Original article **DOI**: 10.29039/2413-5577-2023-2-61-70

Variational Identification of the Initial Field of Chlorophyll A Concentration in the Transport Model according to Remote Sensing Data

V. S. Kochergin *, S. V. Kochergin

Marine Hydrophysical Institute of the Russian Academy of Sciences, Sevastopol, Russia

* *e-mail:vskocher@gmail.com*

Abstract

The work aims at construction of chlorophyll a fields based on variational assimilation of available satellite information for a few days in a transport model. Such information is the most real-time, but most often it has omissions (sometimes significant) in its structure due to the scattering effect of clouds, glares, etc. Therefore, obtaining reliable fields taking into account the available information for the Black Sea is an important and urgent task. In the numerical implementation of the transport model and variational method of measurement data assimilation, the results of calculations based on the MHI dynamic model for the Black Sea were used. In the numerical implementation of the variational assimilation algorithm, iterative gradient methods are used, and the solution of the adjoint problem is used to construct the gradient of the cost function in the parameter space. As a result of the calculations, a field of chlorophyll a concentration was obtained for almost the entire Black Sea area consistent with the measurement data. The paper implements a variational algorithm for the satellite information assimilation, which made it possible to obtain a chlorophyll a concentration field for the Black Sea area, taking into account incomplete coverage with observational data. The procedure can be used to determine concentration fields of various suspended substances in the sea based on data distributed over time and space.

Keywords: chlorophyll a concentration, variational algorithm, adjoint problem, measurement data assimilation, Black Sea, space-time interpolation

Acknowledgements: The work was carried out under state assignment on topic FNNN-2021-0005 "Complex interdisciplinary studies of oceanologic processes which determine functioning and evolution of ecosystems in the coastal zones of the Black Sea and the Sea of Azov" (code "Coastal research").

For citation: Kochergin, V.S. and Kochergin, S.V., 2023. Variational Identification of the Initial Field of Chlorophyll A Concentration in the Transport Model according to Remote Sensing Data. *Ecological Safety of Coastal and Shelf Zones of Sea*, (2), pp. 61–70. doi:10.22449/2413-5577-2023-2-61-70

© Kochergin V. S., Kochergin S. V., 2023

This work is licensed under a Creative Commons Attribution-Non Commercial 4.0 International (CC BY-NC 4.0) License

Вариационная идентификация начального поля концентрации хлорофилла *a* в модели переноса по данным дистанционного зондирования

В. С. Кочергин *, С. В. Кочергин

Морской гидрофизический институт РАН, Севастополь, Россия
* *e-mail: vskocher@gmail.com*

Аннотация
Целью работы является построение полей хлорофилла *a* путем вариационной ассимиляции доступной спутниковой информации за несколько суток в модели переноса. Такая информация является наиболее оперативной, но чаще всего имеет в своей структуре пропуски, иногда существенные, вследствие рассеивающего эффекта облачности, бликов и т. д. Поэтому получение достоверных полей с учетом имеющейся информации для акватории Черного моря является важной и актуальной задачей. При численной реализации модели переноса и вариационного метода ассимиляции данных измерений использовались результаты расчетов по динамической модели МГИ для Черного моря. При численной реализации вариационного алгоритма ассимиляции применяются итерационные градиентные методы, а решение сопряженной задачи используется для построения градиента функционала качества в пространстве параметров. В результате проведенных расчетов получено поле концентрации хлорофилла *a*, согласованное с данными измерений, почти для всей акватории Черного моря. В работе реализован вариационный алгоритм усвоения спутниковой информации, который позволил получить поле концентрации хлорофилла *a* для акватории Черного моря с учетом неполного покрытия данными наблюдений. Процедура может быть использована для определения полей концентрации различных взвешенных веществ в море по данным, распределенным по времени и пространству.

Ключевые слова: концентрация хлорофилла *a*, вариационный алгоритм, сопряженная задача, ассимиляция данных измерений, Черное море, пространственно-временная интерполяция

Благодарности: работа выполнена в рамках государственного задания по теме FNNN-2021-0005 «Комплексные междисциплинарные исследования океанологических процессов, определяющих функционирование и эволюцию экосистем прибрежных зон Черного и Азовского морей» (шифр «Прибрежные исследования»).

