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Calibration and validation of algorithms for the estimation of chlorophyll-*a* concentration and Secchi depth in inland waters with Sentinel-2

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ABSTRACT

Calibration and validation of algorithms for the estimation of chlorophyll-*a* concentration and Secchi depth in inland waters with Sentinel-2

Chlorophyll-*a* concentration and Secchi disk depth are two of the most important biophysical parameters used to assess water quality and determine the ecological state of inland waters. The *Ocean Color 2* and *Dall'Olmo three-band* algorithms were used to estimate chlorophyll-*a* concentration and the calibration of the ratio 490/705 nm was used to produce an algorithm for estimating Secchi disk depth. These algorithms have been calibrated for the Sentinel 2-Multispectral Instrument (S2-MSI) and validated using *in situ* measurements of chlorophyll-*a*, Secchi disk depth and radiometry. This data was taken in the Valencia region reservoirs as part of the project Ecological Status of Aquatic Systems with Sentinel Satellites (ESAQS). The results show that for estimating chlorophyll-*a* concentration, it is better to apply a prior classification based on their trophic status. For eutrophic and hypertrophic waters, the TBDO algorithm had an error of 23 mg/m^3 over a chlorophyll-*a* concentration range of between 10 to 169 mg/m^3. For ultraoligotrophic to mesotrophic waters, the better algorithm was OC2_490, which resulted in an error equal to 0.9 mg/m^3 over a chlorophyll-*a* concentration range of between 0.54 to 5.8 mg/m^3. For the estimation of water transparency by Secchi disk depth, we have obtained good results with the ratio 490/705 nm, with an error equal to 0.88 m over a Secchi disk depth range of between 0.26 to 8.1 m. These algorithms have been applied to S2-MSI images and satisfactory results have been obtained for different reservoirs in the Valencia region (Spain).

Key words: Ocean Color, Dall'Olmo three-band, chlorophyll-*a*, Secchi disk depth, Sentinel-2, HydroLight

RESUMEN

Calibración y validación de algoritmos para la estimación de la concentración de la clorofila*-a *y profundidad de Secchi en aguas continentales con Sentinel-2

La concentración de clorofila-a *y la profundidad del disco de Secchi son dos de los parámetros biofísicos más importantes utilizados para evaluar la calidad del agua y determinar el estado ecológico en aguas continentales. Los algoritmos Ocean Color 2 y triple banda de Dall'Olmo fueron aplicados para la estimación de la concentración de la clorofila*-a. *El ratio 490/705 nm se usó para producir un algoritmo para la estimación de la profundidad del disco de Secchi. Esos algoritmos han sido calibrados para el Instrumento Multiespectral de Sentinel 2 (S2-MSI) y validados usando medidas* in situ *de la clorofila*-a*, profundidad del disco de Secchi y radiometría. Estos datos se tomaron en los embalses de la región de Valencia en el contexto del proyecto Estado Ecológico de los Sistemas Acuáticos con Satélites Sentinel (ESAQS). Los resultados muestran que para la estimación de la concentración de la clorofila*-a *es mejor aplicar previamente una clasificación basada en su estado trófico. Para aguas eutróficas e hipertróficas, el algoritmo triple banda de Dall'Olmo tuvo un error de 23 mg/m^3 sobre un rango de concentración de clorofila*-a *entre 10 a 169 mg/m^3. Para aguas ultraoligotróficas a mesotróficas el mejor algoritmo fue el*

*OC2_490, con el cual se obtuvo un error de 0.9 mg/m³ sobre un rango de concentración de clorofila-*a *entre 0.54 a 5.8 mg/m³. Para la estimación de la transparencia del agua mediante la profundidad del disco de Secchi, hemos obtenido buenos resultados con el ratio 490/705 nm, con un error igual a 0.88 m sobre un rango de profundidad de disco de Secchi entre 0.26 a 8.1 m. Estos algoritmos han sido aplicados a imágenes S2-MSI obteniendo resultados satisfactorios en diferentes embalses en la región de Valencia (España).*

Palabras clave: *Ocean Color, triple banda de Dall'Olmo, clorofila-*a, *profundidad de disco de Secchi, Sentinel-2, HydroLight*

INTRODUCTION

Chlorophyll-*a* concentration [Chl-*a*] is a phytoplankton biomass estimator in water bodies. It is one of the fundamental parameters of water quality used to detect algal blooms and assess eutrophication levels. The anomalous productivity of phytoplankton biomass relative to a "normal situation" (or the ecological optimum, depending on the watershed characteristics and climate of a given water body) is an indicator of eutrophication (Zheng and DiGiacomo, 2017). The [Chl-*a*] derivation from satellite data relies mostly on the absorption signal of phytoplankton. The variability of the [Chl-*a*] specific absorption coefficient is spectrally minimal around the red absorption peak (670 nm), where the influence of accessory pigments is minimal, and is higher around the blue absorption peak (440 nm), where the absorption of accessory pigments and dissolved organic matter is also high (Bricaud *et al.*, 1995; Stramsky *et al.*, 2001, Zheng & DiGiacomo, 2017).

Secchi disk depth (Z_{SD}) is a measurement of water transparency. The depth at which the disk disappears into the water is inversely proportional to the average amount of organic and inorganic materials along the path of sight in the water. The sense of sight is an integral part of the measurement procedure (Preisendorfer, 1986).

The European Water Framework Directive (WFD) establishes a framework for community-wide action for assessing the ecological status, management and conservation of the different water bodies in the member states. In this context, and in view of the need for comprehensive management of the aquatic systems of the Valencia region (south-eastern Spain), the Ecological Status of Aquatic Systems with Sentinel satellites (ESAQS) project was developed. The Regional Water Authority (Confederación Hidrográfica del Júcar, CHJ) collaborates and helps this project. The main objective of ESAQS is to develop and validate algorithms for the estimation of ecological quality indicators of inland waters (i.e. chlorophyll-*a* concentration, Secchi depth, colored dissolved organic matter and suspended solids) using the data provided by the Multispectral Instrument (MSI) sensor on-board the Sentinel-2 (S2-MSI) mission. The MSI scenes have a spatial resolution of 10 m, a high temporal resolution of 5 days and an adequate spectral resolution. Table 1 summarizes the principal features of S2-MSI. These characteristics make this sensor an exceptional instrument for the retrieval of biophysical parameters in inland waters, as compared to other satellite missions designed either for ocean color applications (e.g. the Ocean and Land Colour Imager, OLCI, on Sentinel-3 or the Moderate-Resolution Imaging Spectroradiometer, MODIS-Aqua), or the land-oriented Operational Land Imager (OLI) Landsat-8, which have a lower spatial resolution (300, 1000 and 30 m, respectively). S2-MSI data is suitable for the study of small irregularly-shaped water masses like most reservoirs in the region (Fig. 1) and small area as 80 ha (Regajo reservoir). Remote sensing data adds an extra value to limnological data collected from traditional *in situ* measurements (Giardino *et al.*, 2001), thanks to the synoptic view and frequency of the satellite passes. Remotely-sensed optical imagery over water bodies has been used as a cost-effective way for monitoring water quality.

