Estimation of the Black Sea upper layer thickness and its relationship with atmospheric forcing according to model calculations and in situ measurements

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Abstract. The results of the Black Sea uniform mixed layer (UML) thickness determination are presented in the article and based on using the vertical profiles of seawater temperature obtained by three-dimensional numerical model over a five-year period. The method of adjusting the parameters of automated algorithms to determine the UML depth is proposed with the help of which three known methods of determining this parameter were implemented. The obtained results were used to study the relationship between the UML depth and the changes in the parameters of the atmospheric boundary layer at night time. It is shown that the data of heat fluxes, short-wave solar radiation, wind stress and bulk Brunt-Vaisala frequency can explain of up to 65% UML depth dispersion on the basis of regression analysis by using factor models.

1. Introduction
Investigations of the Black Sea UML thickness variability under the influence of changes in the heat, evaporation, precipitation and components of wind stress fluxes in the atmospheric boundary layer have a definite interest from the point of view of studying the processes occurring at the boundary of the two environments as well as for analysis and forecast of its state. There are a lot of theoretical [1, 2] and experimental [3,4] works devoted to solving this problem. Nevertheless, these results require further clarification and verification. The UML often refers to the upper isothermal layer of the sea. It is this UML definition used in this paper.

The aim of the work is to assess the Black Sea UML depths and clarify the relationship between UML depths and the atmospheric forcing based on large data sets of the hydrophysical and atmospheric boundary layer state parameters obtained by three-dimensional models of the atmosphere and the ocean.

2. Data used
Large arrays of circulation models calculations and in situ data measurements of seawater temperature have been accumulated for the Black Sea [5,6]. There are a number of datasets of the atmospheric boundary layer state obtained by the atmospheric models [7] synchronous in time with in situ measurements and calculations by the circulation model of the Black Sea state. The automatic operational system of Black Sea state analysis and forecast [5] is running in the Monitoring and
Forecasting Center of the Black Sea (BS MFC) of the FSBSI MHI. The model calculations of this system, atmospheric forecasts of the SKIRON system [7] and in situ measurement data [6,8] from 2012 to 2016 were used to solve this task.

The Black Sea UML depth was calculated by using three-dimensional temperature fields produced by BS MFC [5]. The spatial resolution of these fields is about 5 km (238 nodes in longitude, 132 nodes in latitude). The resolution of the model in depth is non-uniform, the data are presented on 38 depth levels distributed from 2.5 to 2100 m. The time resolution is one field a day on 0 hours of the Universal Time Coordinated (UTC). In general, 1827 initial three-dimensional fields of seawater temperature were available from 2012 to 2016. The vertical turbulent diffusivity coefficients, in addition to temperature, were used to calculate the UML depth in one of the methods.

The SKIRON atmospheric forcing initial data – the fields of heat fluxes from the atmosphere to the sea, short-wave radiation, evaporation, precipitation fluxes and components of the wind stress fluxes – have spatial resolution of 0.1° in latitude and longitude. These fields are written in the data archives of the BS MFC for every three hours from 2012 to 2018. The atmospheric forcing data were transformed and spatially interpolated to a horizontal grid of circulation model in order to run the circulation model and obtain seawater temperature fields and other parameters of the Black Sea state.

CTD [6] and SVP-BTC drifters [8] measurements taken in different areas of the Black Sea were used as in-situ data.

3. Estimation of the UML thickness

UML thickness determination methods are considered in [3,4,9]. We used three methods: method based on setting the threshold of the temperature difference $\delta T$ in the UML (TMP method) [3]; method based on setting the threshold of the coefficient of vertical turbulent diffusion of heat ($K_T$), calculated by circulation model [5] (TUR method); method described in [9] (KM method).

It should be noted that the application of UML depth estimation methods requires preliminary adjustment of their parameters in different seawater areas. For example, we were not able to obtain adequate results (the UML depths were too small) when trying to apply the KM method with the parameters specified in [9]. Similarly, the $\delta T$ value should be changed at least each month for the TMP method.

The methods parameters were adjusted based on the results of daily model calculations for each of the 1827 days of the reviewed five-year period in 140 vertical profiles uniformly distributed over the Black Sea. The methods were adjusted by calculating the correlation coefficient $\rho$ or the RMS deviation $\sigma$ between the seawater temperature on the first model depth level and the depth level corresponding to the lower boundary of the UML obtained by methods in use. The choice of the parameters adjustment was carried out by varying their values in the permissible range of variability. The values $\rho$ were calculated for each of the 12 months separately for the whole five-year period to adjust the parameters of the TMP method. As for the KM and TUR methods, $\sigma$ were calculated by using data obtained for the whole five-year period.

The key moment of implementation of the proposed approach to adjusting the parameters of the UML thickness determination methods is to study the features of the dependences of $\rho$ or $\sigma$ on the adjusted parameters. The most important features of these dependences allow us to choose an adequate value of parameter $\delta$ and correspond to the maximum absolute values of the curvature of $\rho(\delta)$ or $\sigma(\delta)$ or their inflection points.

