Earth Observation Data for Science and Innovation in the Black Sea (EO4SIBS)

D3.4 - Regional Algorithms documentation
D3.7 - Error Analysis & Uncertainties

Prepared by TERRASIGNA and Laboratoire d'Océanographie de Villefranche-sur-Mer - LOV

Prepared for the European Space Agency (ESA)

TERRASIGNA
3, Logofat Luca Stroici Str.
020581 Bucharest, Romania

Report Authors

Sorin Constantin and David Doxaran

Approved

Dr. Florin Serban

TERRASIGNA General Manager

Contributions

Name	Company/Institute
Fabrizio D'Ortenzio	LOV
Ioan Daniel Serban	TERRASIGNA

Revision History

Issue	Date	Revised by	Description
1.0	14.11.2020	All	First edition

Table of Content

Abbreviations 4

1 Introduction 4

2 Turbidity estimation algorithm 4

3 Suspended Particulate Matter (SPM) estimation algorithm 9

4 Chlorophyll (Chl) estimation algorithm 13

Abbreviations

Chl - Chlorophyll

EUMETSAT - European Organisation for the Exploitation of Meteorological Satellites

MAPD - Mean Absolute Percentage Difference

MBR - Maximum Band Ratio

NIR - Near infrared

NTU - Normalized Turbidity Unit

OLCI - Ocean and Land Colour Instrument

RMSD - Root Mean Square Difference

SCMF - Sfantu Gheorghe Marine and Fluvial Research Station, University of Bucharest

SPM - Suspended Particulate Matter

T - Turbidity

1 Introduction

The current report refers to the development of regional algorithms for the Black Sea area, for estimation of biogeochemical parameters (turbidity, Suspended Particulate Matter and chlorophyll concentration) based on satellite derived water leaving reflectance. It documents the development of such methods and the associated uncertainties, as depicted by the available match-ups with in-situ collected data. It combines the *D3.4 - Regional Algorithms documentation* and *3.7 - Error Analysis & Uncertainties*. Merging was decided since each regional algorithm is described also in terms of associated statistics based on the calibration datasets, whenever each of them is introduced.

2 Turbidity estimation algorithm

Historical match-ups between in-situ water reflectance and turbidity measurements were not available for the Black Sea area. Therefore, the development of a regional algorithm was based on in-situ data collected in the Danube River plume region (figure 1) by TERRASIGNA in collaboration with the Sfantu Gheorghe Marine and Fluvial Research

Station (SCMF), University of Bucharest, which were then compared with concomitant Sentinel-3 extracted pixel values for water surface reflectance.

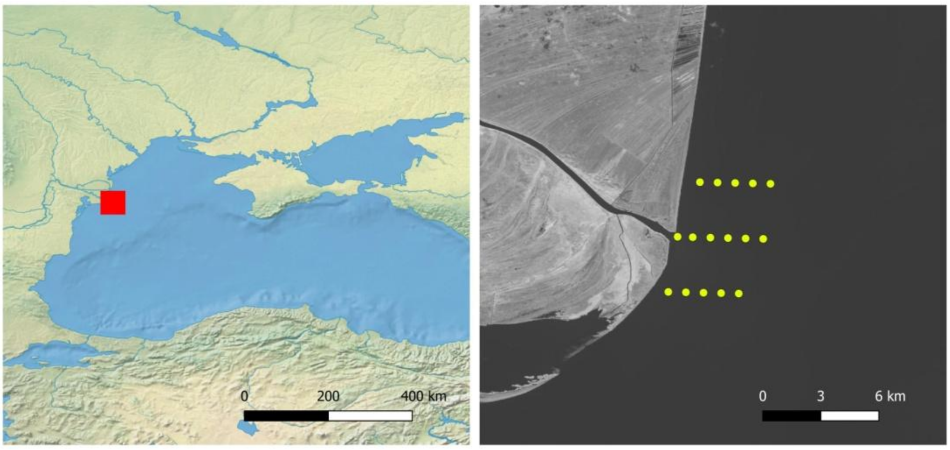

Figure 1 - Locations of sampling collection used for turbidity and SPM in-situ determination (March 18, 2019; June 23 2019; August 7, 2019; November 2, 2020)

In-situ turbidity measurements were collected using a handheld turbidimeter: Hach 2100Q (side scattering at 90°; range 0-1000 NTU; accuracy ±2% of reading plus stray, which is ≤ 0.02 NTU); auto-range function was used, which provides mean values for multiple determinations within a period of couple of seconds. Calibration of the instrument was performed before each field campaign using formazin solutions of 10, 20, 100 and 800 NTU, as indicated by the manufacturer.

A total of 48 in-situ turbidity measurements were available for this exercise, covering a relatively broad range of values, from 2.39 to 74.87 NTU, with most of the readings in the range 2-40 NTU (figure 2).

