Computing complex for modeling the Black Sea

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Abstract. This paper presents a description of a computing complex and results of its use for modeling the Black Sea. The complex is created on the basis of a circulation model and contains blocks of hydrodynamics, energy, and pollutant transport. A numerical experiment is carried out with the Skiron reanalysis data of 2016 as atmospheric forcing. Fields of sea level, velocities of currents, temperature, and salinity are calculated. Comparison of the simulated temperature, salinity, and velocity with contact observations shows good qualitative and quantitative agreement with the in-situ data. The seasonal variability of a basin-scale circulation is reproduced in the velocity field. Mesoscale eddies are reconstructed, and an analysis of the mean current energy and the eddy energy is performed. The most intensive mesoscale variability was observed near the Crimean and Turkish coasts in 2016. The mean current kinetic energy is decreasing during the year, and the formation of mesoscale eddies is associated with baroclinic instability. A test calculation of the radioactive beryllium distribution is also carried out in this experiment. Comparison with real measurements shows that the complex simulates pollutant transport with high degree of accuracy.

1. Introduction

Intensive economic activity in the coastal and abyssal parts of the World Ocean requires realization of environmental events to preserve its resource and recreational capability. If there is knowledge about the structure, regularities, and factors which determine the variability of the Earth's hydrosphere, the negative consequences of climatic, extreme natural and anthropogenic impacts can be sufficiently reduced and sometimes prevented. The main approach in modern fundamental research of the World Ocean is an interdisciplinary principle when physical, chemical, and biological processes are considered together. Now one of the most topical tasks is the diagnosis and prediction of the thermohydrodynamic and biochemical characteristics of water ecosystems. Numerical modeling is an efficient method to solve this problem. Developments of such models are carried out for both global [1 – 3] and regional [4 – 6] basins of the World Ocean.

Analysis and monitoring of the ecological status are impossible without accurate data about the hydrophysical properties and structure of the ocean water. Such data are needed to identify possible scenarios of distribution of pollutants coming to the sea as a result of natural or anthropogenic impacts. The Black Sea is a unique semi-enclosed basin with a maximal depth of about 2 km. Here the circulation is characterized by a basin-scale cyclonic gyre (the so-called Rim Current) covering the abyssal part and mesoscale eddies forming on its periphery. Also, a distinctive feature of the Black Sea is the existence of a hydrogen sulfide layer at mean below 200 m. A number of works are focused on investigations of the water pollution in the Black Sea by numerical modeling (for example, [7, 8]). The goal of the present work is to create a computing complex for simultaneous simulation of both the hydrodynamic and ecological state of the Black Sea with a high spatial resolution.

Section 2 describes the computing complex and the numerical models being used. The results of simulation of the Black Sea state in 2016 and a comparison with in-situ data are given in Section 3. The main conclusions are presented in Section 4.

2. Structure of the computing complex

A flowchart in Figure 1 presents the structure of the complex. It consists of five main blocks: input, hydrodynamics, energy, pollution, and output. The operation of the complex is as follows. The user prepares the initial and boundary conditions at the preliminary step. For this the fields of atmospheric forcing and three-dimensional hydrodynamic initial fields are linearly interpolated into nodes of the model grid. These data are read in the input block. Quasi-geostrophic adjustment between climatic data and atmosphere forcing is accomplished here in the case when starting hydrodynamic fields are absent. Then the parameters of pollutant transport calculation are chosen: its initial distribution, characteristics of the sources and sinks. The complex works automatically after launching. At first the sea level, temperature, salinity, and current velocities are calculated. Then these data are sent to the energy subroutine and the pollutant transport subroutine. This architecture allows one to calculate the pollutant transport at each model time step. Consequently, computational errors which usually arise under velocity interpolation when using horizontal velocity components as input data are excluded. The energetics is computed once a day of the model time. Some integral parameters are evaluated and three-dimensional arrays of all characteristics for their subsequent visualization are written by the output block.