Acceptable values of the permissible absolute deviation of the seawater temperature $\delta T$ within the UML against its value at the sea surface were calculated for each of 12 months based on dependences analysis of $\rho(\delta T)$ for the TMP method. The value of $\delta T$ varies from 0.04 to 0.11°C depending on the month.

The boundary value $K_{Max} = 0.44 \text{ cm}^2/\text{s}$ was obtained for the TUR method based on the analysis of the RMS deviation $\sigma$. It was assumed that the turbulent mixing was caused by processes occurring in the UML above this value. The upper layer of the sea from the first depth level to the last one where $K_T \geq K_{Max}$ was considered as a UML according to this criterion.
Three parameters – $C_1$, $C_2$ and $C_3$ – should be specified for the KM method. The parameter $C_3$ was set to the maximum value of $\delta T = 0.11$ °C obtained by the implementation of the TMP method to determine the UML thickness. The $C_1$ and $C_2$ were determined by the analysis of the features of two-dimensional surface $\sigma^2(C_1, C_2, 0.11)$ generated on regular grid of $20 \times 20$ nodes for $0.001 \leq C_1 \leq 0.02$ °C/m and $0.01 \leq C_2 \leq 0.2$ °C/m. The values $C_1 = 0.008$ °C/m and $C_2 = 0.1$ °C/m were chosen as the result of studying this dependence [9].

4. Comparison results of UML thickness determination

Up to the present, the most reliable estimates of the UML depth $h$ are expert estimates obtained by visual analysis of the shape of vertical temperature profile or other properties of seawater. Thus, we independently obtained expert estimates of the UML depth $h_E$ and compared them with the values obtained by the methods listed above for 120 randomly chosen profiles (10 profiles per month).

We plotted the sea water temperature profile and carried out expert visual analysis for each of the selected profiles. As a result, the expert value of the UML depth was fixed, displayed on the graph of the vertical temperature profile and stored in the UML depth file. Further, the UML depths ($h_{TMP}, h_{TUR}$ and $h_{KM}$) were calculated by methods in use. The obtained values were also displayed on the graph of the vertical profile and recorded in the UML depth file. The statistical analysis of the calculated UML depths deviations from the expert values was performed in addition to graphical comparison. Histograms of the deviations $h_{TMP} - h_E, h_{TUR} - h_E$ and $h_{KM} - h_E$ are presented in figure 1 and additional statistical characteristics are in table 1.

![Figure 1](image)

**Figure 1.** Deviations histograms of the calculated UML depth from expert estimates ((a) – TMP method; (b) – TUR method; (c) – KM method).

The histograms shown in figure 1(a) and figure 1(c) have similar qualitative features. The main part of the deviations is concentrated in a narrow range of values from -2.5 to 2.5 m. This feature is additionally confirmed by percentiles $Q_{2.5}$ and $Q_{5}$ (see table 1) showing the relative number of deviations not exceeding 2.5 and 5 m in absolute value respectively.

| Method | $\mu_{ord} (m)$ | $\sigma_{ord} (m)$ | $\mu_{med} (m)$ | $\sigma_{med} (m)$ | $Q_{2.5} (%)$ | $Q_{5} (%)$ |
|--------|----------------|-----------------|----------------|----------------|-------------|------------|
| TMP    | 0.536          | 4.919           | 0.017          | 0.119          | 85.000      | 91.667     |
| TUR    | 1.172          | 6.711           | -1.233         | 2.210          | 40.000      | 73.333     |
| KM     | 0.536          | 6.613           | 0.017          | 0.177          | 76.667      | 83.333     |

Another feature is related to the presence of outliers. Therefore the classical estimates of the location $\mu_{ord}$ and the scale $\sigma_{ord}$ are ineffective. Robust estimations of the location $\mu_{med}$ and scale $\sigma_{med}$ characteristics of the deviations correspond much more to the observed features of the deviation distributions and are presented in table 1.
The deviations obtained by TUR method are presented in figure 1(b). They have a wider empirical distribution but a fewer number of outliers.

The performed comparison allows us to conclude that the most preferred method is TMP. However, the KM method allows us to obtain not much worse results. At the same time, it is free from the disadvantage of the TMP method – jumping changes of $\delta T$ value from month to month.

In addition, we performed comparisons with expert estimates of the UML depth for 356 randomly chosen profiles of seawater temperature measured by CTD [6] in different seasons in 2012, 2015, 2016 and seawater temperature profiles from [8] in September 2013-January 2014. They confirmed the conclusions made above.

5. Estimation of the UML depth relationship with the atmospheric forcing parameters

The UML depth relationship with atmospheric forcing parameters is given in [1]. However, it is inapplicable to the data used because they refer to the night time when the sea surface layer is cooling due to the heat losses to the atmosphere and convection.

