation results based on the model of multicomponent air medium movement, the hydrodynamics model of shallow water taking into account the wind effect, the flow of the Su-Aran River, water exchange with other waters, the bottom topography, the complex shape of the coastline, friction against the bottom, temperature, salinity, evaporation and precipitation, the Coriolis force, were used as input data [14].

To determine the error estimation of the developed model of pollutant transport in coastal systems, we use the criterion for checking adequacy performed with simultaneous consideration of in-situ data according to the available n measurements using the average absolute error:

$$MAPE = \frac{1}{n}\sum_{k=1}^{n}\frac{|\varepsilon_k|}{s_{k\,nat}}\cdot 100\%, \qquad (4)$$

where s_{knat} is the substance concentration value, obtained using field data; s_k is the substance concentration value of the calculated using the proposed mathematical model (1) – (3), $\varepsilon_k = s_{knat} - s_k$ is an error or forecast error.

Algorithms for numerical implementation of mathematical models of hydrodynamics and biogeochemistry of shallow water, developed in this paper, were implemented in the C++ programming language. The most resource-intensive part of software implementation of a mathematical model is the function of solving a system of linear algebraic equations (SLAE) that arises at model discretization. To accelerate calculations, a software module (library) of iterative solvers for SLAE was developed using the modified alternating-triangular iterative method (ATM) (the self-adjoint and non-self-adjoint cases) for the convection-diffusion problem. It based on decomposition in two spatial directions [15] and used MPI technology for information exchange between computers.

Decomposition methods of grid domains were developed for solving computationally labor diffusion-convection problems taking into account the architecture and parameters of the computer system. An analysis of the effectiveness of the developed parallel algorithms and researches of obtained solutions of water ecology problems were performed [16].

Due to the problem implementation on a high-performance computer system, the calculation time was significantly reduced by a factor of tens with a large amount of input data and, depending on the refining grid along the coastal part of the computational domain and the solved problem, compared to sequential algorithms that implement variational methods [17].

The numerical implementation of fast-converging parallel iterative algorithms for grid equations, obtained by approximating the original problem using schemes of high-order of accuracy with high efficiency coefficients for systems with distributed memory, was proposed.

The developed parallel algorithms implement the pipelined computing process. It makes possible to fully utilize all available computing resources, including high-performance graphics accelerators. Each computing node of the system can contain from 1 to 2 central processing units (CPU) with from 1 to 32 cores, and from 1 to 12 NVIDIA video accelerators with support for CUDA technology (GPU, graphics processing unit) with from 192 (NVIDIA GeForce GT 710) to 5120 (NVIDIA Tesla V100) CUDA cores. The organization of calculations on each node is performed the algorithm that controls all available threads of the CPU and GPU (computers). Each calculator performs calculations only for its own fragment of the computational domain. For this, the computational domain is divided into subdomains assigned to individual computing nodes.

To increase the calculation efficiency of the computational grid fragments assigned to graphics accelerators, the algorithm and its software implementation in the CUDA C language were developed [18].

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Using the graphics accelerator with CUDA technology, we can implement solutions to the problem of efficient resource distribution at solving the 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 was obtained for software implementation of the corresponding algorithm based on NVIDIA CUDA technology. The distinctive feature of software implementation is the use of a more compact data structure for storing a sparse matrix.

4 Software implementation of the problem

A software complex (SC) has been designed to implement the developed mathematical model and the numerical algorithm implement it. It allows to predict the pollutant transport dynamics in water environment in various hydrological and meteorological situations. It focused on high-performance computer systems (Fig. 5).

Interrelated mathematical models of hydrodynamic and biological processes in shallow waters were implemented in the SC. Compared with known models, they make possible to more accurately research the hydrophysics and biological kinetics processes, including sediment transport, primary and secondary pollution by impurities at the rising it from water bottom under the wave processes, eutrophication, to predict the pollutant distribution of various etiologies, biogenic substances (compounds of nitrogen, phosphorus, silicon), dissolved oxygen in water systems with complex spatial structures of currents, and obtain the accurate assessment and predict the ecological situation development of shallow water, especially in emergency.