Для цитирования: *Кочергин В. С., Кочергин С. В.* Вариационная идентификация начального поля концентрации хлорофилла *a* в модели переноса по данным дистанционного зондирования // Экологическая безопасность прибрежной и шельфовой зон моря. 2023. № 2. С. 61–70. EDN UHOSMC. doi: 10.29039/2413-5577-2023-2-61-70

Introduction

Solving the problem of environmental orientation for the Azov-Black Sea Basin requires the creation of systems that make it possible to receive real-time information about the state of the environmental situation. The main constituent elements of such systems are numerical dynamic models [1)] [1], models of transport

1) Marchuk, G.I. and Sarkisyan, A.S., 1988. *Mathematical Modelling of Ocean Circulation*. Berlin: Springer, 292 p.

and transformation of various components of suspended solids [2)], as well as procedures concerning assimilation of available information [3)] [2–7].

An extensive review of measurement data assimilation methods is presented in [8]. In this paper, a variational assimilation algorithm is implemented to assimilate satellite information on the concentration of chlorophyll a in the upper layer of the Black Sea. A characteristic feature of satellite information is that it often contains some omissions, for example due to clouds.

The use of surface values of chlorophyll concentration in the transport and diffusion model makes it possible to complete the missing information in the measurement data. In the algorithm, the applied model plays the role of a space-time interpolant, and the resulting solution of the problem on the time interval used is consistent not only with the model itself, but also with the measurement data. The initial field of chlorophyll concentration was chosen as a desired parameter. When implementing the search procedure for the extremum of the functional that characterizes the deviations of the model estimates from the measurement data, the solutions of the main, adjoint problems and the problem in variations are used to construct the gradient of the functional and organize the iterative process. With difference discretization of the above problems, TVD approximations are used [9]. As input information for the transport model, the results of calculations based on the MHI hydrothermodynamic model [1, 10] with a spatial step of 1.6 km and with realistic atmospheric action were used [11]. 27 horizons are used vertically with the time step of 1.5 min. To simulate the dynamics of chlorophyll a fields in the aquatic environment, the advection and diffusion equation is used.

Transport and diffusion model

Let us write the equation of the impurity transport model in the following form:

$$\frac{\partial C}{\partial t}+\frac{\partial (uC)}{\partial x}+\frac{\partial (vC)}{\partial y}+\frac{\partial (wC)}{\partial z}=A_H\nabla^2 C+\frac{\partial}{\partial z}A_V\frac{\partial C}{\partial z}, \tag{1}$$

where C – concentration; A_H, A_V – coefficients of horizontal and vertical turbulent diffusion, respectively.

On the sea surface ($z = 0$), the following condition is used:

$$A_V\frac{\partial C}{\partial z}=0. \tag{2}$$

At the bottom and solid boundaries, the no-flow condition is taken. In the area of straits, the first type Dirichlet condition is used (homogeneous in this calculation). The concentration field $C^0(x, y, z)$ is set for the initial moment of time.

[2)] Marchuk, G.I., 1986. *Mathematical Models in Environmental Problems*. Amsterdam: Elsevier Science Publishers B.V., 216 p.

[3)] Penenko, V.V., 1981. *Methods of Numerical Modelling of Atmospheric Processes*. Leningrad: Gidrometeoizdat, 352 p. (in Russian).

The finite-different discretization of equation (1) is implemented on grid C [12]. TVD schemes [9] are used to approximate the advective terms. Vertical turbulent diffusion coefficient A_V is set in accordance with [13], with $A_H = 10^7$ cm^2/s.