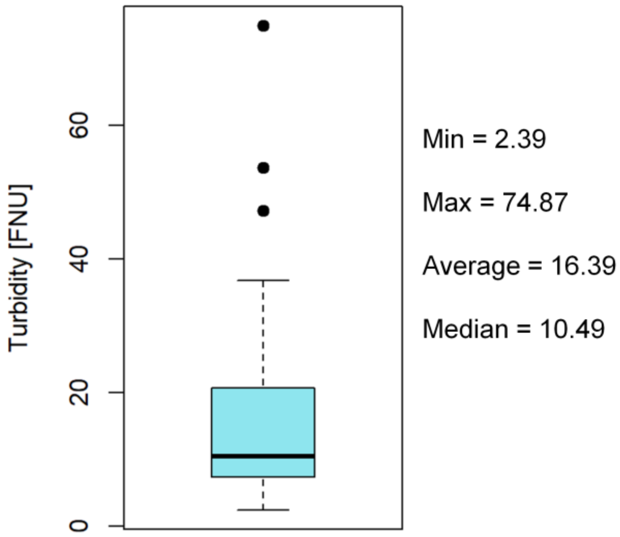

Figure 2 - Distribution and associated statistics for the turbidity in-situ measurements used as match-ups for the regional algorithm development

Four Sentinel-3 images were used to perform match-ups with the in-situ turbidity measurements. As concluded in the deliverable *3.2 - Documentation of the selected algorithms based on a comparative analysis of the performances of existing ocean colour algorithms*, standard Level 2 Full Resolution Ocean Colour (atmospherically corrected) products delivered by EUMETSAT were used. The following scenes were considered:

- March 18, 2019 (S-3A)
- June 23 2019, (S-3A)
- August 7, 2019 (S-3B)
- November 2, 2020 (S-3A)

Water leaving reflectance values were extracted after the identified pixels were masked using the following available flags (descriptions taken from S3 OLCI Marine User Handbook)

- CLOUD - Cloudy pixel
- CLOUD_AMBIGUOUS - Possibly a cloudy pixel, the flag removes semi-transparent clouds and other ambiguous cloud signatures
- SNOW_ICE - Possible sea-ice or snow contamination
- HIGHGLINT - Flag for when the sun glint correction is not reliable
- AC_FAIL - BAC atmospheric correction is suspect

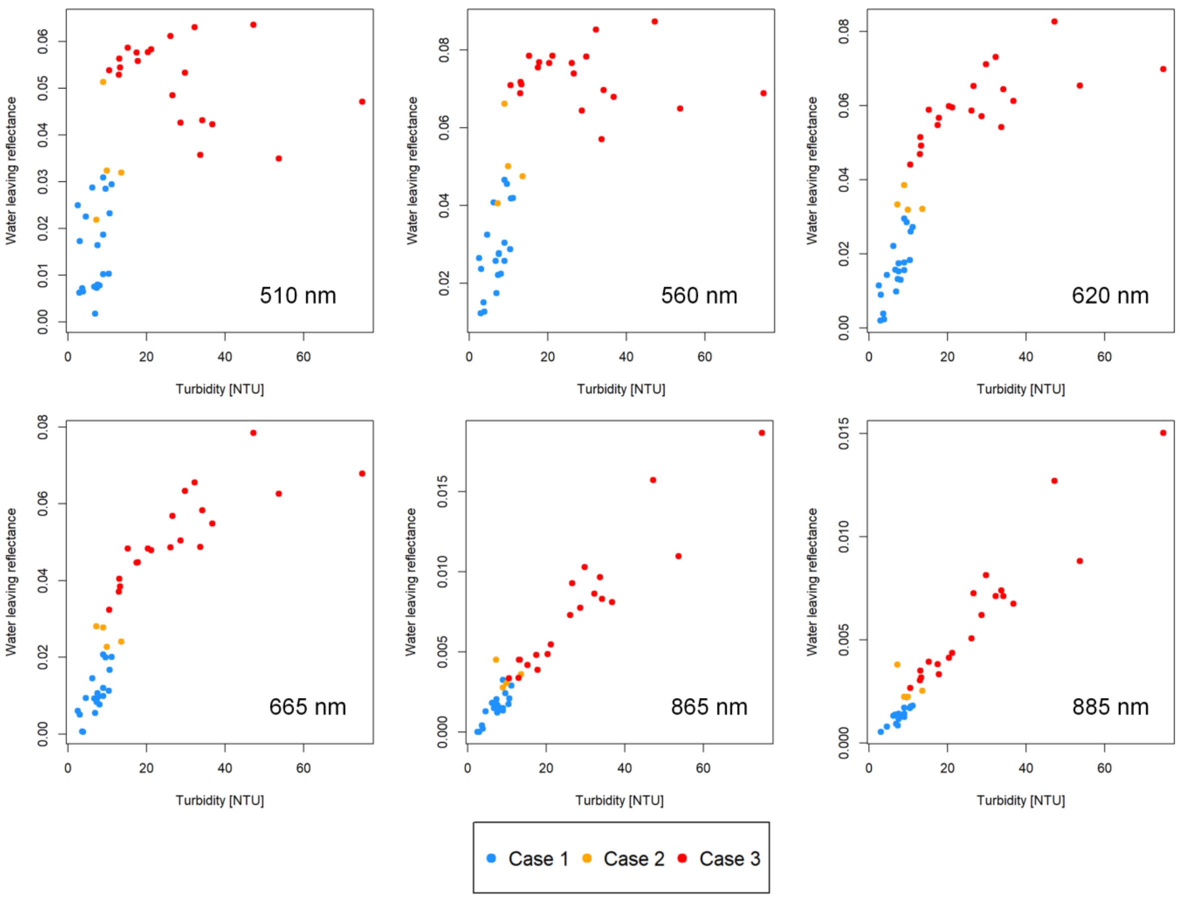

Figure 3 - Scatter plot between satellite-derived water leaving reflectance values (from several OLCI spectral bands) and in-situ turbidity measurements; colours indicate the water case (1, 2 or 3) identified applying the regional classification (D3.3).