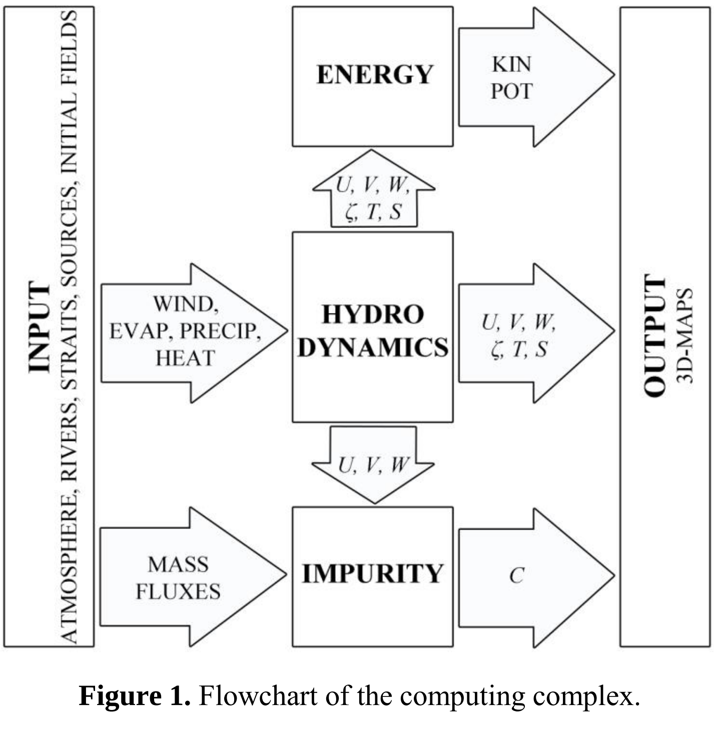

Figure 1. Flowchart of the computing complex.

2.1. Hydrodynamics

The core of the complex is an eddy-resolving z-model of the Black Sea circulation developed at the Marine Hydrophysical Institute of the Russian Academy of Sciences (MHI RAS) [9]. The model is based on the primitive equations of ocean taking into account the approximations of Boussinesq, hydrostatics, and incompressibility of the ocean water:

$$u_t - (\xi + f)v + wu_z = -g\zeta_x - \frac{1}{\rho_0}(p' + E)_x + (\nu_V u_z)_z - \nu_H \nabla^4 u\,, \quad (1)$$

$$v_t + (\xi + f)u + wv_z = -g\zeta_y - \frac{1}{\rho_0}(p' + E)_y + (\nu_V v_z)_z - \nu_H \nabla^4 v\,, \quad (2)$$

$$\zeta_t + \int_0^H (u_x + v_y)dz = (\mathrm{Pr} - \mathrm{Ev})/\rho_1\,, \quad (3)$$

$$u_x + v_y + w_z = 0\,, \quad (4)$$

$$T_t + (uT)_x + (vT)_y + (wT)_z = -\kappa_H \nabla^4 T + (\kappa_V T_z)_z\,, \quad (5)$$

$$S_t + (uS)_x + (vS)_y + (wS)_z = -\kappa_H \nabla^4 S + (\kappa_V S_z)_z\,, \quad (6)$$

$$\rho = \varphi(T, S), \quad (7)$$

$$p = g\rho_0\zeta + g\int_0^z \rho d\mu = g\rho_0\zeta + p'\,, \qquad \xi = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\,, \qquad E = \rho_0 \frac{u^2 + v^2}{2}\,.$$

