Analysis of the distribution of pollution in the Sea of Azov by the results of numerical simulation and data of satellite observations

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Abstract. The paper discusses methods of sharing information obtained by remote sensing of the sea surface from space and model solutions. The estimation of the quality of the model prediction is made depending on the intervals between the assimilation of satellite data. Numerical hydrodynamic modelling of the Azov Sea water area is performed on the basis of the POM model for real atmospheric forcing SKIRON in the period from 2013 to 2014. The peculiarities of spatial and temporal dynamics of the pollution in the Sea of Azov have been studied on the basis of a joint analysis of numerical simulation data and space monitoring data from the Terra/Aqua satellites. Based on the developed new model algorithms, the results of numerical simulation and data of satellite observations on the state of water in the Sea of Azov water area are summarized.

1. Introduction

Ecological problems of the Sea of Azov are given special attention in connection with the continuing significant anthropogenic impact. The scale of pollution becomes threatening to the ecosystem and leads to extremely negative consequences [1]. The emergence of satellite systems that have a sufficiently high spatial resolution and ensure the daily arrival of data for any monitoring area makes it possible to monitor the state and pollution of the marine environment. However, in the situation of a catastrophic black oil spill in the Kerch Strait that occurred on November 11, 2007, the first radar satellite images were obtained only five days after the disaster. Data of the optical range, due to cloudy weather, were not informative. A joint analysis of the results of numerical simulation and satellite radar and optical images seems to be most effective, as it provides more complete information on the transport directions, sizes and concentration of contamination areas, at times of absence of images. The paper summarizes the results of numerical simulation and satellite data on the state of the waters of the Azov Sea for the period from 2013 to 2014. Based on the developed new model algorithms, a numerical study of the dynamics of pollution in the Sea of Azov is carried out.

2. Mathematical model. The model parameters

Numerical studies used the three-dimensional nonlinear hydrodynamic model POM (Princeton Ocean Model) [2], adapted to the conditions of the Azov basin, also applied to the study of marine pollution. The mathematical model is based on the equations of turbulent motion of a viscous fluid in the hydrostatic approximation [3]. The relations for the calculation of the vertical viscosity coefficients...
and the turbulent diffusion according to the semi-empirical model of Mellor-Yamada (level 2.5) are written as follows [4]. The coefficient of the horizontal viscosity is calculated using the Smagorinski model of subgrid viscosity depending on the horizontal velocity gradients [5]. The projections of tangential wind stresses on a free surface are expressed in terms of its velocity values at a standard meteorological altitude, corrected for the coefficient of aero-dynamic resistance of the sea surface, which varies depending on the wind velocity [6]. The normal component of the velocity at the bottom is zero; the bottom tangential stresses are related to the speed according to the logarithmic law. The parameter of roughness is determined using the Grant-Madsen theory [7]. Zero fluid motion and zero fluctuations of the free surface before the atmospheric forcing are specified as the initial conditions. The choice of the integration steps over the temporal and spatial coordinates was performed according to the stability criterion for barotropic waves [8]. The resolutions of the model by latitude and longitude are $(1/59)^0 \times (1/84)^0$, at which the linear sizes of the cell are 1.4 km; the number of sigma levels by the vertical is 11. The initial data for the simulation was the bathymetry map and the configuration of the shoreline of the Azov Sea, built on the basis of digitization of hydrographic maps and subsequent interpolation to the calculated grid. Calculation of the change in the impurity concentration is based on the solution of the transport and diffusion equation, for which conditions on the free surface and in the bottom layer are added to the dynamic boundary conditions for the absence of impurity fluxes [2].

2.1. Information on the atmospheric forcing used in the numerical experiments

As atmospheric forcing fields were used, the wind and the atmospheric pressure obtained according to the regional atmospheric model SKIRON for the period from 2013 to 2014, the Atmospheric model was created and developed at the University of Athens group of Atmospheric Modeling and Weather Forecasting Group [11]. This version of the model gives a detailed 72 h forecast meteorological parameters for the Azov, Black and Mediterranean Seas. At the first 48 h the output data is carried out after at the 2 h, further values are displayed after 6 h on a grid with a step of 0.1°. Data atmospheric model SKIRON was interpolated at the computational grid of the Azov Sea basin.