Figure 3 shows the scatter plots between in-situ turbidity measurements and water leaving reflectance values derived from Sentinel-3 satellite data. Colour codes depict the three water mass classes, as detailed in deliverable *3.3 - Regionalization of the Black Sea waters based on optical properties*. A significant saturation can be observed for the green spectral bands (510 and 560 nm) for turbidity values above 20 NTU. For the red wavelengths (620 and 665 nm), this effect is still visible, while much attenuated. For the NIR bands, the relationship between turbidity and water leaving reflectance shows good linear fit, for all water cases. Therefore, a regional algorithm based on these wavelengths does not require adaptation as a function of optical properties of the water, since a single linear relationship appears to be valid for the three water classes.

Water leaving reflectance at 885 nm (R885) was finally selected as a proxy to derive turbidity, due to the fact that difference between R865 and R885 is negligible and despite the fact that the bandwidth of R865 is 20 nm, thus wider than in case of R885 (10 nm), which (at least in theory) would be less sensitive to noise.

The methodology described in Nechad et al. (2009 and 2010), was used in order to derive the regional algorithm for turbidity (T) estimation based on water leaving reflectance (ρ_w). More precisely, it used the in-situ measurements to adapt the coefficients of the equation used to translate ρ_w to T:

(1) $$T = \frac{A\rho w}{1 - \rho w/C} + B$$

where *C* = 0.2124 from Nechad et al. (2010) and *A* and *B* were regionally adapted, through linear regression using in-situ measurements. The default values of *A* and *B*, for ρ_w (885 nm), as provided by Nechad et al. (2009), are 2390.57 and -0.07. The regional ones, to be used for the Black Sea, are *A* = 4173.201 and *B* = 1.373.

The model yields good results, with associated statistics given in table 1.

Table 1 - Associated statistics for the regional model used to estimate turbidity based on water leaving reflectance values; R is the correlation coefficient, RMSD is the Root Mean Square Difference; MAPD is the Mean Average Percentage Difference; MB is the Mean Bias and MR is the Mean Ratio

R	RMSD	MAPD (%)	MB	MR
0.96	4.05	17.28	0	1.03

The errors associated with the potential use of the default Nechad algorithm, instead of the regional adapted one are illustrated by figure 4. The difference between the two models is shown as a function of turbidity values obtained using the regional approach. It can be observed that significant differences exist. For example, a 20 NTU value would have been underestimated by as much as 10 NTU.

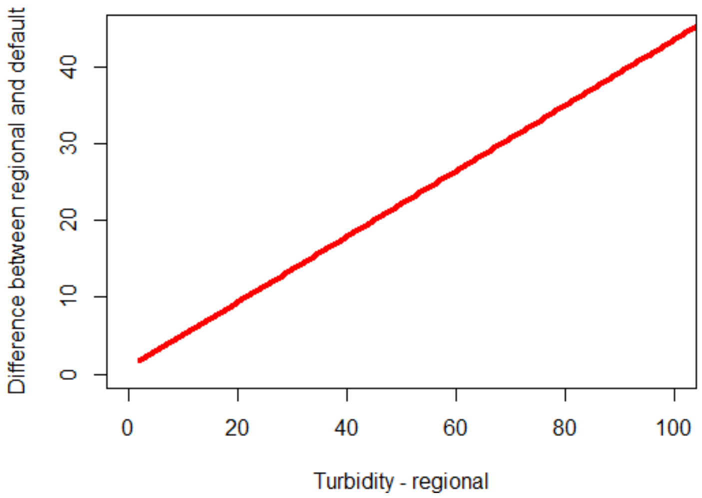

Figure 4 - Differences between default Nechad model and the regional adapted one as a function of turbidity values obtained based on the later one

Given the fact that the in-situ turbidity measurements used to calibrate the regional model based on R885 are above 2 NTU and the Black Sea offshore areas are prone to lower turbidity values, a combined algorithm was further considered. For values above 3 NTU, the regional NIR algorithm should be used, while for values below 2 NTU, the red band at 620 nm will be used instead. For the interval 2 - 3, the two algorithms will be blended, similar to the method proposed by Dogliotti et al. (2015). This methodology addition was proposed since the red band is more sensitive to changes in turbidity, compared to the NIR one, for very low values. Since there are no in-situ data for this range, the default Nechad algorithm will be used. Even if not regionally calibrated, it is expected that differences from reality should be insignificant, given the very low turbidity values accounted for. As a threshold to separate the three distinct classes, values of the red band associated with above mentioned values (2 and 3 NTU) will be used. These were determined to be 0.008 and 0.0125. Finally, the turbidity is computed as:

(2) $T = (1 - w) * T_{620} + w * T_{885}$

where *w* is the weight of the algorithm that changes linearly from 0 at ρ_w(620nm) = 0.008 to 1 at ρ_w(620nm) = 0.0125.

An example of a final turbidity product for Sentinel-3 scene acquired on June 23, 2019 is shown in figure 5.