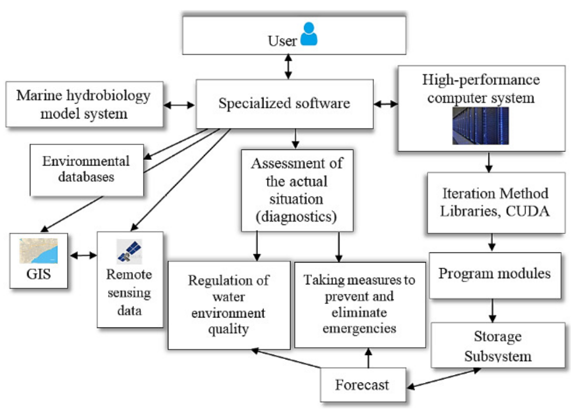

Fig. 5. Block diagram of SC operation.

Calculations based on these models [19] were used for comprehensive interpretation of satellite data and the establishment of causal relationship between hydrodynamic and biotic processes. As a result, approaches have been developed to assess the possibilities of joint use of satellite and model data. The developed complex includes the implementation of 2D and 3D mathematical models on computational grids, consistent with the complex shape of the coastline of the research area. Due to the SC, we can perform calculations for the substance transfer problem in shallow water on various computational grids. The number of computational experiments and researches of the obtained simulation results were performed.

To control the quality of hydrobiological processes simulation, we used the Earth satellite monitoring data obtained by NOAA (National Oceanic and Atmospheric Administration), the Analytical GIS portal system developed by the Institute for Information Transmission

Problems of the Russian Academy of Sciences (IITP RAS, Moscow), literary sources, expeditionary data obtained by the authors in the course of various research works, data from the portal of the Unified State System of Information on the situation in the World Ocean "ESIMO", data from the Federal State Budgetary Institution "Research Center for Space Hydrometeorology" Planeta " Siberian Center [20]. The use of satellite data makes it possible to identify areas of the coastal water zone that are most susceptible to climatic and industrial impacts (Fig. 6, 7).

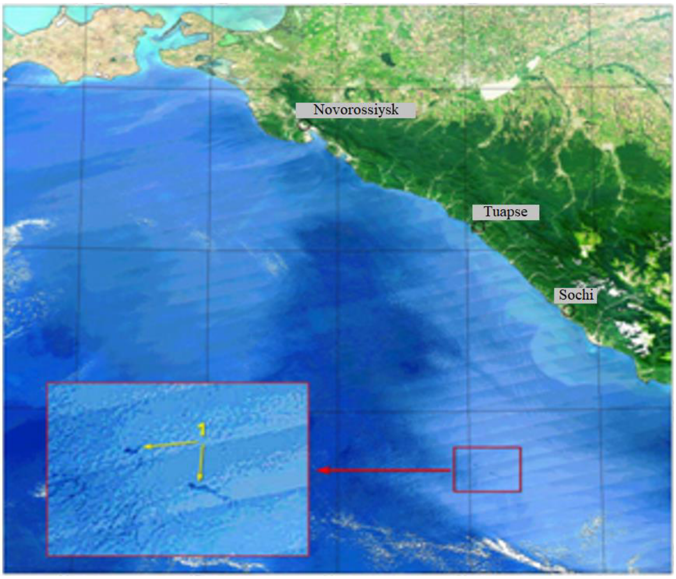

Fig. 6. Decoding of oil films on a color-synthesized image of the Black Sea northeastern part (1 are oil pollution films from ships in the field of solar glare).

Based on satellite data, pollution zones of the coastal regions of the Black Sea northeastern part, in particular, the Gelendzhik Bay, were detected. They appeared due to untreated river runoff. The approximate concentration of pollutants that got into the water and the territory of their distribution were determined [21].