Variational algorithm of identification

Let us consider a functional of the following form:

$$I_0 = \frac{1}{2}\left(P\left(RC_{t_k} - C_{t_k}^{\text{meas}}\right),\ P\left(RC_{t_k} - C_{t_k}^{\text{meas}}\right)\right)_{S_t^0}, \qquad (3)$$

which characterizes deviations of model concentration values from measurement data. In expression (3), R – operator of designing the model solution at the observation point; P – operator of zero expansion of the residuals of the forecast specified at the measurement points; t_k – time points at which the measurement data are received; the scalar product is defined in the standard way in $M_T = M \times [0, T]$; M – area in which the model is integrated on the time interval $[0, T]$; $S_t^0 = S^0 \times [0, T]$, S^0 – sea surface; $\Gamma_t = \Gamma \times [0, T]$, Γ – boundary of area M.

Minimization of expression (3) with the constraints of formulas (1)–(3) is reduced to finding the extremum of the functional of the following form:

$$I = I_0 + \left[\frac{\partial C}{\partial t} + \frac{\partial UC}{\partial x} + \frac{\partial VC}{\partial y} + \frac{\partial WC}{\partial z} - \frac{\partial}{\partial x} A_H \frac{\partial C}{\partial x} - \frac{\partial}{\partial y} A_H \frac{\partial C}{\partial y} - \frac{\partial}{\partial \sigma} K \frac{\partial C}{\partial z},\ C^*\right]_{M_t} +$$

$$+\left(\frac{\partial C}{\partial n},\ C^*\right)_{\Gamma_t} + \left(C - C_0,\ C^*\right)_M, \qquad (4)$$

where $\Gamma_t = \Gamma \times [0, T]$, Γ – boundary of area M.

By varying expression (4) and then integrating by parts, taking into account the boundary conditions and the continuity equation, the following expression can be obtained:

$$\delta I = \left(C - C_0,\ C^*\right)_M, \qquad (5)$$

where C^* – Lagrange multipliers, which are chosen from the solution of the following adjoint problem:

$$-\frac{\partial C^*}{\partial t} - \frac{\partial UC^*}{\partial x} - \frac{\partial VC^*}{\partial y} - \frac{\partial WC^*}{\partial z} - \frac{\partial}{\partial x} A_H \frac{\partial C^*}{\partial x} - \frac{\partial}{\partial y} A_H \frac{\partial C^*}{\partial y} - \frac{\partial}{\partial z} K \frac{\partial C^*}{\partial z} =$$

$$= -P\left(RC_{t_k} - C_{t_k}^{\text{meas}}\right),$$

$$\Gamma : \frac{\partial C^*}{\partial n} = 0,\ z = 0 : \frac{\partial C^*}{\partial z} = 0,\ z = H : \frac{\partial C^*}{\partial z} = 0,\ \ t = T : C^* = 0.$$

The initial approximation is set to zero, and the next approximation can be found by the following formula:

$$C_0^{n+1} = C_0^n + \tau \nabla_{C_0} I,$$

where τ – iterative parameter.

Results and discussion

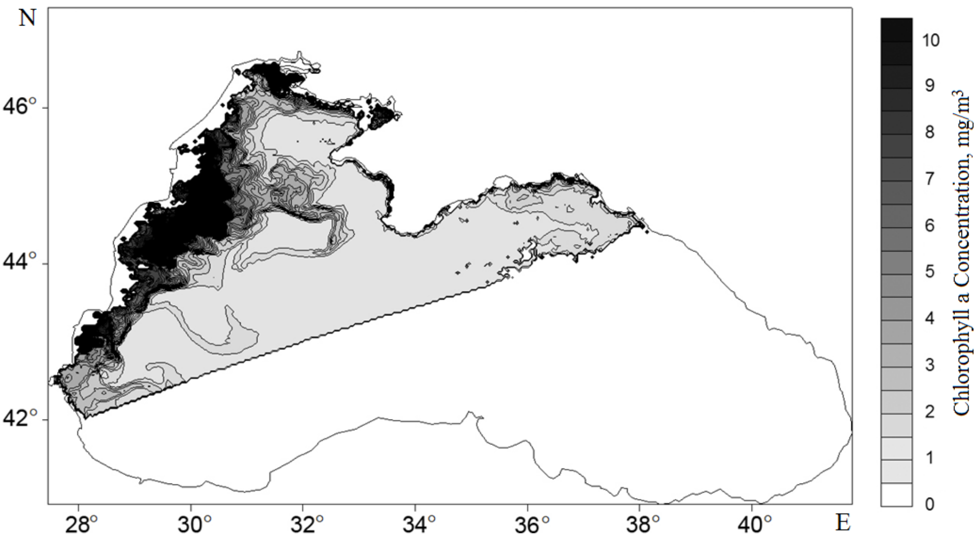
The flow rates for the period from 14 May 2016 to 17 May 2016 were calculated using the MHI model [1, 10] with a horizontal resolution of 1.6 km in latitude and longitude, taking into account the realistic atmospheric action for 2016 (according to ERA5 data with a spatial resolution of 0.25º) [10]. The reanalysis data [14] interpolated onto the model grid were used as initial fields. The obtained flow fields were used as input information.