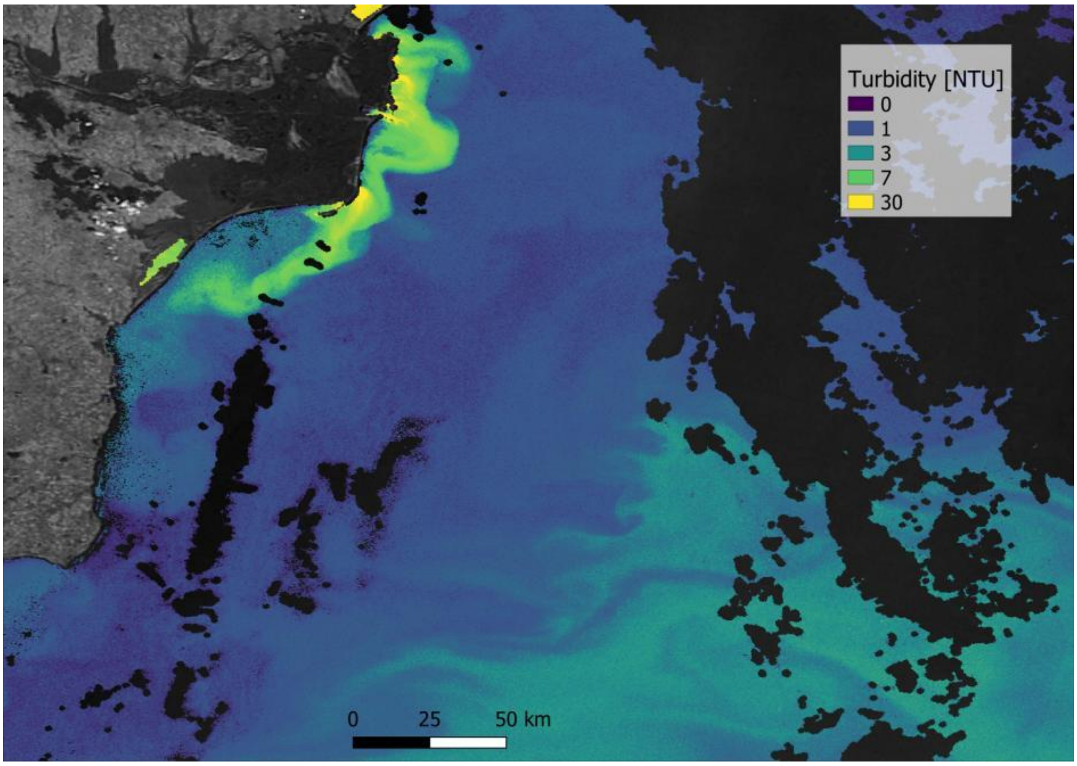

Figure 5 - Turbidity map for the western part of the Black Sea generated using a Sentinel-3 scene (June 23, 2019), using the EO4SIBS regional blended algorithm

3 Suspended Particulate Matter (SPM) estimation algorithm

The same procedure as described above, for turbidity, was used to derive a regional SPM estimation algorithm. The only difference is represented by the availability of in-situ pairs of SPM and radiometric measurements recorded during the BIO-OPT oceanographic cruise, in 2011, 1-11 of July (figure 6). These values cover the lower end of the SPM range. Therefore calibration of an algorithm for low values, based on water leaving reflectance at 665 nm, was also possible.

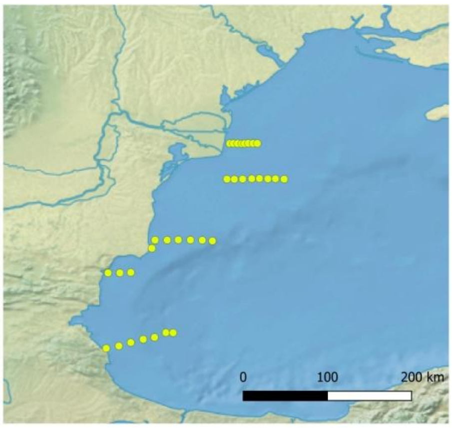

Figure 6 - Sampling locations for in-situ SPM measurements - MERMAID database: PANGAEA database BIO-OPT Cruises

From the MERMAID database, a total of 33 measurements were available (figure 7a). Most of them cover the range between 0 and 1.7, thus being representative for very low SPM concentrations. From TERRASIGNA's database, a number of 34 SPM in-situ determinations (figure 7b) were available for match-ups with Sentinel-3 reflectance data, based on the same scenes mentioned in the previous section of this report. The in-situ SPM measurements were performed taking into consideration the existing protocols, which are described in Neukermans et al. (2012). As it can be observed, the two sets of SPM measurements provide a very good complementary overview, with both low and high values being represented.

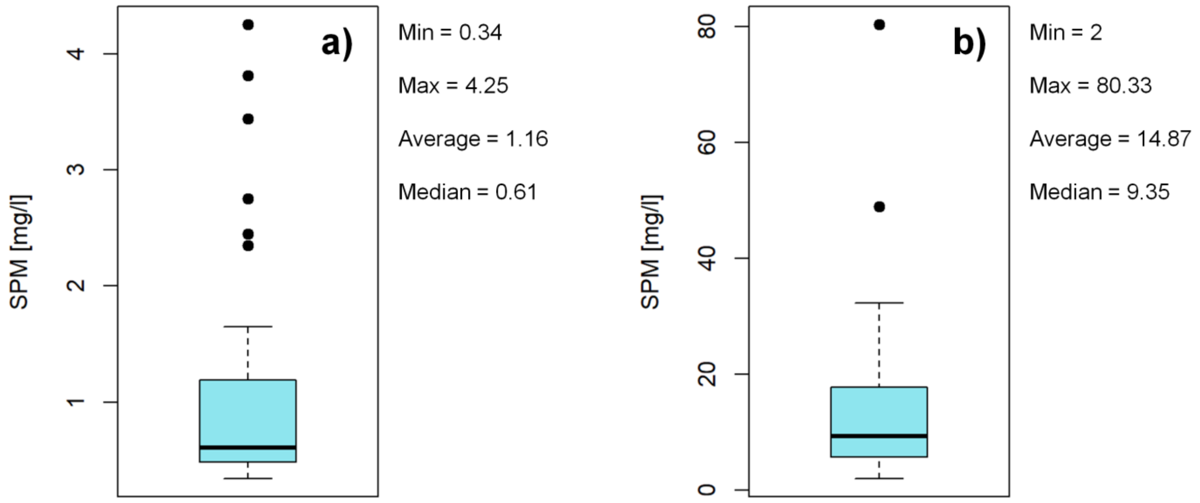

Figure 7 - Distribution and associated statistics for the SPM in-situ measurements used as match-ups for the regional algorithm development; a) data from the MERMAID database; b) data from TERRASIGNA's database