Here u, v, and w are the velocity components; ζ is the sea level; f is the Coriolis parameter; g is the gravity acceleration; p is the pressure; Pr is the precipitation; Ev is the evaporation; T is the temperature; S is the salinity; ρ is the density; $\rho_0 = 1$ g cm^{-3}; ρ_1 is the mean surface density; ν_V and ν_H are the vertical and horizontal viscosity coefficients; κ_V and κ_H are the vertical and horizontal diffusion coefficients. The sea level (equation (3)) is calculated under an assumption of linearized kinematic condition. The density nonlinearly depends on the temperature and salinity (equation (7)). We neglect the density change due to pressure in accordance with [10]. There are several configurations of the model with different horizontal resolution: 5 km, 1.6 km, and 350 m, which can be used for studying processes on wide temporal-spatial scales. Here we apply a model with a resolution of 1.6 km and 27 z-horizons in the vertical. The baroclinic radius of deformation in the coastal zones of the Black Sea varies from 7 to 20 km depending on the depth. Thus, the chosen spatial resolution of the MHI-model is less than the deformation radius that allows us to investigate mesoscale features of the circulation. The wind stress (τ^x, τ^y), the heat fluxes Q^T, the precipitation and evaporation are set on the sea surface as boundary conditions:

$$\rho_0 \nu_V u_z = -\tau^x, \quad \rho_0 \nu_V v_z = -\tau^y, \quad \kappa_V T_z = \mathrm{Q^T}\,, \qquad \kappa_V S_z = \frac{\mathrm{Pr} - \mathrm{Ev}}{\rho_1} S_0 + \beta(S_0 - S^{cl})\,,$$

where S_0 is the surface salinity; S^{cl} is the surface climatic salinity; β is the relaxation parameter. We set a non-flow condition on the solid boundary. The water exchange through the Bosporus and the Kerch Strait and the runoff of the main Black Sea rivers are taken into account by the Dirichlet boundary condition for equations (1), (2), (5), and (6). Bathymetry was built by data of the European Marine Observation and Data Network (EMODnet, available online http://portal.emodnet-bathymetry.eu/).

The model is implemented on a C-grid [11]. The advective terms in equations (5), (6) are approximated by TVD schemes [12]. To provide filtering of computational noise and stabilizing of the numerical solution, we use biharmonic operators for the calculation of the horizontal viscosity and diffusion in equations (1), (2), (5), and (6). The vertical turbulent mixing is parameterized by the Mellor-Yamada turbulent closure model of level 2.5 [13]. A full description of the model, mathematical assumptions, and numerical approximations are presented in [9].

The model release with a resolution of 5 km was successfully used in a system of the European Center for Marine Forecasts within the international project "MyOcean" from 2009 to 2012. The simulated fields were validated by Argo floats (available online http://usgodae.org/argo/argo.html) and the MHI Oceanographic Data Base [14]. The results of the project demonstrated high quality and accuracy of the obtained hydrophysical features and their good agreement with observations [15].

2.2. Energetics
As shown in a number of works [for example 16, 17], analysis of the rates of energy change and conversion allows one to study the mechanisms of formation and evolution of currents, eddies, and density fields in oceans. The terms of the energy change equations indicate to the work of the main internal and external forces which define the variability of the hydrophysical fields. Therefore, to provide a comprehensive approach to the study of regularities of the Black Sea dynamics, the complex was supplemented by a block for calculating the kinetic (E) and potential (P) energy budgets. Note that the energy equations are derived as an exact consequence of the finite-difference equations of the dynamics model. The differential energy equations have the form

$$E_t+[u(g\zeta+p'+E)]_x+[v(g\zeta+p'+E)]_y+[w(g\zeta+p'+E)]_z=g\rho\, w+\nu_V(uu_z+vv_z)_z-\nu_V(u_z^2+v_z^2)$$
$$-\nu_H[(\nabla^2u)^2+(\nabla^2v)^2]-\nu_H(D^u+D^v)\,, \quad (8)$$

$$P_t+(uP)_x+(vP)_y+(wP)_z=-g\rho\, w-\kappa_H(\nabla^4P-gzQ^H)-g(\kappa_V z\rho_z)_z+g(\kappa_V\rho)_z$$
$$-g\rho(\kappa_V)_z-gz\kappa_V Q^V\,, \quad (9)$$

