

Retrospective Analysis of the Black Sea Thermohaline Fields on the Basis of Empirical Orthogonal Functions

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Mathematical method combining optimal interpolation and expansion into the empirical orthogonal functions is developed to implement a retrospective analysis of the Black Sea thermohaline structure using incomplete archival oceanographic data. In order to increase spatial consistency of the resulted hydrologic structure, the earlier applied reconstruction method based on the horizontal empirical orthogonal functions was transformed to the combined one in which the vertical empirical orthogonal functions were the basic elements. The results of computing experiments make it possible to limit the number of the modes by 5 both for horizontal and vertical empirical orthogonal functions. Such a combination significantly reduces the calculation time and **lowers** the error level. This method was applied to reconstruct the monthly fields (spatial resolution is 10' latitude \times 15' longitude) for almost a hundred-year period from 1923–2015. The relative part of the monthly average fields' successful reconstruction constitutes about 70 %. Based on the reanalysis data, the temperature and salinity climatic fields were calculated by various methods both for the entire observational period and for certain decades. It is revealed that in the XX century the gain-phase climatic characteristics of the Black Sea remain very stable whereas general tendencies in the long-term variations of the temperature and salinity seasonal cycles are opposite: when the sea temperature seasonal range rises the phase of annual harmonic of seasonal oscillations diminishes, and in the case of salinity, it increases, i. e. the salt content maximum shifts for the later period. The reanalysis data were used to study various aspects of the inter-annual and inter-decadal variability of the Black Sea thermohaline structure, density stratification, geostrophic circulation etc. The future trends imply application of the thermohaline fields' reanalysis array for studying long-term changes in the Black Sea basin as well as for assimilating observational data in the hydrophysical fields' reconstructions by the hydrodynamic models.

Keywords: Black Sea, thermohaline structure, reanalysis, climate, empirical orthogonal functions.

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Introduction. Along with the widespread arrays of atmospheric field global reanalysis, climate studies now began to use similar arrays of oceanographic characteristics such as *ECWMF-Ocean*, *NCEP/GODAS*, *GECCO*, *SODA*, *Mercator*, etc. A number of regional arrays of the Black Sea hydrophysical field reanalysis, belonging to different historical periods, was created in Marine Hydrophysical Institute of RAS [1–4].

The main method of the ocean retrospective analysis is an application of complete hydrodynamic models and methods of data assimilation of contact and remote observations. Alternative approach consists in the reconstruction of oceanographic fields by mathematical methods based on the statistical data structure only. Such technique, substantiated in the works of L. S. Handin, V. I. Belyaev and I. E. Timchenko [5–8], is applied in modern works [9–17], including the research [18] focused on the Black Sea. Despite various drawbacks of statistical methods, (in particular, a strong dependence on the spatial data structure) they can be used for studying long historical periods with more predictable level of reconstruction errors (degree of uncertainty) than when using hydrodynamic models. This is due to the fact that the modeling results are affected by not only the number and spatial distribution of the assimilated data, but also the quality of the applied atmospheric reanalysis. Recently, atmospheric arrays covering the entire XX century (*ERA-20C*, *NOAA 20CR*) have appeared, but it is still difficult to assess how much they take into account the systematic changes that have occurred in the global meteorological observation system over 100 years.

The purpose of the study was to make the Black Sea reanalysis array over the entire time interval of oceanographic observations covering 100-year period, and to calculate climatic characteristics for various historical periods based on statistical methods for the reconstruction of thermohaline fields.

Methodology for carrying out the retrospective analysis. The calculation of reanalysis array was performed in several stages. At the first stage the primary data, which passed the quality check, were interpolated by the optimal interpolation method onto a regular grid. At the second stage the interpolated values were decomposed into empirical orthogonal functions (EOF). At the third stage the EOF temporal coefficients were calculated for the entire period of observations. At the fourth step monthly average thermohaline fields for the entire volume of the sea were reconstructed by the EOF temporal coefficients and were checked for compliance with predetermined statistical criteria.