Figure 8a depicts the scatter plot between in-situ SPM concentration and water leaving reflectance measurements collected during the Bio-Optics campaign (33 complete cases; the associated best-fitted linear relationship has a determination coefficient of 0.92). Figure 3b shows the relationship between in-situ SPM measurements (TERRASIGNA database) and water leaving reflectance at 885 nm obtained from Sentinel-3 scenes (28 complete cases with a determination coefficient of 0.96). Color codes depict the three water mass classes, as detailed in deliverable *3.3 - Regionalization of the Black Sea waters based on optical properties*.

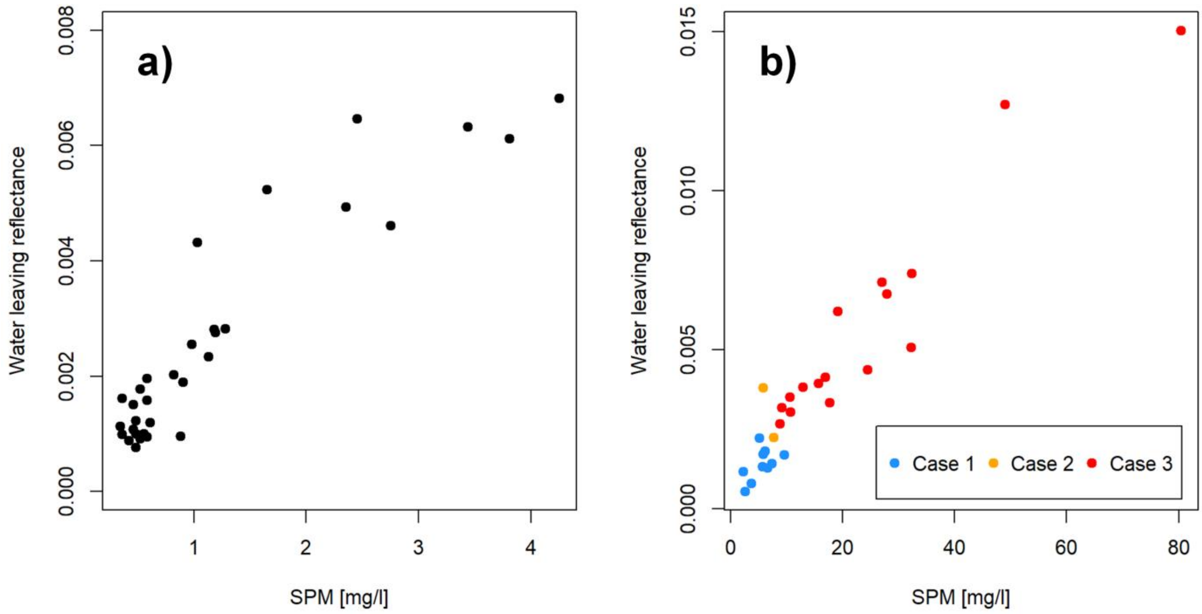

Figure 8 - Scatter plots between water leaving reflectance values and in-situ SPM measurements; a) using the MERMAID database and water leaving reflectance at 665 nm; b) based on TERRASIGNA's measurements and water leaving reflectance at 885 nm (extracted from Sentinel-3 images)

Nechad et al. (2010) algorithm was adapted to the local conditions for both 665 and 885 nm scenarios. Default and updated (regional) coefficients (to be used with equation 1) are given below.

Table 2 - Default and updated / regional coefficients used to derive SPM from water leaving reflectance values

Coefficient	Default 665 nm	Regional 665 nm	Default 885 nm	Regional 885 nm
A	355.85	491.264	3388.53	4424.259
B	1.74	-0.1111	2.68	-1.855

The performance of each regional algorithm and the corresponding uncertainties are shown in table 3.

Table 3 - Associated statistics for the regional models used to estimate turbidity based on water leaving reflectance values; R is the correlation coefficient, RMSD is the Root Mean Square Difference; MAPD is the Mean Average Percentage Difference; MB is the Mean Bias and MR is the Mean Ratio

Model	R	RMSD	MAPD (%)	MB	MR
665 nm	0.93	0.39	27.84	0	1.03
885 nm	0.96	4.71	30.6	0	1.03

For the blending procedure, the same approach as for turbidity was used (see equation 2). Due to the way the two sets of measurements used to derive the regional algorithms overlap, the interval between 2 and 4 mg/l was chosen for blending. Water leaving reflectance in the 665 nm region is used to make the selection of such areas, with set thresholds of 0.004 and 0.008.

The differences between default and regional adapted models can be significant (figure 9a). For the 665 nm model, an overestimation of the default approach is visible for the entire range where this algorithm is intended to be used (0-5 mg/l range). For the 885 nm approach (figure 9b), an overestimation is also present, up to approximately 20 mg/l, switching afterwards to an underestimation behavior, with differences up to 20 mg/l for values close to 100 mg/l SPM.

