

INFORMATION TECHNOLOGIES ИНФОРМАЦИОННЫЕ ТЕХНОЛОГИИ



UDC 519.6

Original Theoretical Research

<https://doi.org/10.23947/2587-8999-2024-8-4-27-34>



Forecasting the Dynamics of Summer Phytoplankton Species based on Satellite Data Assimilation Methods

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Abstract

Introduction. Mathematical tools integrated with satellite data are typically employed as the primary means for studying aquatic ecosystems and forecasting changes in phytoplankton concentration in shallow water bodies during summer. This approach facilitates accurate monitoring, analysis, and modelling of the spatiotemporal dynamics of biogeochemical processes, considering the combined effects of various physicochemical, biological, and anthropogenic factors impacting the aquatic ecosystem. The authors have developed a mathematical model aligned with satellite data to predict the behavior of summer phytoplankton species in shallow water under accelerated temporal conditions. The model describes oxidative-reduction processes, sulfate reduction, and nutrient transformations (phytoplankton mineral nutrition), investigates hypoxia events caused by anthropogenic eutrophication, and forecasts changes in the oxygen and nutrient regimes of the water body.

Materials and Methods. To simulate the population dynamics of summer phytoplankton species correlated with satellite data assimilation methods, an operational algorithm for restoring water quality parameters of the Azov Sea was developed based on the Levenberg-Marquardt multidimensional optimization method. The initial distribution of phytoplankton populations was obtained by applying the Local Binary Patterns (LBP) method to satellite images of the Taganrog Bay and was used as input data for the mathematical model.

Results. Using integrated hydrodynamic and biological kinetics models combined with satellite data assimilation methods, a software suite was developed. This suite enables short- and medium-term forecasts of the ecological state of shallow water bodies based on diverse input data correlated with satellite information.

Discussion and Conclusion. The conducted studies on aquatic systems revealed that improving the accuracy of initial data is one mechanism for enhancing the quality of biogeochemical process forecasting in marine ecosystems. It was established that using satellite data alongside mathematical modeling methods allows for studying the spatiotemporal distribution of pollutants of various origins, plankton populations in the studied water body, and assessing the nature and scale of natural or anthropogenic phenomena to prevent negative economic and social consequences.

Keywords: forecasting, summer phytoplankton populations, coastal system, satellite data, numerical experiment

Funding. The study was supported by the Russian Science Foundation grant no. 22–71–10102, <https://rscf.ru/project/22-71-10102/>

For Citation. Belova Yu.V., Filina A.A., Chistyakov A.E. Forecasting the dynamics of summer phytoplankton species based on satellite Data assimilation methods. *Computational Mathematics and Information Technologies*. 2024;8(4): 27–34. <https://doi.org/10.23947/2587-8999-2024-8-4-27-34>

Прогнозирование динамики летних видов фитопланктона на основе методов усвоения спутниковых данных

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Аннотация

Введение. В качестве основного инструмента исследований функционирования водных экосистем и прогнозирования изменения концентрации фитопланктона в мелководном водоеме в летний период обычно используется математический инструмент с применением спутниковых данных, что позволяет осуществлять корректный мониторинг, анализ и моделирование динамики протекания биогеохимических процессов в пространстве и во времени с учетом совокупного действия ряда физико-химических, биологических и антропогенных факторов, влияющих на изучаемую водную экосистему. Авторами разработана математическая модель, коррелирующая со спутниковой информацией, позволяющая прогнозировать поведение летних видов фитопланктона в мелководном водоеме в условиях ускоренного времени, описывать окислительно-восстановительные процессы водной среды, сульфатредукции, трансформации биогенных веществ (минерального питания фитопланктона), изучать развитие заморных явлений, возникающих в результате антропогенной эвтрофикации, строить прогнозы изменения кислородного и биогенного режимов функционирования водоема.

Материалы и методы. Для моделирования численности видового состава летнего фитопланктона, коррелирующего с методами усвоения спутниковых данных, разработан оперативный алгоритм восстановления параметров качества вод Азовского моря, который базируется на методе многомерной оптимизации Левенберга-Марквардта. Начальное распределение фитопланктонных популяций было получено в результате применения метода LBP (локальных бинарных шаблонов) к космическим снимкам Таганрогского залива и использовано в качестве входных данных для разработанной математической модели.