Optimal interpolation method applied at the first stage is traditionally used in hydrometeorology as it provides taking into account the real correlation structure of the fields, to minimizing the interpolation error and providing its quantitative assessment. The equivalent of optimal interpolation is the variational inverse method, which, in particular, was applied in *MEDATLAS* for the Mediterranean and the Black Sea [19].

In this work, the system of equations of optimal interpolation [5] was solved by the Gaussian elimination. The measure of observation error was estimated as

$$\eta_i = \sigma_f^2 / \overline{x_i^2},$$

where σ_f^2 is an average dispersion of observation error equal to the sum of instrumental error and the variance of mesoscale variability (from [20, p. 150]);

$\overline{x_i^2}$ is an average dispersion of anomalies (deviations of x_i values from the norm \bar{x} at the observation point i). Climatic monthly average fields of temperature and salinity were used as the norm.

It was assumed that the spatial correlation functions in the Black Sea are isotropic [21, 22]. For the autocorrelation function in the system of equations of optimal interpolation, an approximation [21], approximating the structure of Gaussian fields, was applied.

Primary interpolation on a regular grid was deliberately carried out in such a way as to prevent extrapolation when filling in free space, since the following steps were intended for this. As a result of the calculations, the arrays of interpolated values for 1910–2015 observation period with temporal resolution of 10 days and 1 month and $10' \times 15'$ spatial resolution were formed. Relative portion of the sea area coverage (Fig. 1) with data is maximal for the period of late 1950s – early 1990s (up to 80 %) and is minimal in 1930–1940 and after 1995 (less than 20 %).

At the second stage, the total correlation (autocovariance) matrix was calculated first

$$C = \text{Cov}(\mathbf{x}', \mathbf{x}')$$

over the entire set of fields of monthly average anomalies \mathbf{x}' from the optimal interpolation array. The covariance matrices C calculated for each horizon were smoothed by three-point Shapiro filter. Then, a problem of finding eigenvalues and vectors was solved for C :

$$C = E \Lambda E^T,$$

where E is a matrix of eigenvectors; Λ is a diagonal matrix of eigenvalues; E^T is transposed E .

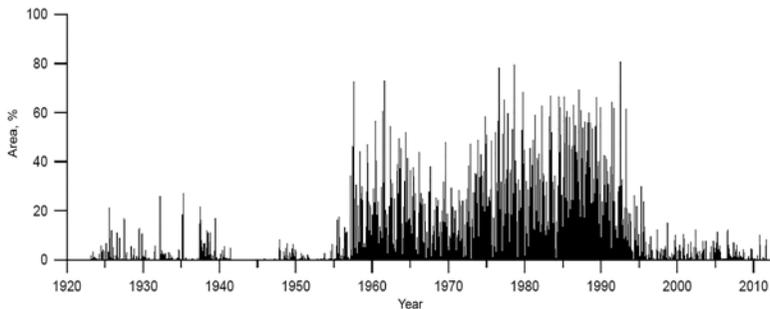


Fig. 1. Relative portion of the Black Sea area covered by the decade-derived values (regular grid) calculated by the method of optimal interpolation

The search for eigenvectors E was performed using QL/QR decomposition algorithms, which are sufficiently effective for calculations [23, 24].

At the third stage, for each time moment temporal coefficients were calculated for all the EOF modes

$$a_{it} = \mathbf{x}'_t \mathbf{e}^i,$$

\mathbf{e}^i is an eigenvector for the i -th mode; \mathbf{x}'_t is a field of monthly average anomalies in time moment t .

Due to the presence of gaps in \mathbf{x}'_t fields, temporal coefficients were determined similarly to the least squares method [25, p. 14]:

$$\hat{\alpha}_i = \frac{\sum_{j \in K} x'_j e^i_j}{\sum_{j \in K} |e^i_j|^2},$$

where $K = \{j: x'_j \text{ are non-missing data}\}$; $\hat{\alpha}_i$ is a symbol of statistic assessment.