The aim of this paper is to present the results of the calibration of water quality algorithms for the estimation of [Chl-*a*] and Z_{SD} from S2-MSI spectral bands and the validation with *in situ* [Chl-*a*] and Z_{SD} measurements. These algorithms cover a wide range of trophic states, from hypertrophic to ultraoligotrophic, in line with the characteristics

Table 1. Main characteristics of S2-MSI spectral bands. *Principales características de las bandas espectrales de S2-MSI.*

Band number	Central wavelength (nm)	Bandwidth (nm)	Spatial resolution (m)
1	443	20	60
2	490	65	10
3	560	35	10
4	665	30	10
5	705	15	20
6	740	15	20
7	783	20	20
8	842	115	10
8a	865	20	20
9	945	20	60
10	1380	30	60
11	1610	90	20
12	2190	180	20

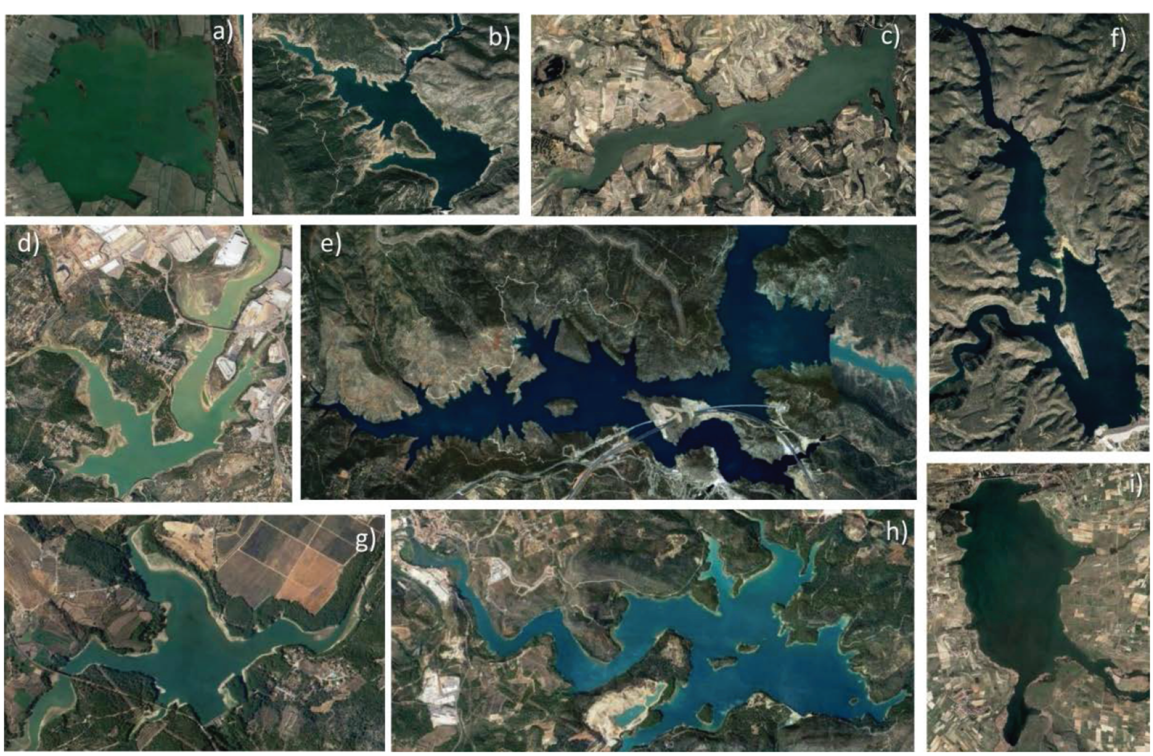

Figure 1. Reservoirs in study area. a) Albufera of Valencia, b) Benagéber, c) Beniarrés, d) María Cristina, e) Contreras, f) Tous, g) Regajo, h) Sitjar and i) Bellús. *Embalses en el área de estudio. a) Albufera de Valencia, b) Benagéber, c) Beniarrés, d) María Cristina, e) Contreras, f) Tous, g) Regajo, h) Sitjar y i) Bellús.*

of reservoirs measured in our study region. This objective fits into the main ESAQS goal of formulating new algorithms for inland water ecological state monitoring from remote sensing.

DATA AND METHODS

Study area

Since 2017, the first year of the ESAQS project, a large number of field campaigns have been carried out in the Valencia region. The study area includes the reservoirs of Benagéber, Bellús, Beniarrés, Contreras, María Cristina, Regajo, Sitjar, Tous and the Albufera of Valencia (Fig. 2), covering a wide gradient of trophic states. For each reservoir, between 1 and 4 *in situ* measuring points were taken at a suitable distance from shoreline to avoid mixed pixels (land-water mixed reflectance). The field campaigns were planned on cloud-free days on which the S2 satellites acquired images over the reservoir region.

In situ data: [Chl-*a*] and Z_{SD}

[Chl-*a*] and Z_{SD} were measured by the Limnology Research Team of the University of Valencia. [Chl-*a*] data were obtained from the water samples by the spectrophotometric method. Samples were filtered through 0.4-0.6 µm GF/F glass

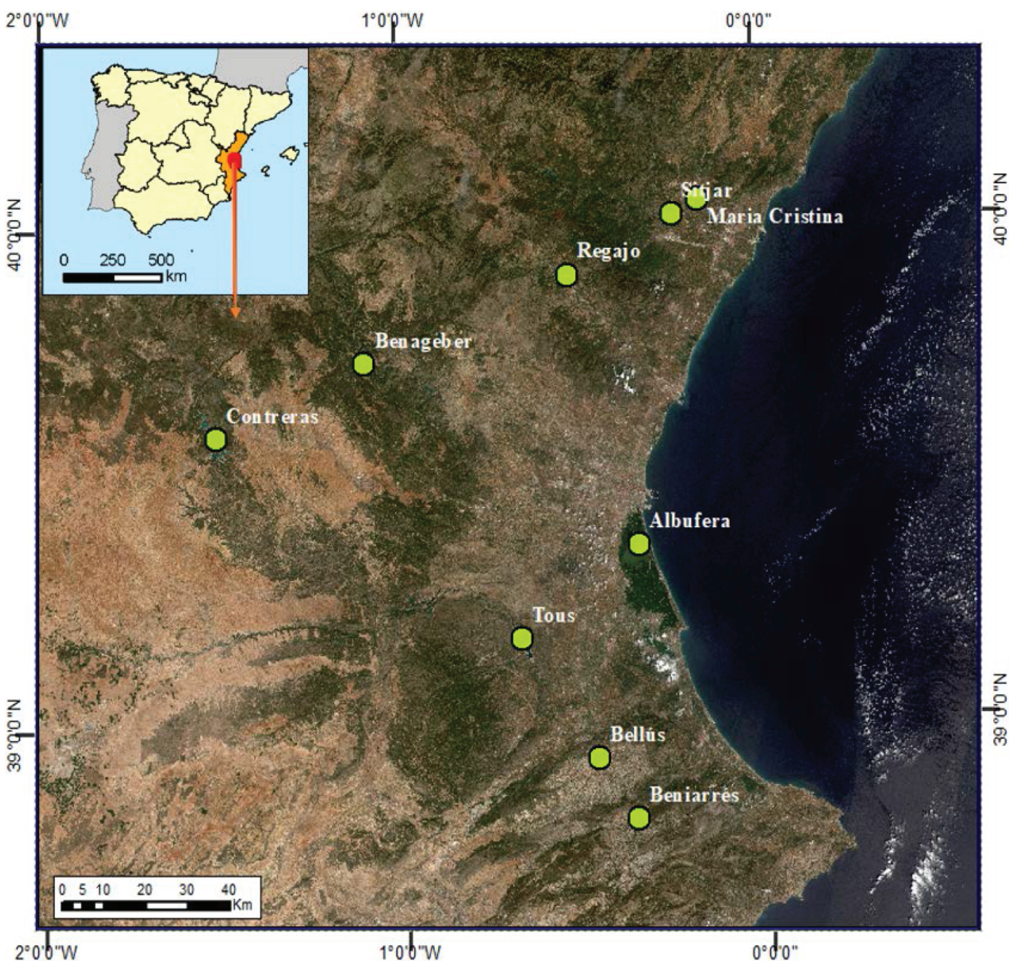

Figure 2. Location map of reservoirs and lakes in study in Valencia region. *Mapa de localización de los embalses y lagos en estudio en la región de Valencia.*