The satellite data are often characterized by some omissions observed in their structure due to, for example, clouds or other factors that significantly affect the quality of incoming information processing. The presence of clouds over the Black Sea can be evaluated based on the information concerning pseudocolor composite MODIS-Aqua (URL: https://earthdata.nasa.gov/labs/worldview/?p=geographic&l=MODIS), which also characterizes the suspended matter concentration in the upper sea layer. As on 15 May 2016, the spatial structure of such fields is characterized by an increased concentration of chlorophyll a in the area of the Danube mouth and the area adjacent to the Dnieper-Bug Estuary. In addition, the composite contains areas of developed clouds in the eastern part of the sea. The increased concentration of impurities along the western coast is stipulated by the dynamics of the waters, namely the Main Black Sea Current. Figure 1 shows the composite as on 16 May 2016. Same as on May 15, the maximum concentration of chlorophyll a is located near the western coast of the Black Sea, and the eastern part of the sea along the Caucasian coast is covered with cloudy fields. On the contrary, clouds cover the central part of the sea on May 17.

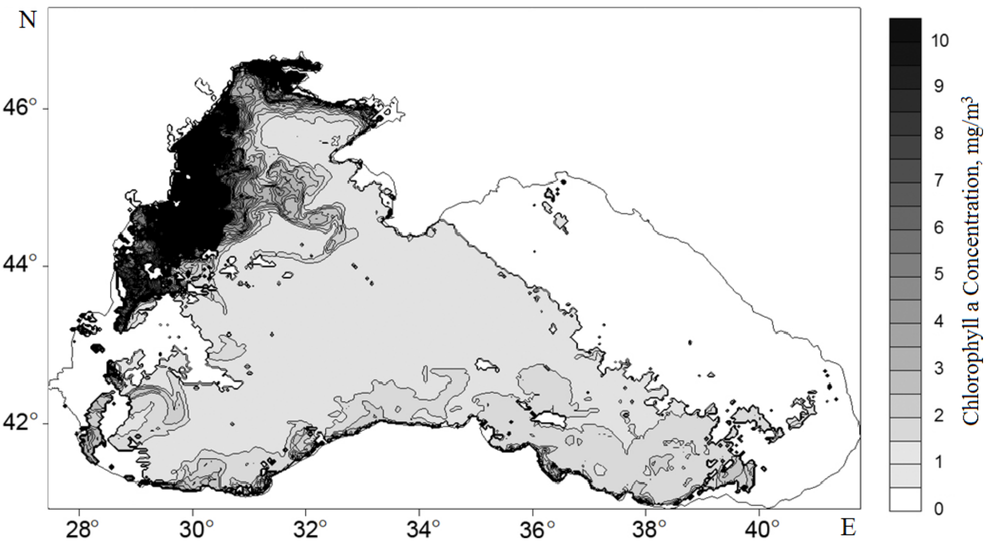
F i g . 1 . Pseudocolour composite MODIS-Aqua, 16 May 2016, the contrasts on the sea are determined by changes in the suspended matter concentration (https://earthdata.nasa.gov/labs/worldview/?p=geographic&l=MODIS)

Fig. 2 shows the chlorophyll a concentration field on 15 May 2016 according to the website http://dvs.net.ru/mp/data/201507vw.shtml.

