Estimation of the numerical modeling accuracy of the Black Sea thermohaline fields based on using ARGO profiling floats

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Abstract. The paper considers the matters of numerical modeling estimation accuracy of temperature and salinity three-dimensional fields in the monitoring and forecasting center of the Black Sea. Automatic system of analysis and forecast of the Black Sea state is run in the center in an operational mode. The data of in situ measurements from ARGO profiling floats regularly provided by the European Marine Forecasting Service – Copernicus – were used to solve the problem. Spatial and temporal mismatch between the model data and in situ measurements was eliminated to form a joint sample of these two data sources. Comparison is performed for the time period from 2012 to 2015. The results show quite good simulation accuracy of the thermohaline fields, however, the problems of modeling the temperature fields in the 5-30 m layer were detected where there is a fairly narrow seasonal thermocline in late spring, summer and early autumn.

1. Introduction

An automatic operational system of analysis and forecasting of the Black Sea state [1] has been run in Marine Hydrophysical Institute since 2012. Daily calculations of the temperature, salinity, current velocities and sea level fields – from the surface to the bottom of the Black Sea – are carried out. Validation subsystem [2] is the integral component of this forecasting system. The task of this subsystem is to estimate the accuracy (reliability) of numerical calculations by the circulation model of the Black Sea on the basis of comparison with in situ measurements. ARGO profiling float is one of the modern technical facilities that allows in-situ measurements of temperature and salinity profiles in the Black Sea on regular basis. The advantage of using them is that at least 5 platforms function regularly in the Black Sea since 2012.

The purpose of this paper is to estimate the accuracy of numerical simulations of the Black Sea temperature and salinity fields by their comparison with in situ measurements of ARGO profiling floats. Several papers were published earlier [3, 4], where short-term experiments of numerical simulations of the Black Sea state fields were performed and verification of them with ARGO profiling float was carried out. In this paper we estimate the accuracy of the numerical simulation of the real forecast system that is functioning in an operational mode in the Marine Hydrophysical Institute of Russian Academy of Sciences from 2012 to the present. The period from 2012 to 2015 was chosen to estimate the accuracy. It allowed us to form a representative joint sample of data and obtain reliable statistical accuracy estimates of the numerical simulation of the Black Sea thermohaline fields.
2. Data used

The work of the automatic analysis and forecasting system of the Black Sea state is based on the three-dimensional basin-scale circulation model which is elaborated by Marine Hydrophysical Institute [5]. The horizontal turbulent viscosity and diffusion are parameterized in the model by the bi-harmonic operator. The state equation includes quadratic terms. The Mellor-Yamada 2.5 model [6] is used to simulate vertical coefficients of turbulent viscosity and diffusion.

The model equations are integrated numerically in the Black Sea area situated between 27.422E and 41.895E along the longitude and between 40.863N and 46.685N along the latitude on the regular horizontal grid with a step of ~ 5 km (11/180 deg lon x 8/180 deg lat). The selected horizontal grid step permits us to resolve well a meso-scale variability of the basin bearing in mind that the Rossby radius is equal to 25 km. The model has 38 vertical levels non-uniformly distributed from 2.5 to 2100 meters.

The finite-difference approximation of the equations is carried out on the C-grid according to the terminology of Arakawa with the second order of accuracy both in space and time in case of a uniform grid. The scheme conserves energy and enstrophy of barotropic motion [7]. The equation describing evolution of the sea level is approximated using a semi-non-explicit scheme. Approximation of the turbulent energy equations permits us to use the conveyer method of their solution. The data of atmosphere forcing are selected every 3 hours from the 5-day SKIRON modeling system [8] and are executed on a bulk daily mode.

Three-dimensional fields of temperature and salinity were validated using the observations carried out by the ARGO profiling floats in the Black Sea in 2012-2015. The measurements of 25 profiling floats were available during this period. Each float performed probing once per five days. Sometimes measurement gaps took place due to low quality of observations or their absence. Measurements performed by profiling floats which functioned in the Black Sea area in 2012-2015 are shown in figure 1.

![Figure 1](image_url)

**Figure 1.** Measurements performed by profiling floats which functioned in the Black Sea area in 2012–2015.
It is seen that the measurements cover almost the whole water area of the Black Sea including the central part. The north-western shelf is the exception. 2166 temperature and salinity profiles were available during the whole study period.