fiber filters, extracted according to standard methods (Shoaf & Lium, 1976) and the calculation methods by Jeffrey & Humphrey (1975) (Soria *et al.*, 2019). The range of *in situ* [Chl-*a*] measurements in the study area reservoirs was between 0.54 to 169 mg/m^3.

Z_{SD} data was measured with a metal disk called a Secchi disk. It is divided into four quarters, each one painted black and white. The measurement procedure for obtaining the Z_{SD} is to slowly lower it into the water until it disappears from sight. When that happens, it is possible to obtain the Z_{SD}. The *in situ* Z_{SD} measurement range in the reservoirs under study was between 0.25 to 10.5 m.

In situ reflectances

The *in situ* reflectances were calculated from above-water *in situ* measurements of: 1) The water-leaving radiance (L_w), 2) the sky radiance (L_{sky}) and 3) the downwelling solar irradiance (E_S). These were measured using a HandHeld2 radiometer, which has a wavelength range of 325 to 1075 nm and a spectral resolution of 1 nm; and an Ocean Optics (HR 4000) radiometer ranging from 200 to 1100 nm at a spectral resolution of ~0.2 nm. According to previous studies (Mobley, 1999) and recommendations done by international remote sensing ocean groups (Fargion & Mueller, 2000), the measurements have been taken with a view zenith angle of ~45 º and an azimuthal angle of ~135 º, with respect to the sun, to minimize the direct and diffuse sunlight reflected by the water surface (Mobley, 1999). Once the measurements were obtained, the *in situ* reflectance spectrum was convolved to the S2-MSI spectral bands (Table 1). This procedure was done to fit the *in situ* reflectance spectral resolution (~0.2 nm or 1 nm) to S2-MSI bandwidth using the Spectral Response Functions database (SRF v2.0) (ESA, 2018a). The SRF determine the position and width of each S2-MSI spectral band (D'Odorico *et al.*, 2013).

S2-MSI imagery

The Cloudless Level 1C S2-MSI images were downloaded from the Copernicus Open Access Hub of the European Spatial Agency (ESA, 2018b) to be concurrent with the *in situ* measurements. SNAP software v.5.0 (ESA, 2018c) was used for the image processing. For the specific case of the Albufera of Valencia, images were atmospherically corrected to Bottom of Atmosphere (BOA) reflectances using the Sen2Cor processor (ESA, 2018d). While this atmospheric correction method was designed for land products, it gives back optimum results in eutrophic waters like the Albufera of Valencia according to Ruescas *et al.* (2016) and Soria *et al.* (2017a). In this respect, we would highlight the importance of atmospheric correction over inland waters. In the ESAQS project, we are evaluating different atmospheric correction methods to obtain an optimum retrieval of the algorithms calibrated and validated to actual S2-MSI images for routine monitoring purposes.

Calibration and validation of established [Chl-*a*] algorithms

To calibrate the [Chl-*a*] algorithms and encompass the variability of the optically active components present in inland waters, we generated a calibration database of simulated data (N = 392) by using the radiative transfer model HydroLight (Mobley, 1994). We carried out simulations with a three-component Case-2 model with ranges of variables characteristics for oligotrophic to eutrophic waters: [Chl-*a*] (1-500 mg/m^3), Colored Dissolved Organic Matter (CDOM) (0.01-4 m^{-1}) and Non-Algal Particles (NAP) (0.1-100 g/m^3). To estimate [Chl-*a*] with S2-MSI spectral bands, we tested the Ocean Color 2_443 nm (OC2_443) and Ocean Color 2_490 nm (OC2_490) (replacing the original 483 band with the 490 band in S2-MSI), the Ocean Color 3 (OC3) (O'Reilly *et al.*, 2000) and the Dall'Olmo three-band algorithm (Dall'Olmo *et al.*, 2003), hereafter called the TBDO algorithm. Following the methodology of Ruiz-Verdú *et al.* (2016), the OC2 and OC3 algorithms, based on the ratio of green and blue bands, have been recalibrated for the S2-MSI spectral bands. The TBDO algorithm, which is based on the evaluation of the reflectance at red and near infrared bands (665, 705 and 740 nm), is used for the estimation of [Chl-*a*] in inland and coastal water (Gilerson *et al.*, 2010). This algorithm has also been calibrated for the S2-MSI spectral bands and validated in a previous work in a hypertrophic coastal lagoon: the Albufera of Valencia (Guibaja *et al.*, 2016).

The [Chl-*a*] algorithms used in this work are described below. The general equation for the OC2 and OC3 models are:

$$\log_{10} [\text{Chl-}a] = a + bX + cX^2 + dX^3 \quad (1)$$

where X is calculated according to:

OC2_443 model (2)
$X = \log_{10} [Rrs\_443/Rrs\_560]$

OC2_490 model (3)
$X = \log_{10} [Rrs\_490/Rrs\_560]$

OC3 model (4)
$X = \log_{10} [\max (Rrs\_443; Rrs\_490)/Rrs\_560]$

The Rrs_443, Rrs_490 and Rrs_560 are reflectances of S2-MSI spectral bands.

The algorithm called OC2_490, fit to the S2-MSI bands, is set to the spectral band 490.

The three-band model of Dall'Olmo *et al.* (2003) (TBDO), takes the form:

$$[\text{Chl-}a] = aX^2 + bX + c \quad (5)$$

where

$$X = [Rrs\_740*((Rrs\_665)^{-1} - (Rrs\_705)^{-1})] \quad (6)$$

The Rrs_665, Rrs_705 and Rrs_740 are reflectances of S2-MSI spectral bands.

Once the different algorithms were calibrated from the HydroLight database, we validated it with the [Chl-*a*] field data, selecting the best method according to different statistical parameters. If a linear trend is maintained, but away from the 1:1 line, the algorithms were recalibrated.