where D^u, D^v are the terms associated with the setting of boundary conditions in the straits and river mouths; Q^H, Q^V are the terms which arise due to a nonlinear form of the state equation (7). Note that equation (8) is obtained at an assumption that $\rho_0 = 1$ g cm^{-3} without limiting the generality (see [19]). The second, third, and fourth terms in the left-hand sides of (8) and (9) are the advective terms, the first term in the right-hand side of (8) is the buoyancy work, the second and third ones are the vertical dissipation of E, the fifth and sixth ones are the horizontal dissipation of E. The second term in the right-hand side of (9) is the horizontal diffusion of P, and the third – sixth ones are the components of the vertical diffusion of P. The vertical and volume integrals of the terms in equations (8), (9) are also calculated in the energy block, which allows one to estimate the energy balance. The derivation of the energy change equations, the properties of their finite-difference approximation are described in detail in paper [18]. Numerical analysis of the intra-annual and seasonal variability of energy characteristics, their influence on the mesoscale processes in the coastal zones of the Black Sea are presented in [19] by using the above-mentioned energy equations. It is found that the buoyancy work and the wind stress work are the most energy-significant fluxes affected to the formation of the mesoscale coastal eddies.

2.3. Pollutant transport
The computing complex can be employed for research associated with ecological monitoring and estimation of marine pollutions. These applied tasks are solved with the help of a block for the calculation of passive pollutant propagation. A standard equation of substance transport taking into account the advective and diffusion transports is realized in this block:

$$C_t+(uC)_x+(vC)_y+(wC)_z=-A_H\nabla^4C+(A_VC_z)_z+F^{\pm}\,, \quad (10)$$

where C is the pollution concentration; A_H is the biharmonic horizontal diffusion coefficient; A_V is the coefficient of vertical turbulent diffusion; $F^{\pm}$ is a function describing the source/sink of the pollutant. If the substance comes from the atmosphere with dry and/or wet precipitation, the mass flux is specified as a boundary condition on the sea surface ($z = 0$):

$$A_VC_z=Q^C(x,y,z,t)\,,$$

where $Q^C(x,y,z,t)$ is the substance flux on the surface.

The absence of a substance flux is set at the bottom and at solid boundaries. It is possible to specify the pollution inflow through the river mouths and straits. It is implemented by the Dirichlet boundary condition. Depending on the type of the simulated pollution, we can take into account the substance deposition on suspension, the flux from a point or distributed source, the processes of oxidation or decay. Earlier on the basis of the model with a resolution of 5 km we obtained estimates of the propagation of oil pollution as a result of a hypothetical instantaneous emergency spill; the change of the radioactive cesium stock in the Black Sea after the Chernobyl disaster; the spatial-temporal variability of the natural content of radioactive isotopes [20].

3. Model results

Let us consider the results of the complex running on an example modeling of the hydrodynamic state and beryllium-7 (7Be) distribution in the Black Sea in 2016. A numerical experiment was performed by using Skiron reanalysis data with a resolution of 0.1° as atmospheric forcing (available online http://forecast.uoa.gr/forecastnew.php). The biharmonic operator coefficients in the terms describing the horizontal turbulence in equations (1), (2), (5), (6), and (10) are $\nu_H = 10^{16}$ cm^4 s^{-1}, $\kappa_H = 10^{16}$ cm^4 s^{-1} and $A_H = 5\cdot10^{16}$ cm^4 s^{-1}. Fields of the sea level, current velocities, temperature and salinity, as well as the 7Be concentration fields were obtained. The 7Be inflow with precipitation and its sedimentation on suspension were taken into account in the pollution block.

The simulated fields of the hydrophysical characteristics were compared with the available data of contact and remote observations. There were data obtained by Argo floats ##6901832, 6901833, online satellite images of the sea surface (http://dvs.net.ru/mp/data/201601bs_mod_ru.shtml), and vessel measurements. We calculated deviations of the model temperature and salinity from in-situ data where the deviation equals the Argo value minus the model value. The deviations averaged over all measurements and RMS are presented in Table 1. One can see that the model temperature exceeds observations at mean of 0.2°C in the upper layer. In contrast, the salinity is less on 0.15 psu than observations in the seasonal pycnocline layer. Below 300 m the mean deviations are about 0.05°C and 0.018 psu for the temperature and salinity, respectively.