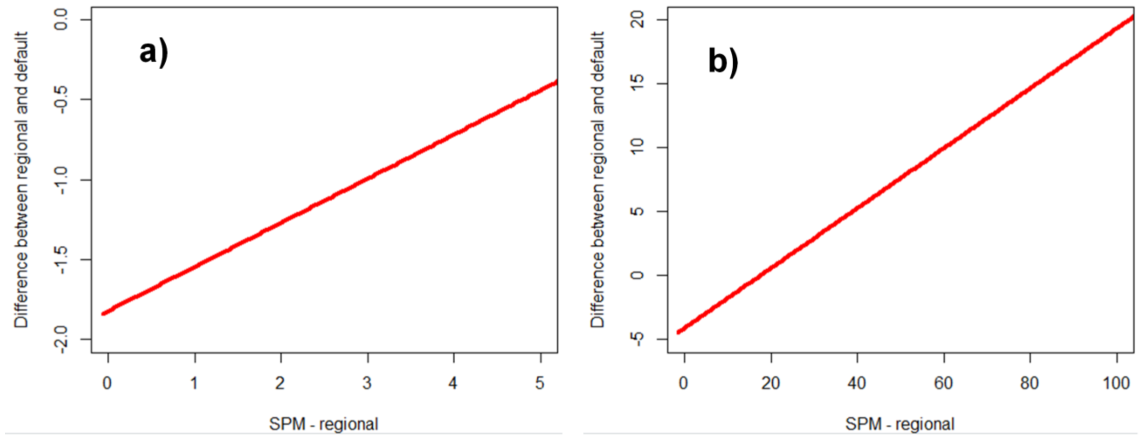

Figure 9 - Differences between default Nechad model and the regional adapted one as a function of SPM values obtained based on the later one; a) for the 665 nm algorithm; b) for the 885 nm algorithm;

An example of a final SPM product for Sentinel-3 scene acquired on June 23, 2019 is shown in figure 10.

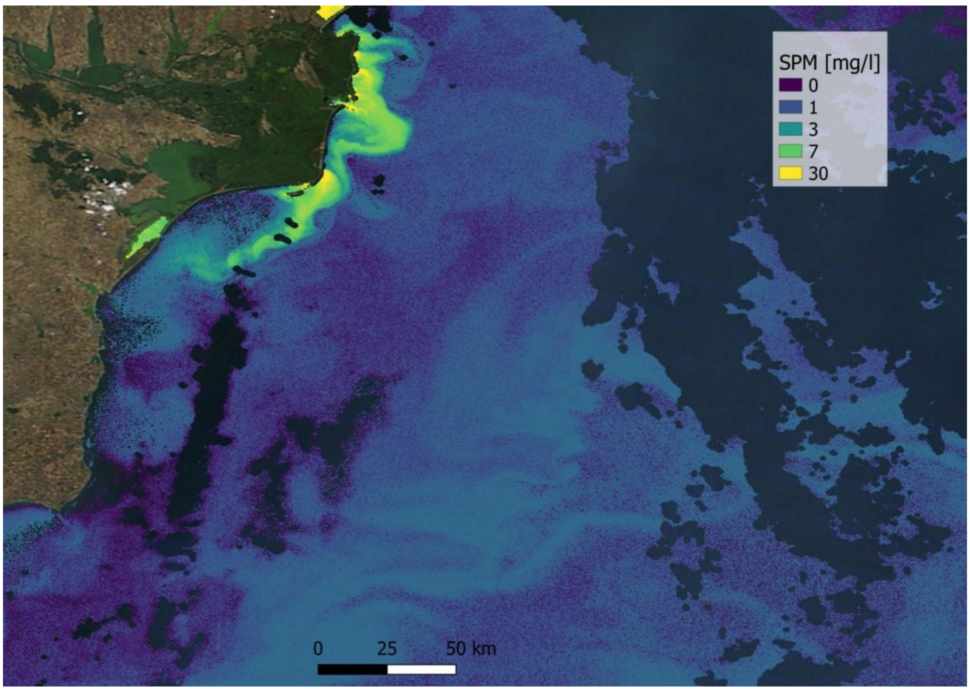

Figure 10 - SPM map for the western part of the Black Sea generated using a Sentinel-3 OLCI scene (June 23, 2019), using the EO4SIBS regional blended algorithm

4 Chlorophyll (Chl) estimation algorithm

For the development and validation of the chlorophyll regional algorithm, both in-situ and satellite derived water leaving reflectance values were available and were evaluated (figure 11). Distributions of Chl values associated with these match-ups are given in figure 12. Only surface determinations were considered and those with a time difference less than 5 hours between in-situ collection and satellite data acquisitions. Both series cover a similar range, from 0.1 to more than 15 mg/m^{-3}. To be noted that the similarities are mainly due to the fact that several samples are common for the two scenario. The differences are given only by the availability of water leaving reflectance match-ups (either in-situ collected or satellite derived).

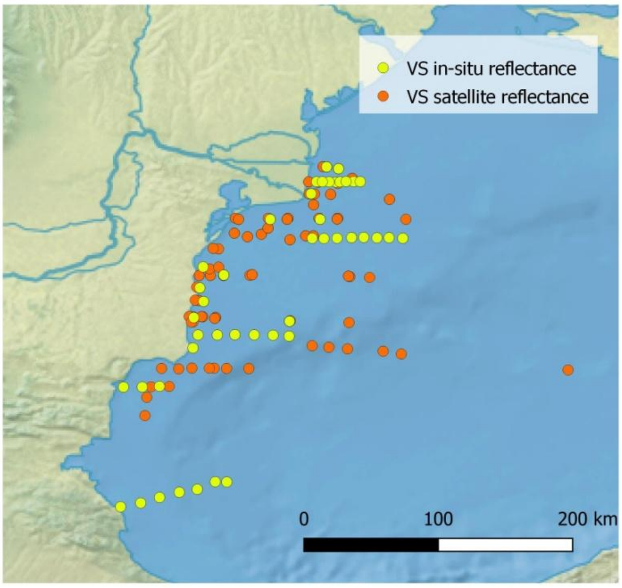

Figure 6 - Sampling locations for in-situ Chl measurements (yellow points - matched up with in-situ water leaving reflectance data; orange ones - matches with satellite derived reflectance)