Calibration and validation of Z_{SD} algorithms

The attenuation of light into water bodies and the vertical visibility (water transparency) is described by the Secchi disk depth (Z_{SD}). It is linked to two optical parameters: the vertical diffuse attenuation coefficient K_d (m^{-1}) and the attenuation coefficient c (m^{-1}) (Antoine, 2010). The vertical visibility is analogous to Z_{SD} and it is the inverse of the sum K_d + c (Doron *et al.*, 2007). Austin and Petzold, (1981) estimated K_d (490 nm) from blue-green water leaving radiances. This algorithm was modified by Kratzer *et al.*, (2008) to estimate Z_{SD} for remote sensing applications (Alikas & Kratzer, 2017). The ratio 490/560 is used to map transparency over clear waters, typically in open ocean waters (Mueller, 2000; Giardino *et al.*, 2001; Antoine, 2010; Soria *et al.*, 2017b). This ratio is a good estimator of Z_{SD} in clear waters in which the phytoplankton is the main contributor to the light attenuation in the water column.

To estimate the transparency of the water in this work, we have performed a process of re-calibration of the 490/560, and 490/705 ratios, plus the hereafter called "Koponen" method (Koponen *et al.*, 2001) after testing different algorithms. We have modified the original Alikas & Kratzer (2017) algorithm. In this paper, the band ratio are not raised to the exponent b. Instead, the b coefficient is added or subtracted depending on the direction of the slope, obtained in the relation between *in situ* Secchi disk depth (Z_{SD}) measurements and band ratio. The algorithm is detailed in equation 7:

$$Z_{SD} = e\text{^} (a*\ln [Rrs\_490/Rrs\_560] + b) \quad (7)$$

where

Rrs_490 and Rrs_560 are reflectances of S2-MSI spectral bands at 490 and 560 nm.

a and b are the coefficients derived by linear regression between the Napierian logarithm of *in situ* Z_{SD} and the Napierian logarithm of 490/560 ratio.

Alikas & Kratzer (2017) applied another model based on ratio 490/705. This model had a better result (R^2 = 0.73) in the Himmerfjärden lake with a 1.9 to 7.5 m Z_{SD} and a 1.2 to 11.6 mg/m^3 [Chl-*a*] range (Baltic Sea). The algorithm is detailed in equation 8:

$$Z_{SD} = e\text{^} (a*\ln [Rrs\_490/Rrs\_705] + b) \quad (8)$$

where

Rrs_490 and Rrs_705 are reflectances of S2-MSI spectral bands at 490 and 705 nm.

a and b are the coefficients derived by linear regression between Napierian logarithm of *in situ* Z_{SD} and the Napierian logarithm of 490/705.

In more turbid waters, where other optically active constituents such as NAP and CDOM are also present in significant concentrations, other spectral regions are more sensitive for estimating the Z_{SD} (Doron *et al.*, 2007). Since this was the present situation in some reservoirs studied in ESAQS, other algorithms were also tested, such as the Koponen *et al.*, (2001) algorithm. This algorithm was validated in Finnish Lakes where the water bodies generally present Z_{SD} values of less than 3 m. We have modified the original algorithm since we have not applied the 783 band. The modified Koponen algorithm is detailed in equation 9:

$$Z_{SD} = e\text{^} (a*\ln [Rrs\_560/Rrs\_705] + b) \quad (9)$$

where

a and b are the coefficients derived by linear regression between Napierian logarithm of *in situ* Z_{SD} and the Napierian logarithm of 560/705.

The Rrs_560 and Rrs_705 are reflectances of S2-MSI spectral bands.

RESULTS

The *C* Z_{SD} measurement range in the water bodies under study was between 0.25 to 10.5 m. The range of Limnetica, 38(1): 467-479 (2019). DOI: 10.23818/limn.38.26 [Chl-*a*] measurements in the study area water bodies was between 0.54 to 169 mg/m^3.

Calibration and validation of [Chl-*a*] algorithms

In the set of simulated data used for calibration, the input [Chl-*a*] presented a very high correlation, according the coefficient of determination (R^2), with the retrieved [Chl-*a*] in all algorithms: OC2_443 with a R^2 = 0.98 (Fig. 3a); OC2_490 with R^2 = 0.97; (Fig. 3b); OC_3 with R^2 = 0.97 (Fig. 3c); and TBDO with R^2 = 0.99 (Fig. 3d). The specific calibration coefficients of each algorithm were obtained by a polynomial fit between the simulated [Chl-*a*] database and reflectance band ratios. Table 2 summarizes the coefficients of each polynomial fit.

To validate these algorithms, the data measured in the field was used. Table 3 shown this dataset. According to Guibaja *et al.* (2015), the TBDO algorithm had an optimum performance on eutrophic and hypertrophic waters. In our study area, this type of water corresponds to reservoirs with [Chl-*a*] > 10 mg/m^3 like the Albufera of Valencia, and the Bellús and Beniarrés reservoirs (Table 3). For [Chl-*a*] < 10 mg/m^3, we have applied the OC2_443, OC2_490 and OC3 algorithm on ultraoligotrophic, oligotrophic and mesotrophic waters. These water types correspond to the Benageber, Tous, María Cristina, Contreras, Sitjar and Regajo reservoirs (Table 3). The error analysis was performed between the calibrated algorithms and *in situ* [Chl-*a*] measurements. For this analysis, we have applied the mean absolute error (MAE) and a systematic direction of the error (bias). Figure 4 shows the [Chl-*a*] measured *in situ* versus the calculated with the 4 algorithms. In the OC2_443, OC2_490 and OC3 algorithms, it can be seen that the slope presented values very far from line 1:1 (0.25 and 0.30) (Fig. 4a, b and c) with a very high bias. This means that in these cases, ocean color models are overestimating the actual chlorophyll concentration, with high error values. For this reason, it was necessary to perform a recalibration process to readjust each of the models. Table 4 shows the final equation, which was obtained from the recalibration process for the [Chl-*a*] estimation, replacing the x of each adjustment (Fig. 4 a, b and c) the formulas obtained in the calibration process. For this, the value of the line slope (coefficient a) was integrated logarithmically in equation 1.

According to Table 4 data, all three algorithms provide similar statistics, but the OC3 was the algorithm which gave back the lowest error equal