At the last stage the resulting fields were reconstructed in all grid nodes by the inverse procedure:

$$x'_t = \sum_{i=1}^M \hat{\alpha}_{ti} e^i,$$

where M is a number of senior modes involved into the calculation.

When analyzing the results of reconstruction it turned out that this approach, previously used for surface fields, is poorly suited for three-dimensional thermohaline structure reconstruction [23]. When increasing the amount of applied modes (up to 20), the range of interannual anomalies increased excessively, the vertical structure of the fields was distorted by strong inversions. With a decrease in the number of modes, the spatial structure of anomalies significantly changed in comparison with the initial fields.

Errors in the sign and absolute magnitude of interannual anomalies are mainly related to the dependence of the assessment of $\hat{\alpha}_{ti}$ temporal coefficients on the initial data spatial distribution. Artificial vertical inversions often occur at the depth data non-uniform coverage. Therefore, in order to increase vertical and horizontal spatial consistency of the thermohaline structure, the reconstruction method was modified by connecting a block of vertical EOF.

Modified method is generally similar to the above-described one, which uses a set of horizontal EOF, but at the same time it has significant differences.

At the first stage vertical EOF Ψ , calculated by the initial vectors x'_t in the form of anomalies from monthly average climate vertical profile in the grid node, become the basic elements. The distribution of the first five vertical EOF of salinity is represented in Fig. 2.

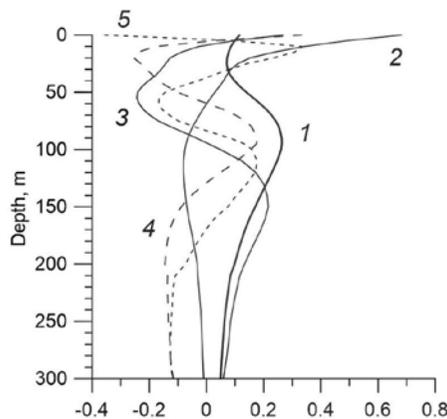


Fig. 2. Vertical EOF of salinity, figures denote the mode numbers

Then the series of vertical EOF temporal coefficients are calculated at each grid node for each vertical mode $\beta_{ii} = x'_t \psi^i$. The essential point is that β_{ii} is taken as initial horizontal fields, not the temperature and salinity anomalies, and E – the matrix of horizontal EOF of the temporal coefficients of EOF vertical modes is calculated for them.

At the last stage, for each β_{ii} field temporal coefficients for all horizontal EOF modes are calculated

$$\alpha_{ii} = \beta_{ii} e^i$$

and, using two inverse procedures, vertical profiles in each computational node are reconstructed:

$$\beta_{ii} \approx \sum_{i=1}^M \hat{\alpha}_{ii} e^i,$$

$$x'_t \approx \sum_{i=1}^L \hat{\beta}_{ii} \psi^i,$$

where M is a number of horizontal modes; L is a number of vertical modes [23, p. 97].

The modified method provided better coordination between the horizontal and vertical structure of the fields and reduction of the number of gross errors. Despite some complexity of the general calculation scheme (the presence of two different sets of modes and their conjugation), the numerical implementation of the algorithm became more efficient. Reduction of the computation time allowed us to carry out a great number of numerical experiments to select the optimal number of vertical and horizontal modes.

The spectra of EOF eigenvalues showed that the first 10 modes provide 98 % of the total dispersion for vertical EOF and up to 60 % for horizontal EOF of the vertical mode temporal coefficients. According to the results of a series of numerical calculations, it was decided to confine final calculation to five vertical EOF modes and five horizontal modes of the vertical EOF mode temporal coefficients. This combination gives minimal deviation from the optimal interpolation basic array with a significant reduction in the number of errors and a considerable saving of computation time.