The maximum values near the western coast reach 18–20 mg/m^3. The values of the central part of the sea are 2–3 mg/m^3. Figure 3 shows the chlorophyll a concentration field on May 16. Omissions in the data correspond to the clouds over the Black Sea in this period (see Fig. 1).



F i g . 2 . Chlorophyll a concentration field on 15 May 2016 (available at: http://dvs.net.ru/mp/data/201507vw.shtml)

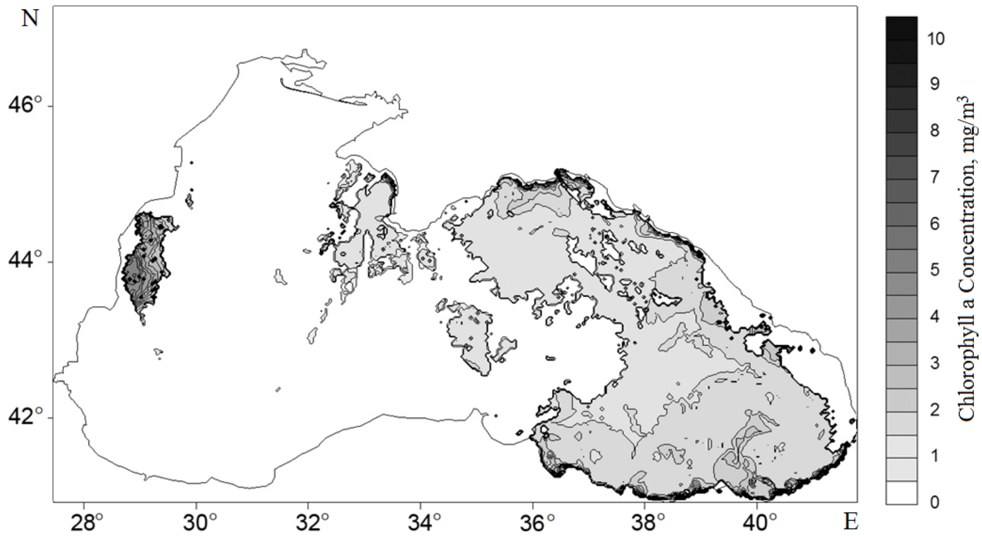


F i g . 3 . Chlorophyll a concentration field on 16 May 2016

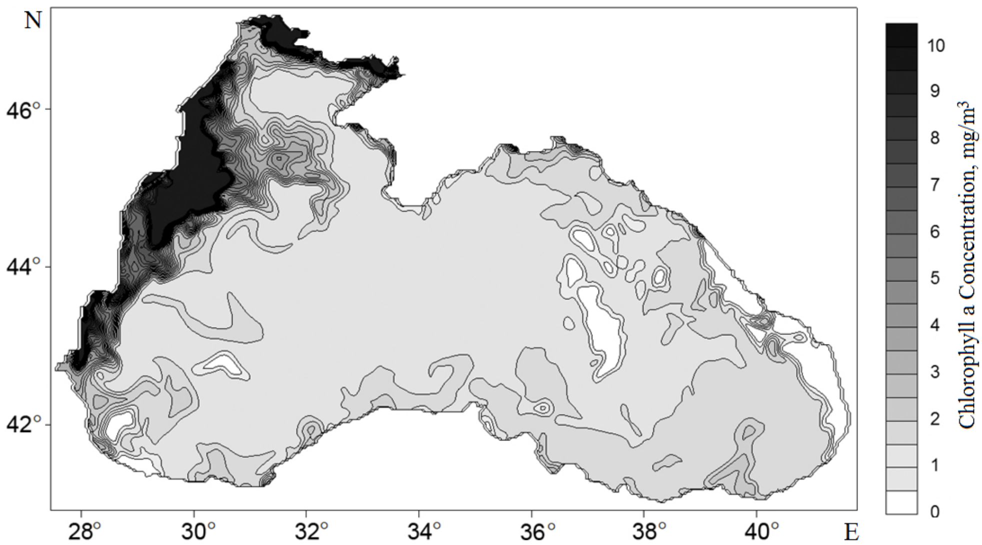
Fig. 4 similarly shows the data on May 17, which are available mainly for the eastern part of the sea.