3. The reconstruction of the primary hydrooptical characteristics in the Sea of Azov according to the colour scanner

Satellite data for the 2013 and 2014 period of the MODIS device from the Aqua satellite [9] with data rejection according to the criteria [10] with a kilometer spatial resolution. To determine the features in the upper layer of the sea, two parameters are calculated. The first is the ratio of the normalized brightness of light emerging from under the water surface ($L_{WN}(\lambda)$), in two spectral channels: $\text{index34} = L_{WN}(531) / L_{WN}(488)$, were $R_{bbp}(531) = L_{WN}(531) / Fo(531)$ and $R_{bbp}(488) = L_{WN}(488)/Fo(488)$ – the coefficients of the brightness of the sea with the central wavelengths of the spectral channels 531 and 488 nm. The physical essence of this parameter is that, in the first approximation, it characterizes the total absorption of all optically active substances contained in the upper layer of sea water. The solar constants $Fo$ for the spectral channels under consideration can be found, for example in [10].

The second parameter is the backscattering coefficient of the particles of suspended matter at 555 nm ($b_{bbp}(555)$), which allows one to observe the peculiarities of light scattering in the upper water layer; in general, this can be a suspension of biological origin (for example, coccolithophoride bloom); so inanimate suspension (for example, a mineral suspension, associated with river discharges or its ascent from the bottom as a result of a strong wind). Calculation of $b_{bbp}(555)$ was carried out by the formula: $b_{bbp}(555) = \{6.76 L_{WN}(555) + 0.03 [L_{WN}(555)]^2 + 3.4 L_{WN}(555) [I_{510}]^{1.8} - 0.84\} \times 10^{-3}$ [m$^{-1}$], were $I_{510} = L_{WN}(555) / L_{WN}(510)$, $R_{bbp}(555) = L_{WN}(555) / Fo(555)$, $R_{bbp}(510) = L_{WN}(510)/Fo(510)$, $R_{bb}$ – the luminance coefficient in the corresponding spectral channel, which is a satellite product of the second level, following [10]. The transition from SeaWiFS spectral channels to MODIS is based on the following expressions: $L_{WN}(555) = 0.9 L_{WN}(547)$ and $I_{510} = 0.8 \text{index34} + 0.11$, were $L_{WN}(547) = R_{bb}(547)/Fo(547)$. 
3.1. *Analysis of time series of parameters index34 and bbp(555) according to the MODIS data*

In the course of the study, satellite images of the surface of the Azov Sea in the infrared range were analyzed for the period from 20013 to 2014, based on the processing of *MODIS* data of the second level (*Level 2*) of R2014.0. The resolution of remote data over time is due to the passage of the satellite over the Azov Sea area with the smallest time step (24 h). The most informative images, most free from the influence of cloudiness and the presence of omissions, are selected from the available satellite data. They are systematized into groups consisting of sequential images with the smallest time interval. Thus, six time groups were obtained, consisting of the most contrast satellite images with a discreteness of 1 to 2 days, which were used in the test calculations. All satellite data is pre-processed so that if there is a pair of images, they are combined into one snapshot. For example, a snapshot of the 4 group was obtained from two consecutive images on June 23, 2013 at the 9:35 and 11:50 (figure 1).

![Figure 1. Combining satellite images in one.](image)

4. *Algorithm for the assimilation of observational data*

The successive recursive algorithm of data assimilation in the problem of estimating the passive pollution concentration fields is based on Kalman's theory of optimal filtration [12]. At times when observations are not available, we believe that the assessment of the analysis coincides with the forecast for the model, and the covariance matrix of the analysis errors is equal to the forecast error covariance matrix. At the time \( t_k \) a vector of a priori estimate \( x_k^m \) is constructed based on the integration of the transport and diffusion equations to solve this problem. It is a short-term model forecast of the investigated parameter from the previous step of assimilation. Its dimension is equal to the number of points in the model space. The data of satellite observations constitute the observation vector \( y_k \), whose dimension is not equal to the dimension of the vector \( x_k^m \). The optimal estimate of the concentration of \( x_k^* \) from the observations and the model is based on the Kalman filter algorithm acting on the forecast-correction system (figure 2).