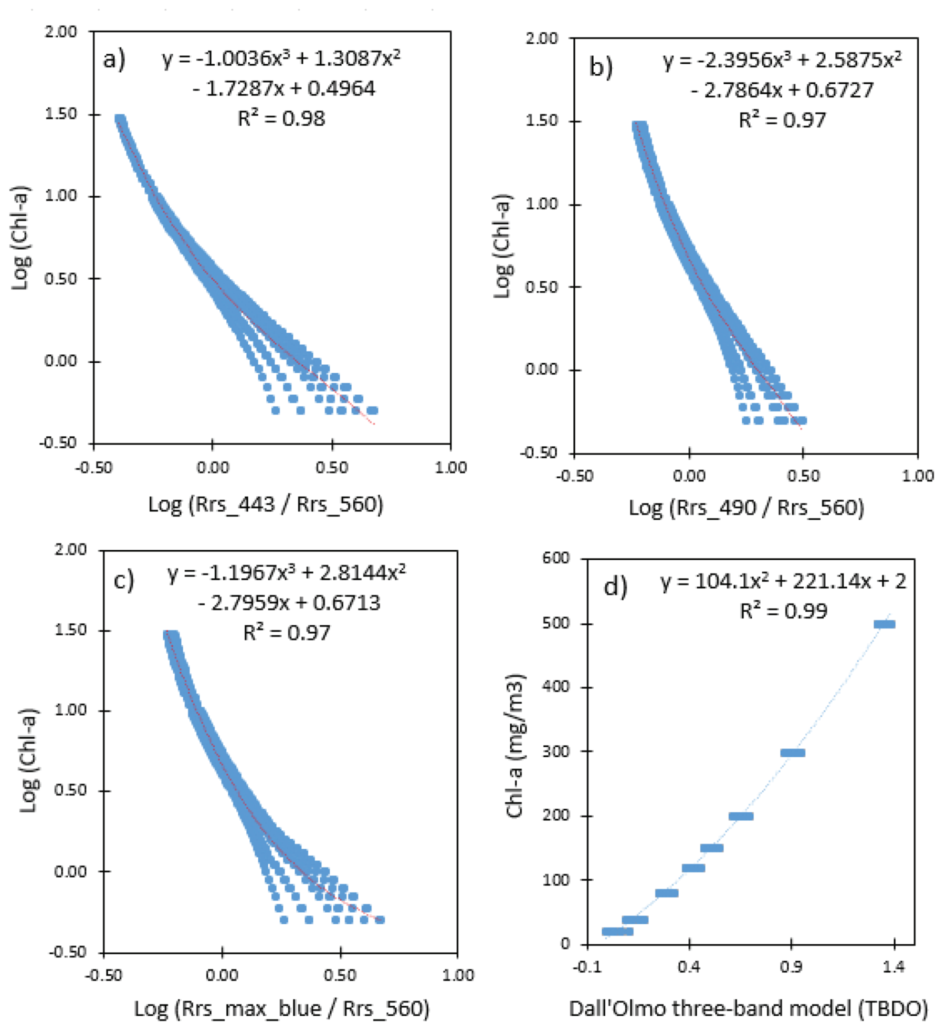

Figure 3. a) OC2_443 algorithm and simulated [Chl-*a*] polynomial fit. b) OC2_490 algorithm and simulated [Chl-*a*] polynomial fit. c) OC3 algorithm and simulated [Chl-*a*] polynomial fit, and d) TBDO algorithm and simulated [Chl-*a*] polynomial fit. *a) Ajuste polinómico entre el algoritmo OC2_443 y la [Chl-*a*] simulada. b) Ajuste polinómico entre el algoritmo OC2_490 y la [Chl-*a*] simulada. c) Ajuste polinómico entre el algoritmo OC3 y la [Chl-*a*] simulada, y d) Ajuste polinómico entre el algoritmo TBDO y la [Chl-*a*] simulada.*

Table 2. Coefficients obtained by polynomial fit for OC2_443, OC2_490, OC3 and TBDO algorithms for [Chl-*a*] estimation (in mg/m^3) from simulated HydroLight dataset. *Coeficientes obtenidos por ajuste polinomial para los algoritmos OC2_443, OC2_490, OC3 y TBDO para la estimacion de la [Chl-*a*] (en mg/m^3) a partir de una base de datos simulada con HydroLight.*

Algorithm	a	b	c	d
OC2_443	0.4964	-1.7287	1.3087	-1.0036
OC2_490	0.6727	-2.7864	2.5875	-2.3956
OC3	0.6713	-2.7959	2.8144	-1.1967
TBDO	104.1	221.1	2.0	

Table 3. Database of *in situ* [Chl-*a*] and Secchi depth disk measurements in Valencia region reservoirs and lakes according by field campaign date. *Base de datos de medidas* in situ *de [Chl-*a*] y profundidad del disco de Secchi en los embalses y lagos de la región de Valencia según fecha de campaña de campo.*

Reservoir	[Chl-*a*] (mg/m³)	Z_{SD} (m)	Date
Albufera	51.3, 53, 54.2, 31.8, 39.1, 43.1		05/08/2015
Albufera	54.8, 56.3, 56.1,52.9,55.2, 58.3		27/08/2015
Albufera	148.9, 157.9, 156, 169.1, 159.4, 154, 93.3		30/11/2015
Albufera	135.6, 138.2, 121.5, 25, 128.7	0.31, 0.31, 0.33, 0.43, 0.32	12/03/2016
Albufera	141.8, 130.4, 140.1, 114.6, 78.1, 84.4, 83.2	0.25, 0.26, 0.3, 0.35, 0.26, 0.33	21/04/2016
Albufera	70.4, 68, 22.4, 10.7, 36.4, 43.5	0.3, 0.32, 0.33, 0.34,0.34, 0.37, 0.5	02/05/2016
Tous	1.27, 1.78, 3.1	5.9, 6, 5.8	27/12/2016
Bellús	31.8	1	16/01/2017
Contreras	2, 1, 0.79, 0.83	1, 1.3, 1.07	08/02/2017
Albufera	39.7, 64.5, 45.1, 47.3	0.27, 0.32, 0.34, 0.36	07/03/2017
Beniarrés	45.45	0.95	27/03/2017
Benagéber	2.48, 2.74	4, 5.2, 7.4	30/03/2017
Ma. Cristina	1.4, 1.33	5.2, 5.6	06/04/2017
Sitjar	0.54, 0.65	9.4, 10.5	06/04/2017
Bellús	61.39, 66.76, 68.01	0.55	15/06/2017
Regajo	8.6, 8.9, 10.2	2, 1.7	05/07/2017
Sitjar	0.68, 0.61	2.7, 3.15	23/10/2017
Benageber	5.4, 5.76, 4.57	3.4, 3.6, 4.1	26/10/2017
Beniarrés	11.13, 17.17	1.15, 1.4	07/11/2017
Tous	0.64, 0.72, 0.69	7.1, 8, 9.1	17/11/2017
Contreras	2.08, 2.42, 2.02, 0.86, 0.98	4.1, 5	30/11/2017
Tous	0.63, 0.58, 0.69	7, 7.75, 8.1	16/01/2018
Ma. Cristina	2.92, 2.72	0.75, 0.75	31/01/2018
Sitjar	0.59, 0.63	2.4, 2.2	31/01/2018
Benageber		4.3, 4.85, 5.5	23/02/2018
Albufera	84.5, 82.1, 81.6	0.31, 0.33, 0.30	07/03/2018
Bellús	41.54, 51.59, 49.09	0.45, 0.45, 0.5	22/03/2018
Regajo	5.57, 4.58, 4.63, 5.12	3, 3.75, 4, 4.25	11/05/2018
Benageber	4.91, 4.91, 4.85, 4.53	3.35, 3.35, 3.7, 3.75	16/05/2018