Fig. 5 shows the result of the variational assimilation procedure.

In its structure, the presented field is in clear line with the image of the pseudocolor composite shown in Fig. 6. The remaining data omissions are determined by the assimilable information. Thus, zero concentration along



F i g . 4 . Chlorophyll a concentration field on 17 May 2016



F i g . 5 . Chlorophyll a initial concentration field on 14 May 2016

F i g . 6 . Pseudocolour composite MODIS-Aqua, 14 May 2016

the Caucasian coast is stipulated by the lack of data for this area in assimilable fields. Most probably, the data omissions on May 17 are stipulated by the quality of the primary processing of satellite information, in which data with increased concentration were erroneously rejected.

As a result of the variational assimilation procedure, an initial field that is well consistent with the available information on the concentration of chlorophyll a and suspended matter in the upper sea layer, was obtained. The resulting field contains the main features of the spatial distribution of concentration with increased values in the area of the Danube and the Dnieper-Bug Estuary and along the western coast of the Black Sea. The spatial structure of the field is characterized by the influence of dynamic structures of a vortex nature on it. To the west of the Bosporus, there is a mushroom-shaped structure, which is partially present in the data on May 15 and 16 and is clearly visible in the composite on May 14 (Fig. 6). The resulting chlorophyll a concentration field is consistent with the model and with the information used for subsequent time moments on the sea surface due to the minimization of the functional of expression (5). 3–4 iterations are sufficient to reach the extremum of the functional on a given time interval.

Conclusion

The performed calculations showed the effectiveness of the algorithm used in initializing the initial chlorophyll a concentration field in the Black Sea. The transport model is used as a space-time interpolant, and the solution of the adjoint problem is necessary to construct a gradient in the parameter space for iterative descent. The concentration fields obtained in this way are consistent with the measurement data distributed over time and space and the available information for the corresponding period of time. The results of the work can be used in order to solve environmental problems concerning the Azov-Black Sea Basin.