Table 1. Mean and RMS deviations of model temperature and salinity from observations.

Depth, m	Temperature, °C		Salinity, psu	
	Mean	RMS	Mean	RMS
5-50	-0.21	0.63	0.097	0.044
50-100	-0.1	0.21	-0.102	0.088
100-300	0.14	0.16	0.158	0.017
300-800	0.05	0.03	0.018	0.006
800-1500	-0.02	0.002	0.003	0.004

Direct measurements of velocity were not performed and, therefore, we evaluated the Lagrangian velocity of the floats and compared it with the model currents velocity at the same points. For example, Figure 2 presents a comparative analysis of the model hydrophysical characteristics and data of Argo float #6901832 (operating period: January 2 – December 27, 2016) along its track. One can see that the maximal deviations are observed in the subsurface layer and reached 2°C and 0.6 psu for the temperature and salinity, respectively. The deviations decreased with depth. Figure 2c demonstrates that the simulated currents velocity is close to real data.

Analysis of the vertical temperature and salinity profiles (not present here) showed that the model reproduces stratification features (such as the core of the cold intermediate layer, the seasonal thermo- and halocline, the boundary of the upper stratified layer, etc.) with a high degree of accuracy. Thus, the comparative analysis of the modeling hydrophysical characteristics shows a qualitative and quantitative agreement with in-situ data.

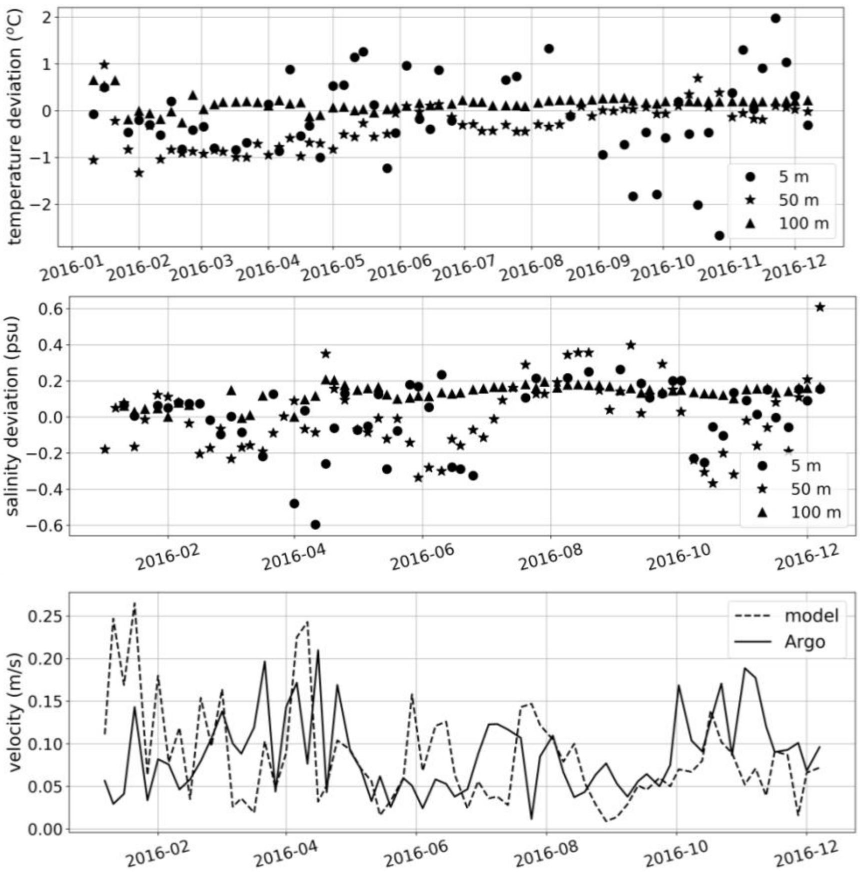

Figure 2. Comparison of simulated parameters with *in-situ* data along the trajectory of Argo float #6901832: a –temperature deviation on depths (°C), b –salinity deviation on depths (psu), c –surface velocity (m s^{-1}).