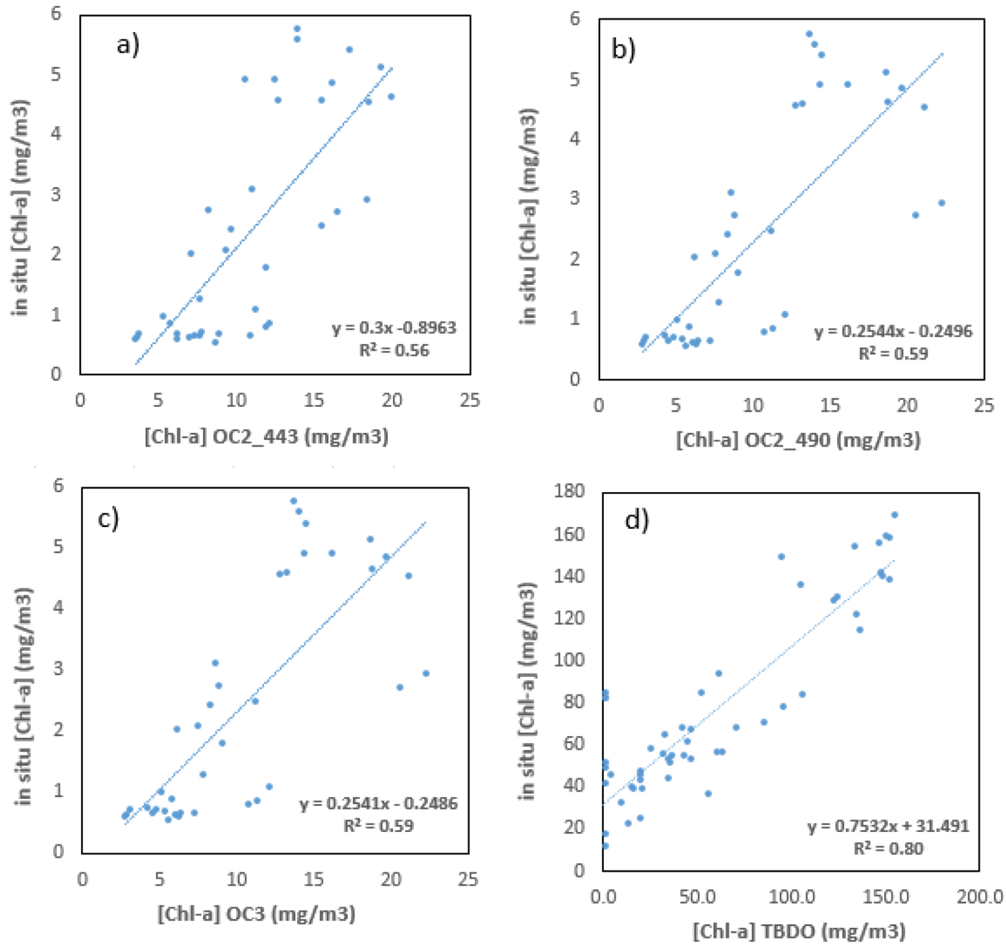

Figure 4. a) OC2_443 algorithm and *in situ* [Chl-*a*] validation. b) OC2_490 algorithm and *in situ* [Chl-*a*] validation. c) OC3 algorithm and *in situ* [Chl-*a*] validation, and d) TBDO algorithm and *in situ* [Chl-*a*] validation. *a) Validación del algoritmo OC2_443 en relación a la [Chl-*a*]* in situ. *b) Validación del algoritmo OC2_490 en relación a la [Chl-*a*]* in situ. *c) Validación del algoritmo OC3 en relación a la [Chl-*a*]* in situ*, and d) Validación del algoritmo TBDO en relación a la [Chl-*a*]* in situ.

to 0.89 mg/m^3. However, the OC2_490 model also has very good results, with the same correlation as OC3 and the advantage that it is easier to calculate, saving processing time and using only one blue band, versus OC3 that he need to use both.

For eutrophic waters with [Chl-*a*] > 10 mg/m^3, the TBDO algorithm (Fig. 4d) gave an $R^2 = 0.80$, a bias = 17.49 and an MAE = 23 mg/m^3, which is a relative low error for high [Chl-*a*] waters, taking into consideration the range of values for this group (10 to 169 mg/m^3). We consider it acceptable for the evaluation of the ecological status in these eutrophic or hypertrophic reservoirs (Guibaja *et al.*, 2016). The validated TBDO algorithm was applied to an S2-MSI image from the Albufera of Valencia acquired on 07/03/2018. This S2-MSI image was atmospherically corrected with Sen2-Cor. Fig. 5 shows the patterns of [Chl-*a*] concentration with medium to high values in nearly the entire lake with a [Chl-*a*] TBDO, between 75 and 90 mg/m^3. The same day, the *in situ* [Chl-*a*] measurements recorded in the Albufera of Valencia were between 81.6 to 84.5 mg/m^3 (Table 3). The green areas correspond to the water contributions with less chlorophyll-*a* coming from the irrigation channels renovating the water, while the central area corresponds to stagnant water, which leads to higher values of [Chl-*a*].

Table 4. Equations for the [Chl-*a*] estimation (in mg/m^3) in the calibration process. *Ecuaciones para la estimación de la [Chl-*a*] (en mg/m^3) en el proceso de calibración.*

Algorithm	**Equation** ([Chl-*a*] in mg/m^3)	**MAE**	R^2
OC2_443	[Chl-*a*] = 10^(-0.02648-1.7287*X+1.3087*X^2-1.0036*X^3)-0.8963	0.93	0.56
OC2_490	[Chl-*a*] = 10^(0.078217-2.7864*X+2.5875*X^2-2.3956*X^3)-0.2496	0.90	0.59
OC3	[Chl-*a*] = 10^(0.076305-2.7959*X+2.8144*X^2-1.1967X^3)-0.2486	0.89	0.59

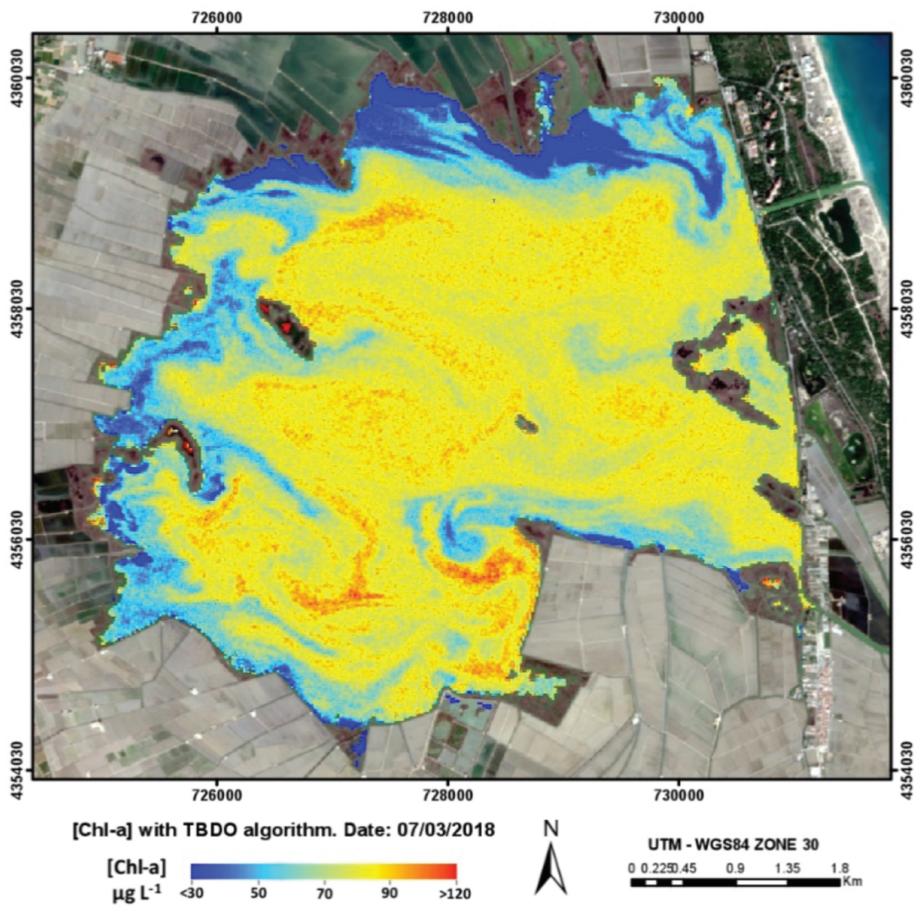

Figure 5. [Chl-a] map by TBDO algorithm in the Albufera of Valencia from S2-MSI image of 07/03/2018. *Mapa de [Chl-a] aplicando el algoritmo TBDO en la Albufera de Valencia obtenido de la imagen S2-MSI del 07/03/2018.*