REFERENCES

1. Demyshev, S.G., 2012. A Numerical Model of Online Forecasting Black Sea Currents. *Izvestiya, Atmospheric and Oceanic Physics*, 48(1), pp. 120–132. https://doi.org/10.1134/S0001433812010021
2. Marchuk, G.I. and Penenko, V.V., 1979. Application of Optimization Methods to the Problem of Mathematical Simulation of Atmospheric Processes and Environment. In: G. I. Marchuk, ed., 2012. *Modelling and Optimization of Complex System.* Lecture Notes in Control and Information Sciences, vol. 18. Berlin, Heidelberg: Springer, pp. 240–252. https://doi.org/10.1007/BFb0004167
3. Semenov, E.V. and Mortikov, E.V., 2012. Problems of Operational Data Assimilation for Marginal Seas. *Izvestiya, Atmospheric and Oceanic Physics*, 48(1), pp. 74–85. https://doi.org/10.1134/S0001433812010124
4. Zalesny, V.B., Agoshkov, V.I., Shutyaev, V.P., Le Dimet, F. and Ivchenko, B.O., 2016. Numerical Modeling of Ocean Hydrodynamics with Variational Assimilation of Observational Data. *Izvestiya, Atmospheric and Oceanic Physics*, 52(4), pp. 431–442. https://doi.org/10.1134/S0001433816040137
5. Shutyaev, V.P., Le Dimet, F.-X. and Parmuzin, E., 2018. Sensitivity Analysis with Respect to Observations in Variational Data Assimilation for Parameter Estimation. *Nonlinear Processes in Geophysics*, 25(2), pp. 429–439. https://doi.org/10.5194/npg-25-429-2018
6. Kochergin, V.S., Kochergin, S.V. and Stanichny, S.V., 2020. Variational Assimilation of Satellite Data on Surface Concentration of Suspended Matter in the Azov Sea. *Sovremennye Problemy Distantsionnogo Zondirovaniya Zemli iz Kosmosa*, 17(2), pp. 40–48. doi:10.21046/2070-7401-2020-17-2-40-48 (in Russian).
7. Demyshev, G.S., Dymova, O.A., Kochergin, V.S. and Kochergin, S.V., 2020. Determination of Location of the Concentration Initial Field of a Possible Contamination Source in the Black Sea Water Area near the Gerakleisky Peninsula Based on the Adjoint Equations Method. *Physical Oceanography*, 27(2), pp. 210–221. https://doi.org/10.22449/1573-160X-2020-2-210-221
8. Shutyaev, V.P., 2019. Methods for Observation Data Assimilation in Problems of Physics of Atmosphere and Ocean. *Izvestiya, Atmospheric and Oceanic Physics*, 55(1), pp. 17–31. doi:10.1134/S0001433819010080
9. Harten, A., 1984. On a Class of High Resolution Total-Variation-Stable Finite-Difference Schemes. *SIAM Journal on Numerical Analysis*, 21(1), pp. 1–23. https://doi.org/10.1137/0721001
10. Demyshev, S.G. and Dymova, O.A., 2013. Numerical Analysis of the Mesoscale Features of Circulation in the Black Sea Coastal Zone. *Izvestiya, Atmospheric and Oceanic Physics*, 49(6), pp. 603–610. https://doi.org/10.1134/S0001433813060030
11. Kallos, G., Nickovic, S., Papadopoulos, A., Jovic, D., Kakaliagou, O., Misirlis, N., Boukas, L., Mimikou, N.G.S.J.P., Sakellaridis, G., Papageorgiou, J., Anadranistakis, E. and Manousakis, M., 1997. The Regional Weather Forecasting System SKIRON: An Overview. In: University of Athens, 1997. *Proceedings of the Symposium on Regional Weather Prediction on Parallel Computer Environments*. Athens, Greece: University of Athens. Vol. 15, pp. 109–123.
12. Arakawa, A. and Lamb, V.R., 1981. A Potential Enstrophy and Energy Conserving Sheme for the Shallow Water Equations. *Monthly Weather Review*, 109(1), pp. 18–36. https://doi.org/10.1175/1520-0493(1981)109<0018:APEAEC>2.0.CO;2

13. Demyshev, S.G., Zapevalov, A.S., Kubryakov, A.I. and Chudinovskikh, T.V., 2001. Evolution of the ^{137}Cs Concentration Field in the Black Sea after the Passage of the Chernobyl Cloud. *Russian Meteorology and Hydrology*, (1), pp. 37–46.
14. Korotaev, G.K., Ratner, Y.B., Ivanchik, M.V., Kholod, A.L. and Ivanchik, A.M., 2016. *Izvestiya, Atmospheric and Oceanic Physics*, 52(5), pp. 542–549. https://doi.org/10.1134/S0001433816050078

Submitted 19.01.2023; accepted after review 16.03.2023;
revised 03.05.2023; published 26.06.2023

About the authors:

Vladimir S. Kochergin, Junior Research Associate, Marine Hydrophysical Institute of RAS (2 Kapitanskaya St., Sevastopol, 299011, Russian Federation), **ORCID ID: 0000-0002-6767-1218, ResearcherID: AAG-4209-2020**, *vskocher@gmail.com*

Sergey V. Kochergin, Senior Research Associate, Marine Hydrophysical Institute of RAS (2 Kapitanskaya St., Sevastopol, 299011, Russian Federation), Ph.D. (Phys-Math.), **ORCID ID: 0000-0002- 3583-8351, ResearcherID: AAG-4206-2020**, *ko4ep@mail.ru*

Contribution of the authors:

Vladimir S. Kochergin – problem statement, programme code writing and debugging, data preparation, analysis of calculation results, article text preparation

Sergey V. Kochergin – problem statement, analysis of calculation results, article text preparation

All the authors have read and approved the final manuscript.