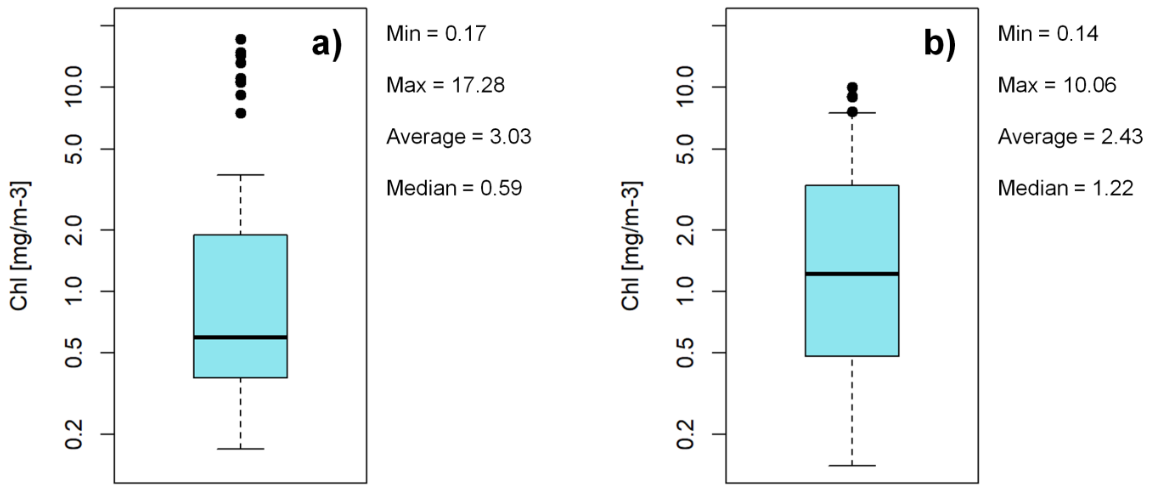

Figure 12 - Distribution and associated statistics for the Chl in-situ measurements used as match-ups for the regional algorithm development; a) that have match-ups with in-situ water leaving reflectance data; b) that have match-ups with satellite derived water leaving reflectance values

As mentioned above, datasets shown in figure 12a were initially considered for model development (57 measurements). The following wavelengths were available, in terms of in-situ water leaving reflectance measurements: 412, 443, 490, 510, 560, 665 and 681 nm. Thus, the development of an algorithm taking advantage of the red edge bands (which OLCI is adapted with) is not possible using the in-situ measured reflectance dataset. Also, given other uncertainties associated with in-situ data collection, these datasets were not used for model calibration. Uncertainties refer mainly to difficulties in extrapolating in-water upwelling radiance measurements to above water reflectance and unknown spectral response functions and bandwidths of the instruments used to collect in-situ data. Therefore, the match-ups obtained from OLCI imagery with in-situ chlorophyll measurements were finally considered for algorithm development.

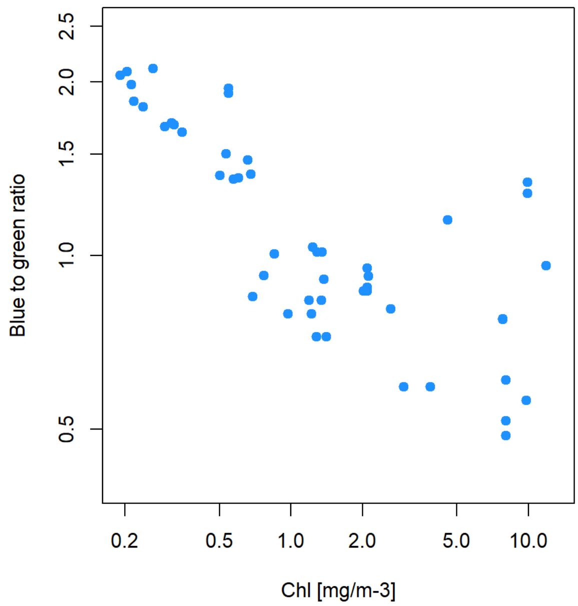

Figure 13 - Scatter plot between log transformed satellite water leaving reflectance values and in-situ Chl measurements

The scatter plot between in-situ Chl measurements and a maximum blue to green ratio (MBR) based on OLCI derived water leaving reflectance (figure 13) shows, as expected, a good relation between the two variables for low concentrations. The MBR was determined as the highest value between R490/R560 and R510/R560. All points were classified as Case 1. Therefore no conclusions can be drawn to this regard based on the current available dataset. Nevertheless, a significant scatter is noticed for values of Chl higher than 2 mg/m^{-3}. Based on this observation, a regional adapted algorithm based on the MBR was first developed.

A fourth-order polynomial relationship between maximum band ratio of water leaving reflectance and Chl concentration (OC4-type) was established:

(3) $$\log_{10}(Chl) = a_0 + \sum_{i=1}^{4} a_i (log10(MAXBR))^i$$

where MAXBR is the maximum band ratio between R490/R560 or R510/R560, and the corresponding coefficients (a0 - a4) are given in table 4.