Calibration and validation of Z_{SD} algorithms

The calibration-validation process of algorithms for the Z_{SD} estimation, has been based on the relationship between the 490/560, 490/705 and 560/705 ratios and *in situ* Z_{SD} measurements. Inspired by the algorithms described earlier, we have tested several regression models. The dataset collected in field campaigns over the study area consist of 79 measurements. It has a wide Z_{SD}

range from 0.25 to 10 m. For the calibration and validation process, the dataset was divided into 2 groups: 75 % of the data (N = 60) was used to calibrate and 25 % (N = 19) to validate the ratios. In a first attempt, we tested the three algorithms applying the trophic classification followed in the [Chl-*a*] algorithm calibration, differentiating ultraoligotrophic-mesotrophic waters and eutrophic-hypertophic waters, but the results were not optimum due to the limited dataset used.

Figure 6 shows the results of the calibration process. Here, the logarithm of measured Z_{SD} is represented, depending on the logarithm of each of the three indices. In Fig. 6 it is observed that the best fit is the linear one, and that for the calibration process, the 490/705 and 560/705 ratios showed the best performance in both cases.

To validate the Z_{SD} algorithms, we applied the coefficients obtained in the calibration process to the different band ratios, as explained earlier. The validation data set consists of 19 measurements (25 % of total). Figure 7 show the results. To select the best method, Table 5 shows the three formulas obtained in the calibration process and the statistics of the validation process. Considering all the statistics, the algorithm with the lowest error and the best correlation is 490/705.

According to these results, the 490/705 ratio is the most appropriate for estimating Z_{SD} with an error MAE of 0.88 m. We have applied this algorithm on the same S2-MSI scene that was used in the application of the [Chl-*a*] algorithm. We obtained a map that shows the different values of the water transparency of this hypertrophic lake (Fig. 8). For the Albufera of Valencia (Fig. 5 and Fig. 8), it can be observed that according to the 490/705 ratio, a vast majority of the lagoon had values between 0.30 to 0.36 meters. Once again, the correct match-up with the *in situ* Z_{SD} was confirmed. According to the data measured this day, the Z_{SD} was between 0.30 and 0.33 m (Table 3).

As can be seen in the [Chl-*a*] and the Z_{SD} maps, the expected relationship between the minimum value of chlorophyll concentration and maximum water transparency is given in areas near shoreline. In the northern region, the concentration of chlorophyll is minimum, taking into account the values normally measured in Albufera of Valencia (See Table 3). Here the values are between 50 to 70 mg/m^3, coinciding with maximum transparency, Z_{SD} up to 0.38 meters, again matching-up with the values registered in this lagoon (Table 3). This high transparency is probably due to the early opening of water gates for rice crops that usually starts in May.

DISCUSSION

To estimate [Ch-*a*] and according to the error analysis (MAE = 0.89 mg/m^3), the OC2_490

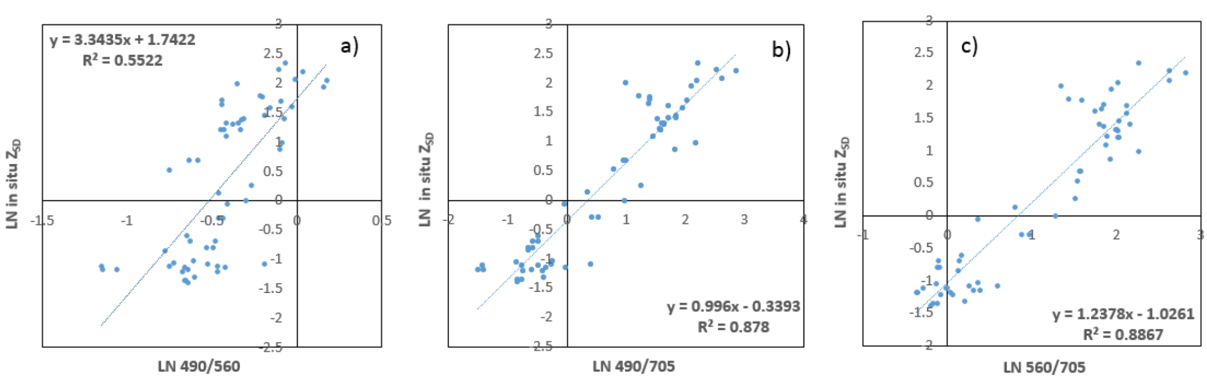

Figure 6. Calibration of the Z_{SD} algorithms. a) 490/560 algorithm and *in situ* ln(Z_{SD}) linear fit. b) 490/705 algorithm and *in situ* ln(Z_{SD}) linear fit. and c) 560/705 algorithm and *in situ* ln(Z_{SD}) linear fit. *Calibración de los algorimos para Z_{SD}. a) Ajuste lineal entre el algoritmo 490/560 y ln(Z_{SD})* in situ. *b) Ajuste lineal entre el algoritmo 490/705 y ln(Z_{SD})* in situ, *y c) Ajuste lineal entre el algoritmo 560/705 y ln(Z_{SD})* in situ.

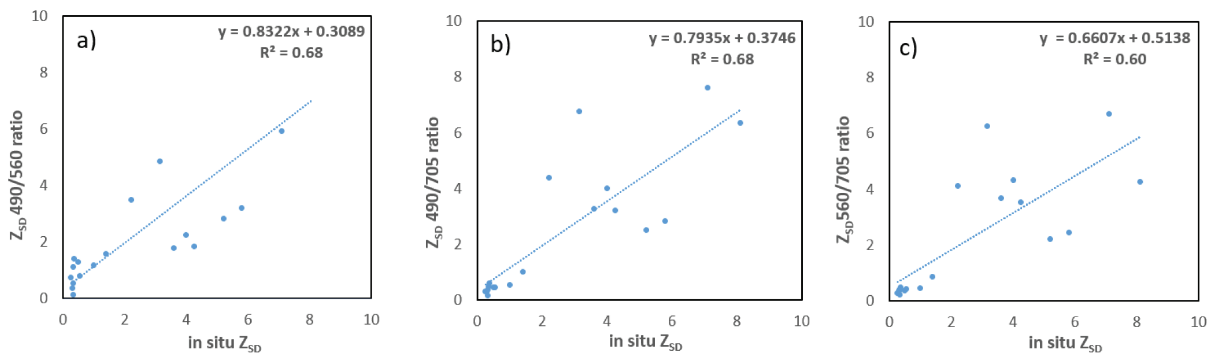

Figure 7. Validation of the Z_{SD} algorithms. a) Z_{SD} calculated with the 490/560 ratio in relation with *in situ* Z_{SD}. b) Z_{SD} calculated with the 490/705 ratio in relation with *in situ* Z_{SD} validation. c) Z_{SD} calculated with the 560/705 ratio in relation with *in situ* Z_{SD}. *Validación de los algorimos para* Z_{SD}*. a)* Z_{SD} *calculada con el ratio 490/560 en relación a* Z_{SD} *medida* in situ*. b)* Z_{SD} *calculada con el ratio 490/705 en relación a* Z_{SD} *medida* in situ*. c)* Z_{SD} *calculada con el ratio 560/705 en relación a* Z_{SD} in situ.