![Figure 2. Data assimilation algorithm.](image)
5. Results of experiments
The simulation was carried out at a real atmospheric exposure to SKIRON corresponding to the selected time period of a group of satellite images of the surface in the Sea of Azov. Numerical experiments were carried out in two scenarios: without further assimilation of satellite distributions of parameters index34 and b_h(555) and with the assimilation of distributions at times corresponding to the available satellite data.

5.1. The first experiment
In the course of the study, the propagation of these parameters was simulated with the assimilation of satellite data only at the initial time. Consider the satellite and model distributions of index34, referring to a group of images from April 26 to May 2, 2013 (figure 3).

Figure 3. The distribution index34 in the surface layer in the Sea of Azov by satellite data (left column) and model data (right column).
Assimilation of observational data was carried out using the satellite image A20131161035000. The left column contains satellite images. In the right-hand side are the corresponding distributions of the index34 parameter, and also the surface velocities of the flows, constructed from the numerical simulation data for a near instant of time (the time difference does not exceed 2 h). Here, the white areas correspond to either the clouds or the gradient zones that were cut out during data processing. Date and local time are indicated for model distributions, the name of the MODIS file is given in the corresponding satellite data. The color scales closely correspond to each other in which satellite and model data are presented. In figure 3(a) shows the experimentally accepted satellite distribution of parameter index34 of April 26, 2013 at 10:35. Here regions with a high concentration index34 can be clearly traced. They spread from the coastal regions at the base of the Taganrog Bay towards the high seas. Analysis of wind speed showed a north-easterly wind speed of 10 – 12 m/s is developed 2 days before the point in time. Hydrodynamic scenario, confirm the results of the model. Surface velocity of currents directed towards the active wind. In a day, a fairly large area on the satellite image is occupied by cloudiness (figure 3(c)). The modeling data (figure 3(d)) allow us to estimate the character of the propagation of parameter index34 in this region. The direction of the wind changed to the west, a stream of currents appeared in the central part of the sea, a capturing impurity from the shore and transferring it to the center of the basin to the north and northeast. After 2 days, a large amount of contamination occurs in the Taganrog Bay area on a satellite image (figure 3(e)). The model distribution of this parameter, obtained without the subsequent assimilation of satellite data, has a significant discrepancy with the actual situation (figure 3(f)). The next satellite image, which corresponds on April 30, 2013 at 10:15, practically does not contain information (figure 3(g)). The corresponding model solution figure 3(h) makes it possible to estimate the spatial distribution of parameter index34. On the image relating to the date 02.05.2013 (figure 3(i)), in the region adjacent to Taganrog Bay, and near the coast of Berdyansk there is a region of the greatest concentration. The corresponding model distribution poorly reflects the real distribution as seen (figure 3(j)).

5.2. The second experiment
In the second numerical experiment, a consistent assimilation of observational data was carried out at times when information satellite information images were present. The correlation between the observational data and the simulation carried out for these two experiments was evaluated (figure 4).

![Figure 4. The correlation coefficient between the satellite and model distributions of the parameter index34 in the surface layer in the Sea of Azov.](image-url)
The root-mean-square error in the concentration estimate was calculated during this experiment. This error was compared with the root-mean-square error of the concentration estimate without data assimilation. To solve the problems of assimilating the observations of the use of the parameters index34 and $b_{bbp}(555)$, an algorithm based on the Kalman filter was applied. On the basis of the analysis of the conducted experiments it follows that the evaluation of the field of concentration of parameters index34 and $b_{bbp}(555)$ with subsequent assimilation leads to a significant decrease in the mean square error and an increase in the correlation coefficient.

6. Conclusion
A system for assimilation of observational data is proposed, which is a set of applied programs designed to solve the problem of estimating the spread of the pollution in the Sea of Azov. The complex of programs implements the algorithm for assimilation of observational data and makes it possible to perform a prediction of the process of contamination spread in the absence of satellite imagery based on the model of transfer and diffusion of a passive impurity. Numerical experiments have shown the effectiveness of the algorithms proposed in this paper for estimating the evolution of the parameters index34 and $b_{bbp}(555)$.

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