Результаты исследования. На основе скомплексированных моделей гидродинамики и биологической кинетики, а также методов усвоения спутниковых данных, разработан программный комплекс, который позволяет строить кратко- и среднесрочные прогнозы экологической обстановки мелководных водоемов на основе различных входных данных, коррелирующих со спутниковой информацией.

Обсуждение и заключение. В рамках проводимых исследований состояния водных систем установлено, что одним из механизмов повышения качества прогнозирования биогеохимических процессов морских экосистем является уточнение начальных данных. Установлено, что использование спутниковых данных наряду с методами математического моделирования позволяют изучать пространственно-временное распределение загрязнений различной природы, планктонных популяций исследуемого водного объекта, оценивать характер и масштабы природного или техногенного явления для предотвращения негативных последствий экономического и социального характера.

Ключевые слова: прогнозирование, популяции летнего фитопланктона, прибрежная система, спутниковые данные, численный эксперимент

Финансирование. Исследование выполнено за счет гранта Российского научного фонда № 22–71–10102, <https://rscf.ru/project/22-71-10102/>

Для цитирования. Белова Ю.В., Филина А.А., Чистяков А.Е. Прогнозирование динамики летних видов фитопланктона на основе методов усвоения спутниковых данных. *Computational Mathematics and Information Technologies*. 2024;8(4):27–34. <https://doi.org/10.23947/2587-8999-2024-8-4-27-34>

Introduction. Remote sensing of the Earth (RSE) represents a modern and promising method for assessing the biological state of shallow water bodies, as well as the dynamics of biogeochemical processes, including the behavior of phytoplankton populations during the summer in shallow aquatic systems. A key challenge in this domain is developing and implementing computationally efficient forecasting algorithms and providing them with real-world input data. Addressing this challenge is fundamental to solving numerical modelling problems in hydrobiology for water bodies in southern Russia.

Research in this field is actively conducted by both Russian and international scientists. For example, [1] describes the application of remote sensing methods to map cyanobacterial blooms in lakes in northern Italy. The study in [2] demonstrates the effectiveness of the Maximum Peak Height (MPH) algorithm of MERIS in extracting chlorophyll-a (chl-a) concentrations as a tool for monitoring water body eutrophication. G.I. Marchuk, V.P. Shutyaev, G.K. Korotaev,

and V.B. Zalesny have significantly contributed to data assimilation methods in atmospheric and ocean physics problems [3, 4]. A.A. Zelenko and Yu.D. Resnyansky have studied marine observation systems [5]. O.I. Krivorotko and S.I. Kabanikhin developed algorithms for reconstructing disturbance sources in the nonlinear shallow water equations system [6].

The works of G.I. Marchuk and V.P. Shutyaev focus on iterative algorithms based on the theory of adjoint equations, allowing the solution of variational data assimilation problems [7]. Y. Chao, H. Zhang, et al., in [8], proposed a three-dimensional ocean modelling system for the California region that processes satellite data in real time. This ocean model features a horizontal resolution of approximately three kilometers and employs a multi-scale three-dimensional variational data assimilation methodology.

In [9], researchers Robertson R. and Dong C. compare several vertical mixing parameterization algorithms for oceanic waters: modifications of the Nakanishi-Niino Mellor-Yamada algorithm (NN), the Large-McWilliams-Doney's Kpp algorithm (LMD), Mellor-Yamada 2.5 (MY), and four versions of the Generic Length Scale (GLS) algorithm. Algorithms for processing satellite images to parameterize hydrodynamic and hydrobiological models and identify pollution zones are also actively developed. Study [10] describes algorithms and provides code for automatic detection of upwelling filaments (AFD) based on image processing and pattern recognition. Study [11] explores the potential use of Sentinel-2 satellite images with unmanned aerial vehicles for obtaining multispectral aerial photographs to detect marine surface debris for monitoring, collection, and removal.

The aim of this study is to integrate effective mathematical modeling methods with satellite data assimilation techniques to conduct detailed investigations into the functioning of aquatic ecosystems and forecast the dynamics of summer phytoplankton population changes in shallow water bodies. This approach enables the observation and analysis of the spatiotemporal dynamics of biogeochemical processes in shallow systems while accounting for the combined influence of physicochemical, biological, and anthropogenic factors affecting the studied aquatic ecosystem.