3. Comparison methodology
Joint sampling of the results of numerical modeling of the temperature and salinity fields of the Black Sea and in situ measurement of ARGO profiling floats was formed in order to compare them. One of the central problems in its formation was due to the fact that the location of in situ measurements and the nodes of the model grid are spaced apart in space and time. Therefore, it is necessary to combine the data in the best way in order to minimize the comparison errors due to space and time mismatch.

The temporal mismatch between the compared data is 0.75 hour on average. The spatial mismatch between compared sources of information takes place for two reasons: 1) the nodes of the horizontal grid of the model do not match the points of ARGO profiling floats in situ measurements. In this case, the average distance between the nearest model node and the profile measurement point is 1.25 km; 2) the vertical depth levels on which model calculations are performed generally do not match the depths at which temperature and salinity measurements are made by the ARGO profiling float. Taking into account the variability of the temperature and salinity fields, a linear interpolation method was used to form a joint sample and eliminate the space and time mismatch. As a result, a joint sample of data was formed and analyzed for outliers. These outliers were excluded from further analysis.

4. Results
The total volume of the joint sample was 46720 joint measurements contained in 2166 temperature and salinity profiles.

The accuracy of model seawater temperature and salinity are presented in tables 1 and 2 respectively. These results are obtained by statistical averaging of deviations in 0-5, 10-30, 30-100, 100-300, 300-800, 800-1500 m layers, between model and ARGO in situ data. Accuracy values are given by bias, standard deviation (SD), 2.5%, 97.5% quantile errors ($Q_{2.5}$ and $Q_{97.5}$), minimum (Min) and maximum (Max).

In general, samples were carried out within the layer from the sea surface to 1500 m. However, in a number of cases the samples covered a thinner depth interval. Tables 1 and 2 (column Number of measurements) contain information on a number of measurements in each of six layers and provide accuracy estimates of the modeling seawater temperature and salinity. It is seen that the number of measurements was the lowest in the near-surface sea layer. The major quantity of measurements lies in the 5-300m layer. The measurement number considerably reduces in deep layers. Thus, the results for 0-5m and 800-1500m depth layers are less reliable due to the lack of data.

Six pairs of outliers in sea surface temperature values were detected during analyzing the joint sampling on homogeneity. The temperature values exceeded the limits of acceptable values. These pairs were excluded from the joint samples when estimating the modeling accuracy of the temperature of the Black Sea upper layer.

4.1 Temperature
Estimations accuracy of the numerical simulation of three-dimensional temperature fields for different layers of the sea are presented in table 1.
Table 1. Estimated accuracy of the Black Sea water temperature.

| Depth layer (m) | Number of measurements | Bias (°C) | SD (°C) | Q_{2.5} (°C) | Q_{97.5} (°C) | Min (°C) | Max (°C) |
|-----------------|------------------------|-----------|---------|-------------|--------------|----------|---------|
| 0-5             | 257                    | -0.05     | 0.62    | -1.06       | 1.80         | -1.90    | 2.53    |
| 5-30            | 10551                  | 0.46      | 2.19    | -2.83       | 6.78         | -15.78   | 14.86   |
| 30-100          | 12673                  | 0.18      | 0.79    | -1.10       | 1.85         | -8.92    | 7.75    |
| 100-300         | 13882                  | -0.02     | 0.15    | -0.24       | 0.31         | -1.92    | 2.33    |
| 300-800         | 6927                   | -0.02     | 0.03    | -0.09       | 0.05         | -0.28    | 0.18    |
| 800-1500        | 2424                   | -0.01     | 0.10    | -0.21       | 0.16         | -0.28    | 0.20    |

Satellite sea surface temperature data are assimilated by the system, so surface errors are relatively small: SD error is 0.62 °C. Below the surface, according to ARGO buoy comparisons, the biggest errors are found at 5-30 m depth, where a warming bias of 0.48 °C and SD error of 2.19 °C are detected. Such big errors are caused by very sharp seasonal thermocline in the late spring, summer and early autumn (Fig 1 c, d). In the 30-100 m layer, the bias is about 0.18 °C, with relatively high SD differences of ~ 0.79 °C.