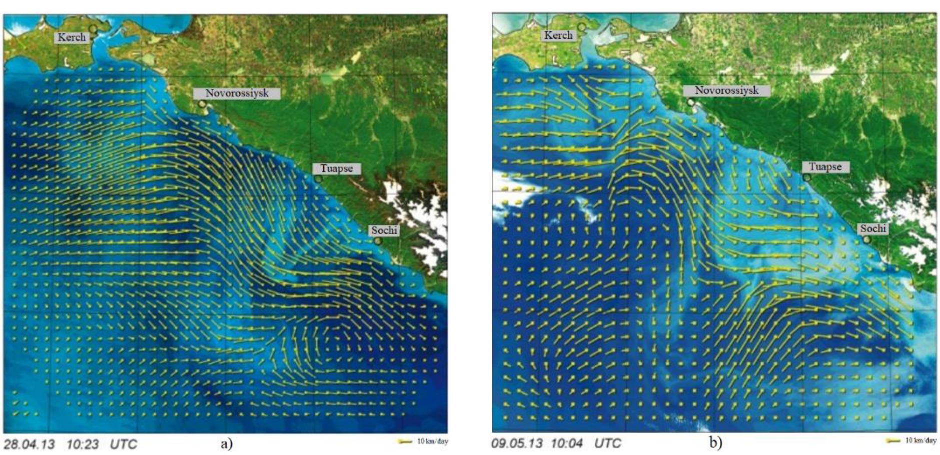

Fig. 7. Map of large-scale movement of the Black Sea water mass combined with a color-synthesized image for 1 day: a) 27.04.13 (11:18) – 28.04.13 (10:23); b) 08.05.13 (11:00) – 09.05.13 (10:04).

Using the developed SC, we can assess and predict the ecosystem conditions of shallow waters; calculate the risk factor associated with water, determinate the type and concentration of pollutants and microparticles, biogenic substances, heavy metals, oil and oil products; assess the probability of ingress and accumulation of fine (including oil) and other pollution microparticles into the organisms of the main commercial fish, depending on the places of their spawning and feeding; assimilate methods of measurement data; diagnose the developed models quality; reconstruct the state function; research the sensitivity of models to input data variations; integrate models of various scales; plan, observe and assess the information content of monitoring systems, detect, assess the pollutant sources power and their management; use the developed mathematical models and it numerical implementation. We can predict both the spread of suspended plumes in water environment and the change in the bottom topography due to the precipitation of suspended soil particles during the operation of various types of dredging equipment; organization and research to identify trends and patterns of changes in water ecosystem conditions under the influence of natural and anthropogenic factors, including assessing risks and vulnerability to anthropogenic impacts, assessing the observability of areas, zoning a reservoir in accordance with the levels of anthropogenic loads; develop a number of proposals and measures for prevention; environmental design from the standpoint of sustainable development, elimination of negative consequences of climatic and industrial challenges.

Previously developed methods that take into account satellite information use simplified models for the development of environmental events. Often, the equations in the model take into account only the diffusion component, and use the Gaussian approximation. This is fundamentally wrong at model development for real waters. At creation the predictive models of ecological situation development (distribution of pollution biogenic substances, oil slicks on the water surface, phyto- and zooplankton), the developed PC uses not only satellite information, but also additional ground-based measurement data, a priori information on pollution parameters with an accuracy, sufficient for environmental modeling and presenting the results in the form of a digital map as part of GIS.

In further, we plan to replicate the SC on other shallow waters in the South of Russia. The developed software and algorithmic tools will increase the prediction accuracy of shallow water ecosystem situation by 20 – 30%.

To simulate the pollutant transport processes in water environment, the real pollutant distribution was researched. It occurred in the Gelendzhik Bay at October 5, 2011. Heavy rainfalls was in the coastal areas of the Black Sea northeastern part; as a result, floods formed on the rivers of the region. A large amount of polluted river water ended up in the sea. Due to the increased cloudiness, satellite images were obtained only by the end of the first ten days of October. The fragment of the radar image on October 11, 2011 (Fig. 8) shows films of mixed (biogenic and anthropogenic) origin caused by coastal runoff (the current velocity and direction during the period of satellite imagery, colored in blue).

The section of the pollution film of the bay was allocated to simulate the pollution transport process (Fig. 9).

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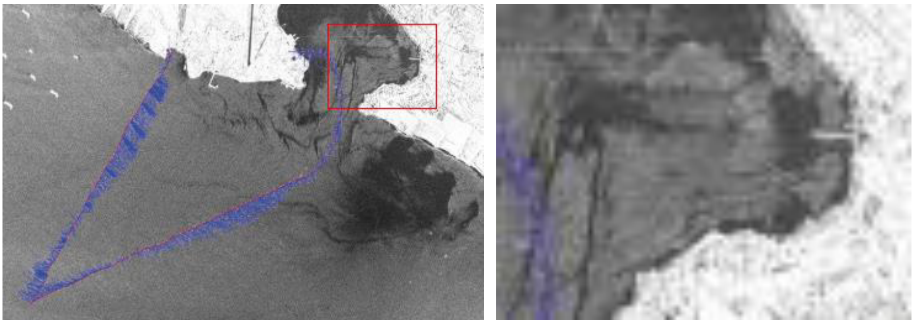

Fig. 8. Fragment of the radar image of Gelendzhik Bay.