Materials and Methods. The developed 4D mathematical model of summer phytoplankton evolution in coastal systems is based on a system of unsteady partial differential equations with nonlinear source terms ψ_i :

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

where u, v, w are the components of the velocity vector for convective transport; μ_i, ν_i are the coefficients of turbulent transport in the horizontal and vertical directions, respectively; w_{gi} is the gravitational settling velocity of the i -th component in suspension; Δ is the two-dimensional Laplace operator; ψ_i are nonlinear source functions describing chemical and biological processes; i is the type of substance, $i \in M = \{P, MP, N, D, BT, BD, H_2S, S, SO_4, O_2\}$. The set of modeled substances is detailed in Table 1.

Table 1

Set of Modeled Substances

No.	Symbol	Description
1	P	Summer phytoplankton species
2	MP	Phytoplankton metabolite
3	N	Nutrients
4	D	Detritus
5	BT	Aerobic bacteria <i>Thiobacillus</i>
6	BD	Anaerobic bacteria <i>Desulfovibrio</i>
7	H_2S	Hydrogen sulfide
8	S	Elemental sulfur
9	SO_4	Sulfates
10	O_2	Dissolved oxygen

The source functions and model parameters are described in detail in [12]. Appropriate initial and boundary conditions are incorporated into the model.

The presented mathematical model builds upon the foundational works of prominent researchers, including A.I. Sukhinov, B.N. Chetverushkin, G.G. Matishov, E.V. Yakushev, and E.R. Weiner, among others [13, 14].

Development of a Software Suite for Research and Forecasting. The forecasting of phytoplankton dynamics in a shallow waterbody during the summer period was carried out using the developed research and forecasting complex (RFC), equipped with an integrable algorithm for interaction with geographic information systems (GIS). The software

and algorithmic framework is designed to analyze and evaluate the scale of natural disasters (including eutrophication, “blooming”, pollution by components of various etiologies, etc.) and to generate short- and medium-term forecasts of their development in accelerated time frames, with the potential for mitigating economic and social impacts.

Given the rapid escalation of factors adversely affecting the progression of hazardous and emergency events (climatic and anthropogenic), the use of modern and efficient forecasting methodologies integrated with GIS and satellite data is highly relevant today.

Modelling the dynamics of biological and geochemical indicators of the shallow waterbody (the Azov Sea and the Taganrog Bay) was carried out by solving direct and inverse remote sensing (RS) problems for aquatic environments. The solution to the direct problem of remote sensing in the visible range involves determining the spectral dependence of the reflection coefficient $R_{rsw} = (\lambda, -0, \theta_0, \beta)$ as a function of the concentrations of water system components and their optical properties [15]:

$$R_{rsw}(\lambda, -0, \theta_0, \beta) = T_{surf} L_w(+0, \theta_v, \beta_v, \lambda) / E_d(+0, \lambda), \quad (8)$$

where λ is the wavelength; β is the viewing angle of the water surface by the satellite sensor; θ_0 is the solar zenith angle; T_{surf} is the solar light attenuation factor when passing through the “water-air” interface; $E_d(+0, \lambda)$ is the illumination of the water surface, and $L_w(+0, \theta_v, \beta_v, \lambda)$ is the brightness of the water surface, determined using remote sensing data.

The solution to the inverse problem is based on developing an algorithm for retrieving water parameters from satellite data. Optical properties of water are influenced by living organisms, dissolved and suspended substances, micro-turbulent inhomogeneities, and bubble gases. This study highlights the primary color-forming components (water, dissolved organic matter (DOM); chlorophyll from phytoplankton (Chl), and mineral suspension (MS)), as well as the primary hydro-optical water parameters (a — absorption coefficient; b_b — backscattering coefficient). These parameters are convolutions of the optical properties of the color-forming components, characterized by additive properties:

$$a = \sum_{k=1}^K C_k a_k^*; \quad b = \sum_{k=1}^K C_k b_{bk}^*, \quad (9)$$

where a_k^* , b_{bk}^* are the primary hydro-optical characteristics of the k -th component; C_k is the specific concentration of the k -th component. The set of spectral values of the a^* , b_b^* coefficients constitutes the hydro-optical model of the Azov Sea. The coefficient $R_{rsw} = (\lambda, -0, \theta_0, \beta)$ is determined as a secondary hydro-optical characteristic of the aquatic environment, describing water properties and brightness characteristics. It is calculated at the horizon based on the surface layer of the water column and shows minimal dependency on θ_0 and β :

$$R_{rsw}(\lambda, C, a, b_b) = a_0 + a_1 \{b_b(\lambda) / a(\lambda)\} + a_2 \{b_b(\lambda) / a(\lambda)\}^2, \quad (10)$$

where $a_k, k = \overline{0, 2}$, $b_b(\lambda)$, $a(\lambda)$ are the known coefficients for each component of the aquatic environment (hydro-optical model of the Azov Sea).

Let us describe the developed algorithm for retrieving water parameters of the Azov Sea, which is based on the efficient Levenberg-Marquardt (LM) multidimensional optimization method. The concentration vector of color-forming components was represented as:

$$\mathbf{C} = (C_{chl}, C_{ms}, C_{pog})^T.$$

To find the optimal concentration vector $\mathbf{C}$ an absolute minimum of the residual function $f(\mathbf{C})$ was sought:

$$f(\mathbf{C}) = \sum_j [S_j - R_{rsw}(\lambda, \mathbf{C}, a, b_b)]^2. \quad (11)$$

The expression for calculating the optimal vector $\mathbf{C}$ is as follows:

$$\mathbf{C}_{k+1} = \mathbf{C}_k + \lambda_k (F_k^T F_k + \mu_k D_k)^{-1} F_k^T R_{rsw}(\lambda, \mathbf{C}_k, a, b_b), \quad (12)$$

where $F_k = \left(\frac{\partial R_{rsw}(\lambda, \mathbf{C}_k, a, b_b)}{\partial \mathbf{C}_k} \right)$ is the matrix; μ_k is the direction of minimization; D_k is the diagonal of the matrix $F_k^T F_k$;

λ_k is the step size of the optimization; τ denotes the transpose operation.

Expressions (9) and the parameterization in (10) were used to calculate the spectral value of the reflectance coefficient of the water column based on the concentration vectors of color-forming components. Calculations were performed for the wavelengths 412, 443, 490, 510, 590, and 670 nm (corresponding to the Sea Viewing Wide Field Sensor (SeaWiFS) channels).

In addition to synchronous remote sensing data from SeaWiFS sensors and the MODIS spectrometer, in situ measurements of hydrodynamic, hydro-optical, and biogeochemical parameters of the studied water body were used to verify the accuracy of the retrieved vector C_{opt} obtained using the LM algorithm. These measurements included scattering, absorption, and attenuation coefficients for nine wavelengths in the spectral range of 412–715 nm, collected at each station during field expeditions.

A comparison of the measured and retrieved concentrations of color-forming components from satellite monitoring data showed agreement, with a correlation coefficient averaging 0.75.

Results. A computational experiment was conducted based on integrated hydrodynamic and biological kinetics models. The Taganrog Bay was chosen as the real modelling area since this part of the Azov Sea produces the majority of phytoplankton biomass during the summer. A module for calculating biological kinetics processes was developed and integrated into the “Azov3D” software suite [16–18].

The input data for the calculations included salinity and temperature distributions derived from cartographic information, water flow velocity calculated using a hydrodynamic mathematical model, and processed long-term observational data on the concentrations of nutrients and key phytoplankton species [19]. Additionally, the spatial distribution of phytoplankton populations, obtained using the Local Binary Patterns (LBP) method applied to satellite images, was used as input data. The method was developed by the authors of this research [20].

The LBP method enables the detection of the boundaries of phytoplankton “blooms” and pollutants, including oil and petroleum products, in satellite images. Figure 1 *a* shows the initial satellite image captured on August 6, 2020, by the Sentinel-2 L2A satellite [21]. Figure 1 *b* presents the initial distribution of phytoplankton populations, derived using the LBP method, which serves as input data for the program module. The concentration values reflect typical summer phytoplankton levels based on long-term observations.

The results of the software suite’s operation for a 30-day time interval and uniform initial distributions of phytoplankton and nutrient substances are shown in Figure 2.