The main peculiarities of the Black Sea circulation, such as the Rim Current, the Sevastopol and Batumi anticyclones, the coastal mesoscale eddies are reproduced in the velocity fields and are confirmed by satellite images and float trajectories. The Rim Current is most intensive in the winter of 2016, the cyclonic gyre is traced to a depth of about 500 m. The winter-mean currents velocity is about 22 cm s^{-1}, the maximal values exceed 60 cm s^{-1} near the Crimean and Caucasus coasts. Weakening and strong meandering of the Rim Current are observed in spring and summer. During this period several sub-basin eddies of different signs are revealed in the central part, and intensive mesoscale variability is observed in shelf zones (the Crimean and Turkish coasts, the North-Western Shelf). In autumn the velocity and width of the Rim Current increase again and it acquires features of a steady jet stream.

The Sevastopol anticyclone is formed quasi-periodically toward the south-west from the Crimea. The development of this eddy is associated with barotropic instability of the Rim Current. A characteristic property of the eddy is motion along the continental slope to the south-west. The Sevastopol anticyclone is dissipated near the Bulgarian coast. Its lifetime is about 3 – 4 months, and its mean size is about 80 km. The Batumi anticyclone is a quasi-stationary eddy in the south-eastern part of the Black Sea. Its generation and development are due to an impact of the mesoscale eddies coming from the Anatolian coast. The anticyclone is detected from spring to the middle of winter. Usually its size reaches 170 – 200 km and the orbital velocities are about of 40 – 50 cm s^{-1}. However, the modeling results have shown that in 2016 the Batumi anticyclone was weaker: its diameter not exceeded 100 km and the mean orbital velocity was about 30 – 35 cm s^{-1}. The eddy was displaced to the vicinity of 38°E, and only the coastal mesoscale anticyclones were observed in the south-eastern part at the end of autumn, which was confirmed by observations. A fragment of the simulated velocity field and an image of the chlorophyll concentration from the satellite MODIS-AQUA (http://dvs.net.ru/mp/data/modis/1611/161121lg.gif) at the same date are presented in Figure 3.

As mentioned above, the mesoscale eddies are formed on the periphery of the Rim Current. The sizes and penetration depths depend on the generation place, atmospheric forcing, and the basin-scale circulation structure. Thus, the eddies observed on the North-Western Shelf and near the Crimean coast are smaller than near Turkey. The eddies in the northern part have diameters of about 10 – 30 km and are detected to a depth of 60 – 100 m, their lifetimes are from several days to weeks. The eddy sizes near the Anatolian coast are more than 60 – 80 km and the orbital velocities exceed 40 cm s^{-1} (see inset picture in Figure 3). They are observed to a depth of 300 m.