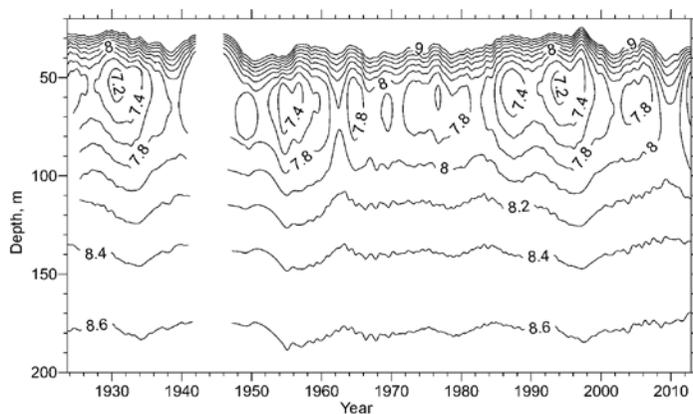


Fig. 3. Multi-year variations of the Black Sea water temperature in 20–200 m layer, the isotherms exceeding 9 °C are not shown

As a result, the reanalysis array of monthly average thermohaline fields for the 1922–2015 period was calculated, the number of omissions made up 13 %. Horizontal spatial distribution of the array is $10' \times 15'$ (latitudinal – 18.5 km and longitudinal – 19–21 km), vertical one – 67 horizons (in 0–100 m layer – every 5 m, then the step varies from 10 to 200 m). After filtering the spikes by statistical criteria, about 20 % of the array values were rejected.

The reconstruction of a continuous series of monthly average hydrological fields for the entire observation period in the Black Sea (since 1890) using this method is not possible. For adequate field reconstruction throughout the sea area the measurement data from multiple representative areas of the sea are required.

Later on, the reanalysis array was applied to study various aspects of the interannual and multi-year variability of the Black Sea thermohaline structure (Fig. 3, 4), density stratification, geostrophic circulation, etc. [26, 27].

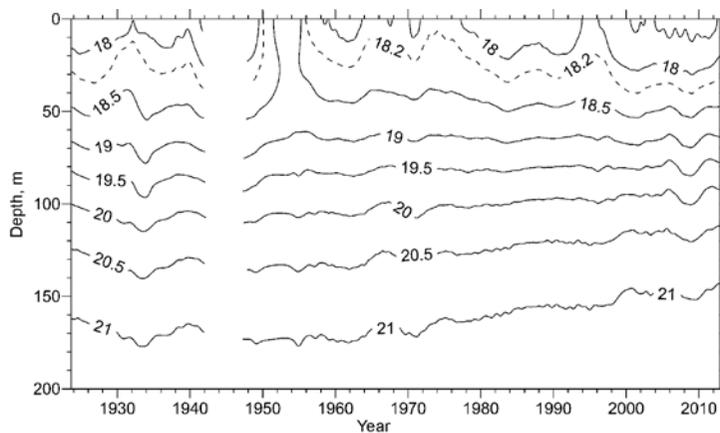


Fig. 4. Multi-year variations of the Black Sea water salinity in 20–200 m layer

Climatic arrays. In order to calculate the climatic fields of temperature and salinity, several methods were used. The simplest and most obvious is the arithmetic averaging of the reanalysis array data at the regular grid nodes for each month. The second method consists in the approximation of averaged values of reanalysis array or optimal interpolation array by annual and semiannual harmonics. The third method is based on the above-described algorithm of thermohaline field reanalysis with fundamental difference in the fact that vertical and horizontal EOF are calculated not by inter-annual anomalies, but by seasonal ones.

Comparison of climatic arrays calculated by different methods showed that when the main features of the field spatial structure coincide, there are regional differences in intra-annual evolution of thermohaline characteristics, especially in salinity. Nevertheless, spatial distribution of the hydrological seasonal cycle amplitude-phase characteristics retains its general regularities not only for different arrays, but also for different ten-year periods.

One of the characteristic features of the seasonal temperature cycle is a decrease in annual harmonic phase with an increase in the seasonal amplitude. Seasonal variation amplitude increased after 1980s and by now it reaches its maximum values (Fig. 5).