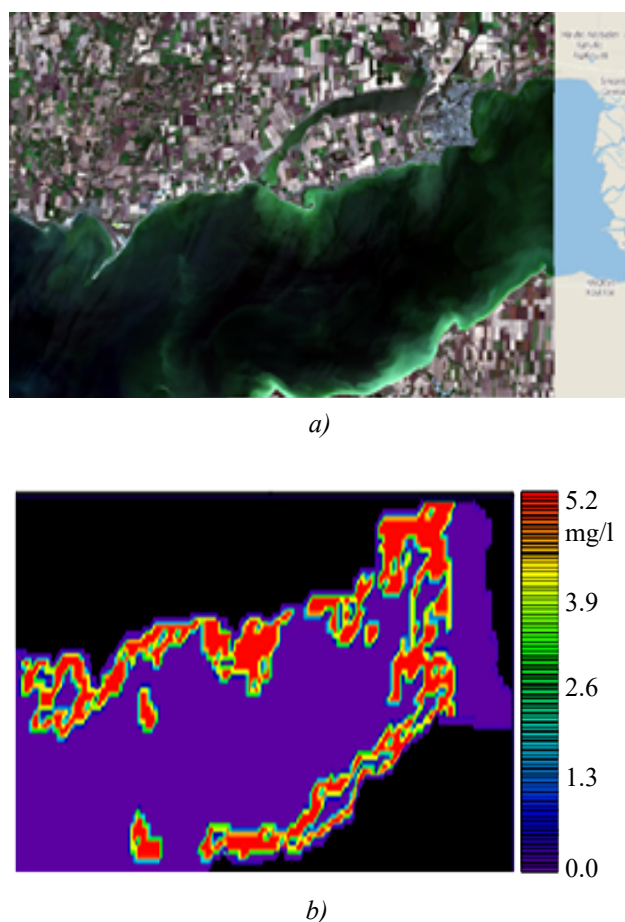


Fig. 1. Phytoplankton Images

a — Satellite image of the modeled area;