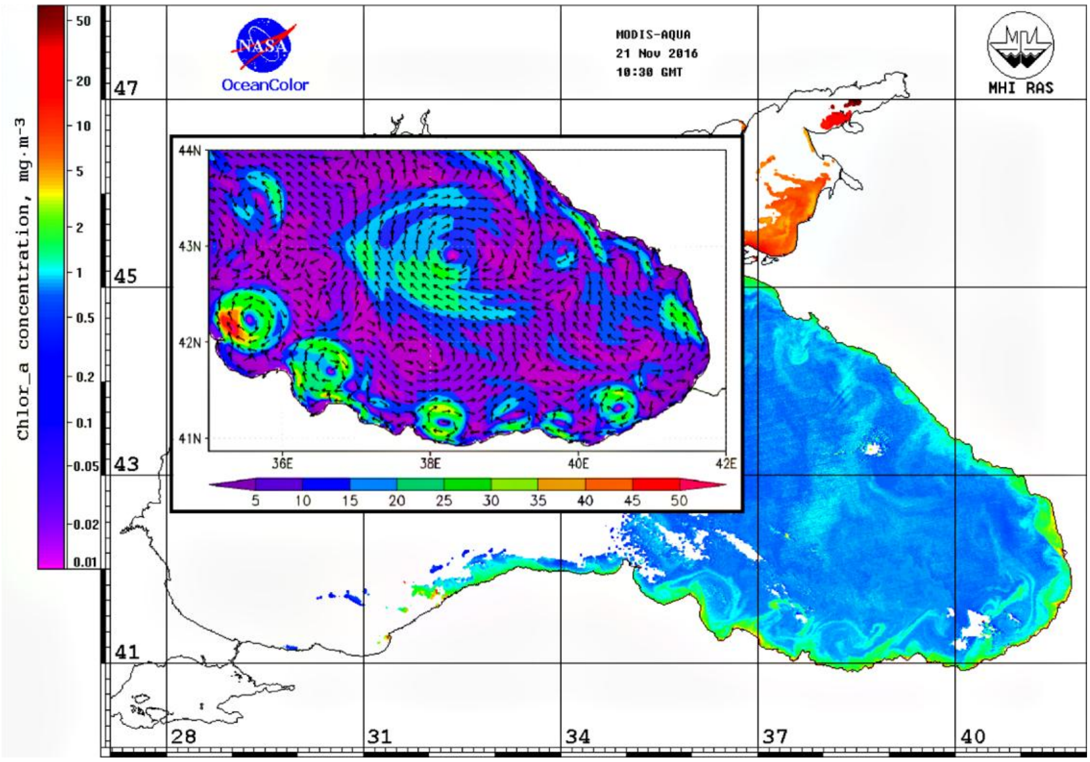

Figure 3. Satellite image of chlorophyll concentration (mg m^{-3}) on November 21, 2016. Fragment of simulated surface velocity field (cm s^{-1}) at the same date in inset picture.

We compute the energetic circulation characteristics and the rates of conversion between the kinetic and potential energy to investigate the mechanisms of eddy generation. It is found that the eddy kinetic energy comprises almost half of the total kinetic energy in 2016. The mean current kinetic energy decreased during the year. Its increase is observed from the middle of October 2016 due to enhancement of the wind. Growth of the eddy kinetic energy is revealed in February, from April to June and in August – September. Recall that the conversion between the mean current kinetic energy and the eddy kinetic energy (denote BT) is associated with the barotropic instability, and the conversion between the eddy kinetic energy and the available eddy potential energy (denote BC) is associated with the baroclinic instability. Analysis of the BT and BC temporal variability showed that the eddy kinetic energy is increased due to the mean current and the available eddy potential energy in the spring and summer of 2016, but the BC flux is more than the BT flux approximately two times. The maximal values of the BC flux are observed in winter and autumn and exceed the BT flux 3 – 4 times. Thus, the mesoscale eddies are generated in 2016 predominately due to the baroclinic instability of the Rim Current.

The pollutant transport is simulated on an example of calculation of the 7Be concentration in the Black Sea in 2016. Beryllium-7 is a radionuclide of natural genesis with a half-life period of 53 days. The spatial-temporal and seasonal distribution of the isotope is evaluated. The analysis showed that the central and the south-eastern sea parts are characterized by higher concentrations. The maximum values are revealed in the eastern sector in the summer of 2016 owing to heavy rainfall. Accuracy estimation of the modeling results are performed using data of the 87th and 89th cruises of the research vessel "Prof. Vodyanitsky", which made measurements near the Crimean coast in July and October 2016. Figure 4 presents the 7Be surface concentration at station points obtained by the computing complex and in-situ data. A measurement error of 25% is indicated for the curves describing observations. It can be seen that the majority of the modeling values are obtained within the confidence interval. The greatest deviations are observed for the stations located near the shore in shallow zones. Thereby the modeling results are in good agreement with measurements.