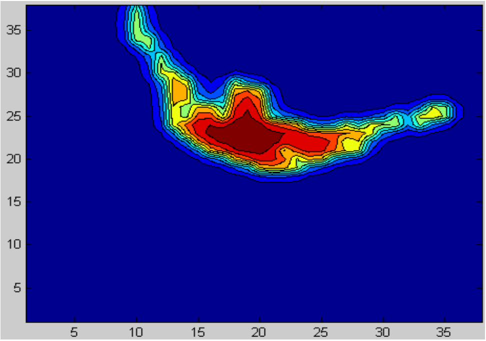

Fig. 9. Image of a film area of mixed origin pollution.

Figure 10 shows the results of numerical experiment for pollutant transport simulation. The research of similar applications that numerically implement pollutant transport models showed that the prediction accuracy of pollutant distribution dynamics, including phytoplankton, in shallow water increases by about 10%.

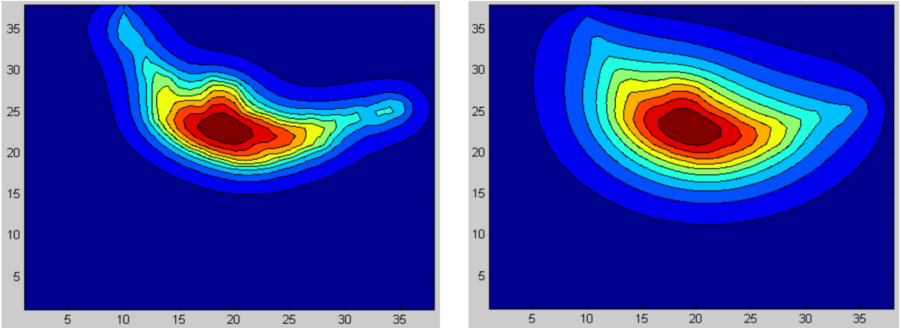

Fig. 10. The pollution spread dynamics in the presence of convective transport at the velocity 5 m/s (the time interval is equal to 1.5 s).

The analysis of SC efficiency, implements the constructed scenarios of ecological situation development in the Gelendzhik Bay using the numerical implementation of biological kinetics model problems, was performed with similar works in the field of mathematical modeling of hydrobiological processes. It was found that the obtained simulation results are qualitatively and quantitatively consistent with satellite monitoring data.

5 Conclusion

The mathematical model of pollution transport by various etiologies, including oil and oil products, in water environment has been developed, researched and numerically implemented taking into account a number of determining hydrodynamic and hydrophysical factors, including destruction and bottom sedimentation, which significantly affect the nature of their flow. The effective methods for its numerical implementation were proposed for prediction the dynamics of pollution spread in shallow water systems in limited time on high-performance computer systems. Due to the use of high-performance computer systems, the numerous highly reliable calculations that arise at solving this class of water ecology problems can be performed in a limited time. This is one of the main conditions for construction both short-term and long-term forecasts of ecological situation in water. In addition, the main advantages of the problem implementation in this paper on high-performance computer systems are taking into account the multidisciplinary nature of real processes, the complex geometry of the simulated domain, the high accuracy of calculations, and performing a large number of calculations in a short time at simulation the processes and environmental phenomena.

The computational experiments and reseaches of obtained simulation results were performed. It showed the possibility of effective use of the developed SC at research the dynamics of pollutant transport processes of various etiologies in natural and technological systems.

The test and optimization of parallel algorithms and programs were performed taking into account the architectural features of high-performance systems; verification and validation of the developed models and programs that implement them were performed using various environmental databases, available field data, including the remote sensing data [20]. The developed parallel algorithms for solving the hydrodynamics and biological kinetics problems in this paper make it possible to reduce the calculation time by tens to hundreds of times; development the recommendations and proposals for their further improvement.

Parallel algorithms for solving the biological kinetics problem on the sequence of condensing grids were developed, and their efficiency was analyzed in the case of a different number of involved flows. 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, the algorithm and software module that implements it were developed for solving SLAE arising at model discretization of the hydrodynamics problem of shallow water. MPTM using NVIDIA CUDA technology. The developed software toolkit makes it possible to more efficiently use the GPU computing resources to solve computationally labor three-dimensional hydrophysical problems.

The computational and software and analytical experiments and calculations have shown the adequacy and efficiency of the developed mathematical model of pollutant transport in shallow water, integrated into the SC. SC can to be used in planning prognostic calculations for determining water quality in different time.

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