b — Initial distribution of phytoplankton populations

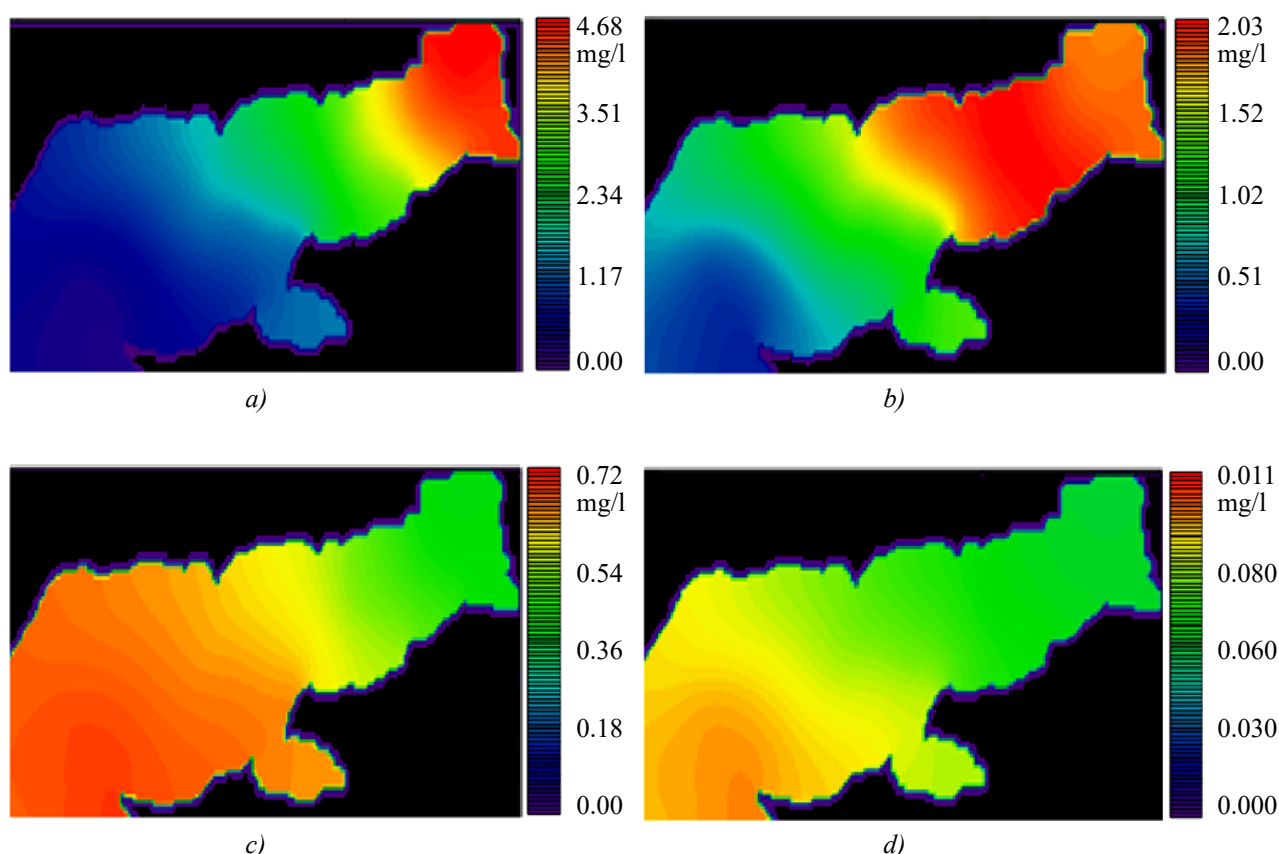


Fig. 2. Distribution of Concentrations in Taganrog Bay During the Summer Period

a — *Chlorococoides vulgaris* green algae; *b* — *Aphanizomenon flos-aquae* cyanobacteria; *c* — Phosphates; *d* — Nitrates

Discussion and Conclusion. The research on the state of aquatic systems has revealed that one of the mechanisms for improving the quality of biogeochemical process forecasting in marine ecosystems is refining initial data. In data assimilation systems, alongside stationary measurements, methods for processing and assimilating satellite information, which have been actively developed in the country over the past decades, have gained significant importance. It has been established that using satellite data in conjunction with mathematical modelling methods enables the study of the spatiotemporal distribution of various pollutants and plankton populations in the studied water body. This approach also helps assess the nature and scale of natural or anthropogenic events to prevent adverse economic and social impacts.

The authors have developed a spatially heterogeneous mathematical model of summer phytoplankton evolution in a shallow water body, numerically implemented in a research and forecasting complex (RFC). This complex integrates with various GIS platforms and satellite data. The model provides real-time forecasting of changes in density and spatial distribution of plankton populations. It also facilitates the study and analysis of redox processes, the transformation of nutrients (mineral feeding of phytoplankton), and sulfate reduction occurring within the water column. Additionally, the model examines the development of fish-kill events caused by anthropogenic eutrophication and predicts changes in the oxygen and nutrient regimes of the water body.

The RFC enables the development of comprehensive preventive measures to ensure environmental safety and mitigate economic damage in the studied region. The study also constructed an efficient and rapid algorithm for restoring water parameters in the shallow region (Azov Sea), based on the effective Levenberg-Marquardt multidimensional optimization method.

The developed RFC can be effectively applied to generate short- and medium-term environmental forecasts for shallow water bodies in Southern Russia. It utilizes diverse input information, such as the spatial distribution of phytoplankton during the summer period, obtained using the Local Binary Patterns method applied to satellite imagery.

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Claimed Contributorship:

Yu.V. Belova: software implementation, visualization and analysis of calculations.

A.A. Filina: numerical and software implementation, analysis of results.

A.E. Chistyakov: problem statement, development of research methods.

Conflict of Interest Statement: the authors declare no conflict of interest.

All authors have read and approved the final manuscript.

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Заявленный вклад авторов:

Ю.В. Белова: программная реализация, визуализация и анализ расчетов.

А.А. Филина: численная и программная реализация, анализ результатов.

А.А. Чистяков: постановка задачи, разработка методов исследования.

Конфликт интересов: авторы заявляют об отсутствии конфликта интересов.

Все авторы прочитали и одобрили окончательный вариант рукописи.

Received / Поступила в редакцию 11.11.2024

Reviewed / Поступила после рецензирования 26.11.2024

Accepted / Принята к публикации 02.12.2024