a

b

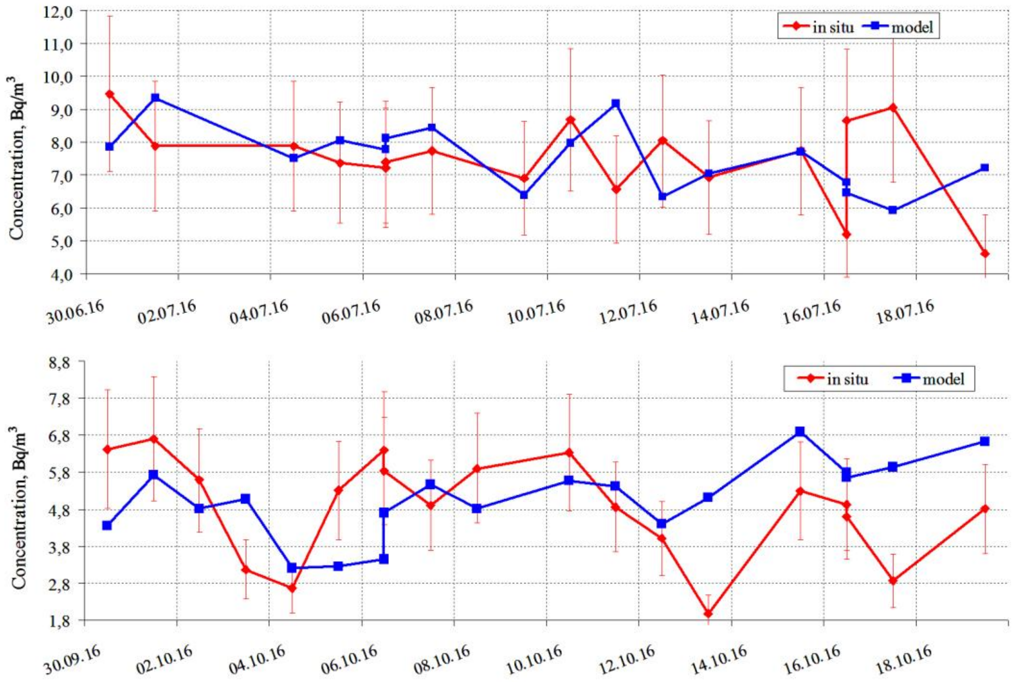

Figure 4. 7Be surface concentration (Bq m^{-3}) by the modeling results and *in-situ* data:
a – 87th "Prof. Vodyanitsky" cruise in July 2016,
b – 89th "Prof. Vodyanitsky" cruise in October 2016.

4. Conclusions

Testing results of a computing complex for the Black Sea modeling have been presented. The hydrophysical fields, energy and 7Be concentration fields of 2016 have been calculated with a high spatial resolution of 1.6 km. The temporal-spatial variability of the thermohaline structure and circulation has been reconstructed. Good agreement of the thermohydrodynamical parameters with the available measurements data has been shown.

It has been found that the Rim Current is observed as a continuous stream with a mean velocity of 20 – 25 cm s^{-1} in winter and autumn. The basin-scale circulation weakens and the mesoscale activity enhances in warm seasons. The Sevastopol anticyclone characteristics in 2016 are typical: the size is about 80 – 100 km and the orbital velocities reach 35 – 40 cm s^{-1}. A reduced Batumi anticyclone is revealed in 2016: its size and the orbital velocities declined by about 30% compared with the usually observed parameters. Such behavior is caused by a displacement of the eddy to the north-west in the second half of the year and, as a result, the energy inflow from the Anatolian mesoscale eddies has been terminated. Energy analysis showed that the mean current kinetic energy is decreasing during 2016. The eddy kinetic energy grows in spring and summer predominately due to the development of baroclinic instability.

The available accurate data about the circulation structure allow us to diagnose the evolution of pollution in the sea, which is mainly determined by advection and diffusion transport. The modeling results on the 7Be concentration in 2016 demonstrate that the complex can be used for the calculation of pollution transport. It has been found that the majority of the simulated values are inside a measurement confidence interval of 25%. Thus, the computing complex allows us to carry out fundamental research and solve problems associated with environmental monitoring in the Black Sea region.

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