Table 5. Equations for the Z_{SD} estimation and statistics of the validation process. *Ecuaciones para la estimación de* Z_{SD} *y estadísticos del proceso de validación.*

Algorithm	**Equation** (Z_{SD} in m)	**R²**	**MAE**	**Bias**
490/560	Z_{SD} = e^(3.3435*ln (Rrs_490/Rrs_560) + 1.7422)	0.68	1.16	0.12
490/705	Z_{SD} = e^(0.996*ln (Rrs_490/Rrs_705) - 0.3393)	0.68	0.88	0.15
560/705	Z_{SD} = e^(1.2378*ln (Rrs_560/Rrs_705) -1.0261)	0.60	0.96	0.35

algorithm should be preferred for low values ([Chl-*a*] = < 10 mg/m³), as is the case of the reservoirs of Benagéber, Contreras, Sitjar, Tous, Beniarrés, María Cristina and Regajo. While Ocean Color algorithms have a longer tradition in ocean studies, the optimum results achieved in this study suggest they could have broad applicability on some types of inland waters. The validation of the TBDO algorithm gave a good result in eutrophic to hypertrophic water mass with [Chl-*a*] > 10 mg/m³, such as the Albufera of Valencia and the Bellús reservoir. The results obtained in this study ratify the ones obtained by Guibaja *et al.* (2016) on the applicability of this algorithm on eutrophic to hypertrophic water masses. The match-up obtained between the TBDO application over the S2-MSI image and the values measured *in situ* the same day confirms the validity of the TBDO algorithm in water masses with high value of chlorophyll-*a*.

To estimate the Z_{SD}, we have obtained an optimum result with the 490/705 band ratio. While it is true that the environment and natural conditions between the Baltic Sea and the reservoirs of the Valencia region are different, the Z_{SD} range (0.25 to 10.5 m) measured in our study area is similar to that measured by Alikas & Kratzer (2017) in Himmerfjärden Lake (1.9 to 7.5 m). As happened with the [Chl-*a*], the match-up obtained between the 490/705 ratio application over the S2-MSI image and the values measured *in situ* the same day confirms the validity of this algorithm in water masses with lower water transparency value.

Regarding the applicability of the three algorithms by trophic states as we did for the [Chl-*a*] algorithms, we concluded that is not appropriate due to a) the limited dataset for the calibration-validation process and b) the composition of suspended solids of water, due to similar Z_{SD}

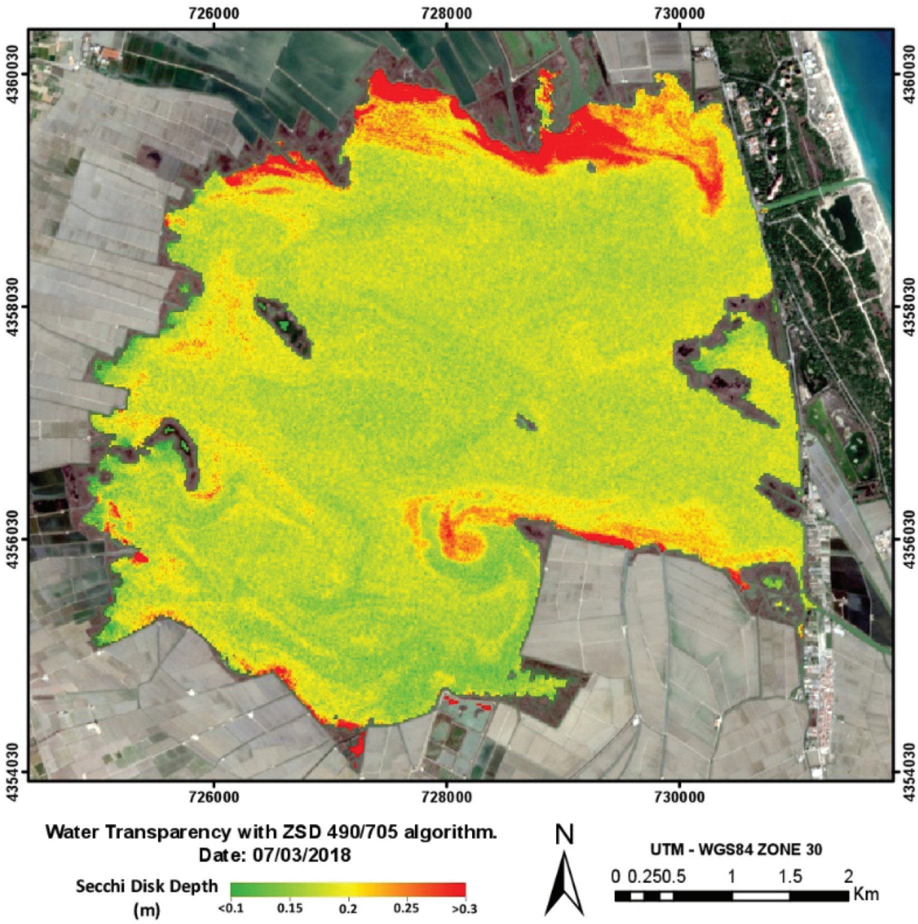

Figure 8. Z_{SD} map by 490/705 ratio in the Albufera of Valencia. S2-MSI image of 07/03/2018. *Mapa de Z_{SD} aplicando el ratio 490/705 en la Albufera de Valencia. Imagen S2-MSI del 07/03/2018.*

values have different [Chl-*a*]; this is produced by the presence of NAP giving turbidity to water but without pigments. In this way, Yang *et al.* (2013) also proposed two quasi-analytical algorithms to retrieve total absorption and backscattering coefficients based on a semi-analytical estimation model for clear and turbid inland waters, and these models could be proved in future works. There are many works were Z_{SD} is not well estimated, as Devi Prasad & Siddaraju (2012) in some Indian hypertrophic lakes; Borkman & Smayda (1998) in coastal areas of Rhode Island and Lahtrop (1992) were algorithms derived from samples in Lake Michigan cannot be extrapolated to Yellowstone and Jackson Lakes.

CONCLUSIONS

The accuracy of the algorithms estimated in the reservoirs studied so far is sufficient for most of the applications related to the ecological status assessment. The S2-MSI images showed that they are optimum for performing ecological monitoring on inland waters from space.

It is important to emphasize the relevance of the atmospheric correction method used: Sen2-Cor, which in our case was accurate enough, allows the algorithms to be applied to actual S2-MSI data for routine monitoring purposes, which is the ultimate goal of the ESAQS project. In this context, the next step of the research is to evaluate and validate several atmospheric correction methods for different types of inland water in order to determine the one best suited for achieving the ESAQS objectives.

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