The analysis of $Q_{2.5}$ and $Q_{97.5}$ and their comparison with minimum and maximum errors in this layer show that the relative portion of large deviations in the layer is small. The observed rare but large deviations are possibly associated with the epizootical penetration of the thermocline to the upper depth levels of this layer. A similar situation is observed in the 100-300m layer. Large deviations in this layer may be caused due to the incomplete account of processes in the permanent pycnocline, what will be discussed further.

Results are rather accurate below 300m depth.

Figure 2. Simulated and measured by ARGO float profiles of seawater temperature (a, c) and difference between them (b, d) depending on depth.

Figure 2(a) shows the temperature profile measured by ARGO profiling float No.6900804 2012-04-17 07:55 and simulated by model. Figure 2(b) shows their difference. It can be seen that these profiles are in good agreement. Figure 2(c) shows the temperature profile measured by ARGO profiling float No.6901959 2013-08-24 06:28 and simulated by the model. Figure 2(d) shows their difference. There is a big error in the upper layer due to the fact that the model incorrectly reproduces the thermocline which took place in the summer.

4.2 Salinity

It is known that density stratification in the Black Sea is determined mainly by seawater salinity. Estimated accuracy of the Black Sea water salinity simulation in different layers is presented in table 2.
Table 2. Estimated accuracy of the Black Sea water salinity.

| Depth layer (m) | Number of measurements | Bias (‰) | SD (‰) | Q<sub>2.5</sub> (‰) | Q<sub>97.5</sub> (‰) | Min (‰) | Max (‰) |
|----------------|------------------------|----------|--------|---------------------|---------------------|--------|--------|
| 0-5            | 263                    | 0.04     | 0.28   | -0.53              | 0.54                | -0.77  | 1.12   |
| 5-30           | 10551                  | -0.07    | 0.24   | -0.60              | 0.39                | -1.32  | 1.59   |
| 30-100         | 12673                  | 0.09     | 0.43   | -0.67              | 1.02                | -1.96  | 1.86   |
| 100-300        | 13882                  | 0.04     | 0.25   | -0.33              | 0.75                | -1.04  | 3.29   |
| 300-800        | 6927                   | -0.007   | 0.02   | -0.05              | 0.03                | -0.11  | 0.09   |
| 800-1500       | 2424                   | -0.006   | 0.02   | -0.05              | 0.03                | -0.06  | 0.06   |

According to the comparison with ARGO float observations salinity biases are negligible in the two upper layers, SDs are about 0.24-0.28‰. Errors increase in the layers between 30-100 and 100-300m where the permanent pycnocline is located. Bias around 0.04-0.09‰, SD – 0.25-0.43‰ are detected. Below 300m depth, results are rather accurate.

Figure 3. Simulated and measured by ARGO float profiles of seawater salinity (a, c) and difference between them (b, d) depending on depth.

Figure 3(a) shows the salinity profile measured by ARGO profiling float No.6901961 2015-06-06 06:43 and simulated by the model. Figure 3(b) presents their difference. It can be seen that these profiles are in good agreement. Figure 3(c) shows the salinity profile measured by ARGO profiling float No.7900590 2014-04-13 06:00 and simulated by the model. Figure 3(d) shows their difference. A large error is seen in the 30-100m layer.

The difference between SDs in this depth layer is less than in 0-5 m depth layer. However, SDs values are comparable with the 5-30 m depth layer. This can be explained by the fact that we have a permanent pycnocline in this layer and the model does not adequately describe the processes in it.

5. Conclusions

Estimations of the numerical simulation accuracy of the thermohaline fields in the monitoring and forecasting center of the Black Sea are given in the paper. Estimates are obtained on the basis of the accumulated archive of model calculations from 2012 to 2015. The results confirm, update and improve the reliability of similar estimates obtained earlier. According to these results, the main problems of inadequate modeling of thermohaline fields are observed in the layers where seasonal thermocline, the permanent halocline and pycnocline are located. In the first case, the most probable problems can be related to the low vertical spatial resolution of the model incapable of the accurate reproducing the temperature distribution in a narrow layer of sharp temperature gradient observed from mid-April to mid-September. In the second case, the more likely causes may be insufficiently accurate...
parametrization of physical processes in the permanent halocline and pycnocline. It follows that it is necessary to improve the vertical resolution of the model and parameterize more accurately the physical processes in the layer of the permanent pycnocline in order to further improve the reliability of model calculations.

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