As for other literary sources, we did not find similar formulas given in [1]. We will try to estimate this relationship by the data available to us. We used the data related to one of the horizontal grid nodes of the circulation model situated approximately in the center of the Black Sea (35.48°E, 43.31°N) and UML depths determined by the KM method to solve this task.

The values $Q_d$, $S_d$, $Q$, $\tau$ and $N_h^2 = g(\rho_{po} - \rho_{ph})/(\rho_{pm} h)$ were taken as the main influencing factors. The first two variables are the average heat flux and the average flux of short-wave solar radiation over the previous day. The UML has a seasonal trend consistent with the seasonal variability of these parameters. The remaining parameters refer to the group of "instantaneous" values calculated at the beginning of the current day (0 hours UTC). $Q$ and $\tau$ are the heat flux and the wind stress respectively. The variable $N_h^2$ is the bulk Brunt-Vaisala frequency, characterizing the stability of water masses stratification in the UML having the depth $h$. $\rho_{po}$, $\rho_{ph}$ and $\rho_{pm}$ – are sea water potential density on the sea surface, sea water potential density on the last model depth level corresponding to the lower boundary of the UML and the mean value of sea water potential density within UML.

The functional relationship between the chosen influence factors and the UML depth was approximated in the class of factor models:

$$ h(x_1, x_2, x_3, x_4, x_5) = a_0 + \sum_{i=1}^{5} a_i x_i + \sum_{i=1}^{5} \sum_{j=1}^{i-1} a_{ij} x_i x_j + \cdots, $$

where $x_1 = N_h^2$, $x_2 = \tau$, $x_3 = Q$, $x_4 = S_d$, $x_5 = Q_d$.

The unknown coefficients were obtained by regression analysis. The complete model and all of its particular cases (when some coefficients were set to zero) were investigated. Determination coefficients $R^2$ for some of the most interesting models are given in table 2.

### Table 2. Determination coefficients for some of the factor models.

| Model number | Model function | $R^2$ |
|--------------|----------------|-------|
| 1            | $h = a_0 + a_1 N_h^2 + a_2 \tau + a_3 Q + a_4 S_d + a_5 Q_d$ | 0.57  |
| 2            | $h = a_0 + a_1 N_h^2 + a_4 S_d + a_5 Q_d$ | 0.56  |
| 3            | $h = a_0 + a_1 N_h^2 + a_2 \tau + a_3 Q + a_4 S_d + a_5 Q_d + a_6 N_h^2 \tau + a_7 N_h^2 Q + a_8 \tau S_d + a_9 S_d Q_d + a_{10} Q_d$ | 0.64  |

The first linear model contains all five factors and six coefficients. It allows us to explain 57% UML thickness dispersion.

The second model contains two interacting factors and four coefficients. It makes possible to account for 56% UML thickness dispersion that is practically as much as explained by the first model.
It is important to emphasize that it includes the $N^2_h$ parameter associated with the stability of water masses stratification in the upper layer of the sea.

The third model is the best of the models with five pairwise interacting factors. It explains 64% UML thickness dispersion almost as much as explained by the complete five-factor model where $100R^2 = 66%$.

In conclusion it should be highlighted that even the full four-factor model explains only 44% of the variation of UML thickness dispersion when the parameter $N^2_h$ is excluded from the list of interacting factors.

The time series of $h$ and $\tilde{h}$ are shown in figure 2(a). Histogram of deviations between the UML depth estimates $\tilde{h}$ and its values calculated by the KM method $h$ is shown in figure 2(b). The scatterplot of $h$ и $\tilde{h}$ is shown in figure 2(c). These graphs additionally illustrate the reproducibility of UML depth changes by the third model from table 2. The presented dependences will make it possible to conclude that used factor models underestimate the UML depth in the winter season.

**Figure 2.** Validation results of the model 3 from table 2 ((a) – time series: (+) – $h$; (o) – $\tilde{h}$; (b) – histogram of the $\tilde{h} - h$ values; (c) – scatterplot of the $\tilde{h}, h$ values).

### 6. Conclusions

The approach to adjusting the parameters of the automated methods used to determine the UML depth by using vertical temperature profiles allowed the improvement of three different methods for determining UML depth. The comparison of the results of the UML depth determination obtained by these three methods showed a satisfactory consistency between the obtained values.

The analysis of factor models including five variables $Q_d$, $S_d$, $Q$, $\tau$ and $N^2_h$ shows the possibility of explanation of up to 65% variation of UML thickness dispersion by changes of the selected factors. The inclusion of parameter $N^2_h$ in the set of main influencing factors is important for a more adequate reproduction of changes in the depth of this sea layer. The analysis of time series, histogram and scatterplot shows that the models defined by (1) on average underestimate the UML depth in the winter season.

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