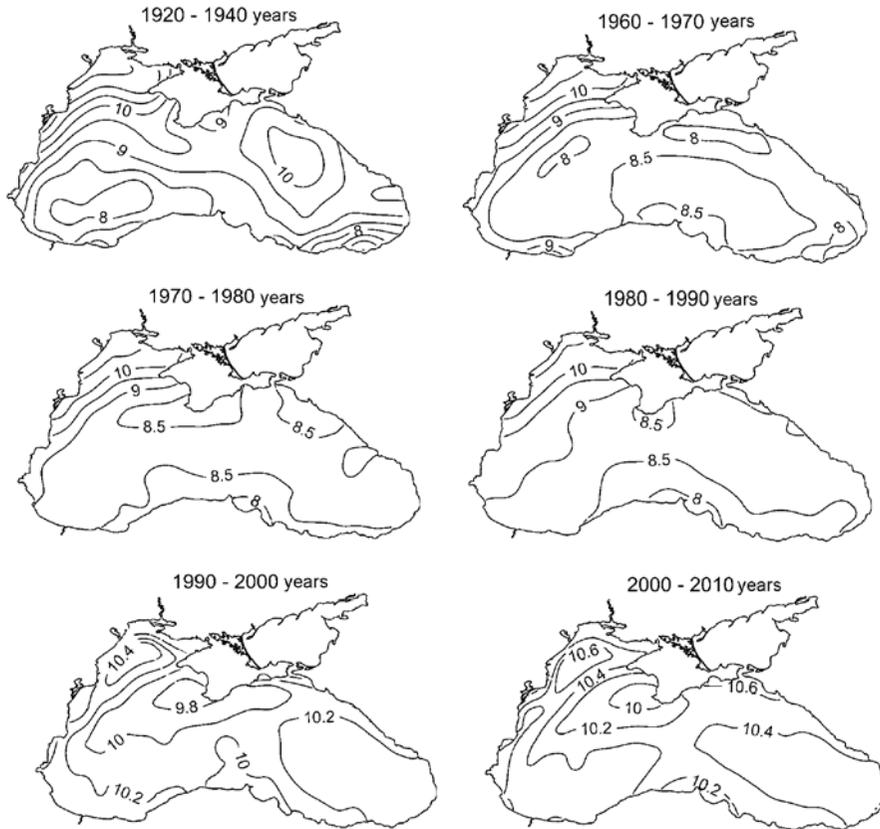


Fig. 5. Spatial distribution of the annual harmonic amplitude of the water temperature seasonal variations on the sea surface ($^{\circ}\text{C}$) for various ten-year periods

An increase in the seasonal amplitude of salinity occurs during the periods of general desalination of the sea. The main regularity of multi-year variations in the amplitude-phase characteristics of salinity is a positive correlation of phase and amplitude of the seasonal variation, which is the opposite of the changes in the water temperature seasonal variation.

Conclusions. Application of a new method for reconstructing the thermohaline fields of the basin according to irregular sets of observational data, combining optimal interpolation and decomposition into EOF functions, provided the calculation of the Black Sea hydrological structure reanalysis array for a long 1923–2015 period and climate fields for separated ten-year periods. Taking into account the significant omissions of observations in some years and the adopted criteria for filtering the errors of calculation results, relative portion of complete reconstruction cases of monthly average fields was about 70 % of the studied period.

The comparison of climatic fields for separated ten-year periods showed that seasonal hydrologic cycle in the Black Sea remains sustainable during the entire XX century, spatial distribution of seasonal variability characteristics retains its

general regularities for different ten-year periods. General trends of multi-year variations of amplitude-phase characteristics for temperature and salinity are different. With an increase in the water temperature seasonal variation amplitude, annual harmonic phase decreases, while the salinity is characterized by an inverse dependence.

In the future, this array of thermohaline field reanalysis can be used as a basis for more detailed study of the Black Sea long-term variability, and also can be applied in assimilating the observational data in the hydrophysical field reconstruction using hydrodynamic models.

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