Table 4 - Coefficients used for equation (3)

a_0	a_1	a_2	a_3	a_4
0.01880849	-0.5604981	-5.61988818	-27.98195094	101.21078387

Based on 31 match-ups (figure 14), the statistics associated with the observed versus predicted Chl values are R=0.91, RMSD=0.17 and MAPD=20.33%.

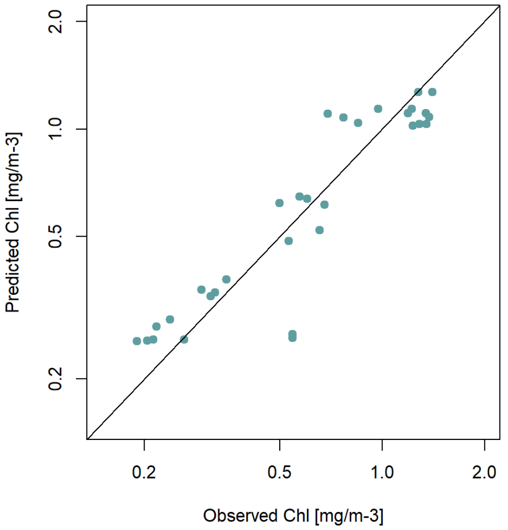

Figure 14 - Observed versus predicted Chl values, using the MBR regional approach

For values higher than 2 mg/m^{-3}, development of a regional algorithm was not possible using the available in-situ datasets. The proposed solution for the Black Sea area is to use the above mentioned method, based on the MBR, for low values, and to combine it (using a merging scheme) with the results of the neural network algorithm (proven to perform better that other approaches) for higher chlorophyll concentrations.

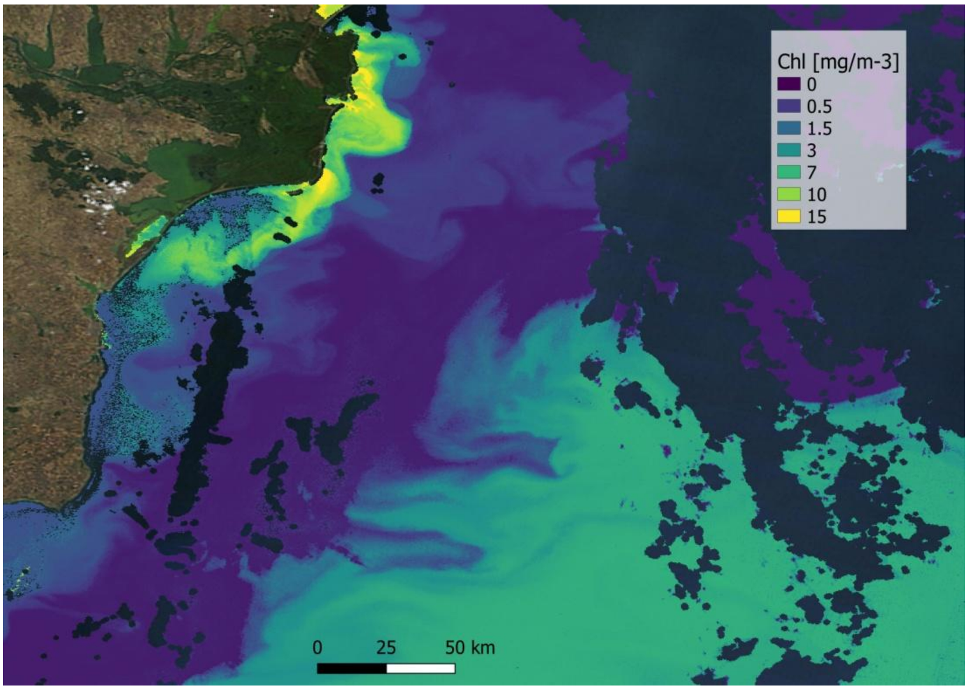

Figure 10 - Chl map for the western part of the Black Sea generated using a Sentinel-3 OLCI scene (June 23, 2019), using the EO4SIBS regional blended algorithm

Acknowledgements

Turbidity and SPM in-situ measurements were performed by TERRASIGNA in collaboration with the Sfantu Gheorghe Marine and Fluvial Research Station (University of Bucharest).

References

Dogliotti, A. I., Ruddick, K. G., Nechad, B., Doxaran, D., & Knaeps, E., 2015. A single algorithm to retrieve turbidity from remotely-sensed data in all coastal and estuarine waters. Remote Sensing of Environment, 156, 157–168. https://doi.org/10.1016/j.rse.2014.09.020

EUMETSAT, 2018. S3 OlCI Marine User Handbook, EUM/OPS-SEN3/MAN/17/907205

Nechad, B., Ruddick, K. G., & Neukermans, G., 2009. Calibration and validation of a generic multisensor algorithm for mapping of turbidity in coastal waters. Remote Sensing of the Ocean, Sea Ice and Large Water Regions, 7473. https://doi.org/10.1117/12.830700

Nechad, B., Ruddick, K.G., Park, Y., 2010. Calibration and validation of a generic multisensor algorithm for mapping of total suspended matter in turbid waters. Remote Sens. Environ. 114, 854–866. doi:10.1016/j.rse.2009.11.022

Neukermans, G., Ruddick, K., Loisel, H., & Roose, P., 2012. Optimization and quality control of suspended particulate matter concentration measurement using turbidity measurements. Limnology and Oceanography: Methods, 10(DECEMBER), 1011–1023. https://doi.org/10.4319/lom.2012.10.1011