

Evaluation of MODIS-Aqua and OLCI Chlorophyll-*a* products in contrasting waters of the Southwestern Atlantic Ocean

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Satellite chlorophyll-*a* concentration (Chl-*a*) estimations provide a valuable tool to study marine phytoplankton dynamics with unprecedented spatial and temporal coverage. Standard empirical Chl-*a* algorithms perform well where phytoplankton is the dominant optically active component in seawater, but usually fail in those regions where there is a high optical influence from multiple dissolved and particulate components that are not covariant with Chl-*a* (Prieur and Sathyendrenath, 1981). Therefore, in coastal regions, where colored dissolved and suspended particulate matter are dominant, it is crucial to perform an accuracy assessment of satellite Chl-*a* products to ensure their reliable use.

The water masses on the Northern Patagonian continental shelf (Figure 1) have sub-Antarctic

origin, mixed with regional coastal inputs, and are influenced by the temperate thermal cycle and NW prevailing winds, making this region a complex oceanographic and ecological system (Lucas et al., 2005). Its coastal zone presents temperate (15°C), high saline (35) and turbid waters (35 NTU) with pronounced seasonal variability (Delgado et al., 2017). The Bahía Blanca Estuary is a tidally dominated, turbid and mixed system that is a main source of fine sediment to the inner shelf (Menendez et al., 2016) towards the eastern coastline (Delgado et al., 2017). Phytoplankton is mainly dominated by diatoms, comprising more than the 50 % of the cell abundances and biomass, followed by dinoflagellates (Guinder et al., 2018) and coccolithophores, both also highly abundant (Guinder et al., 2018; Delgado et al., 2019).

Long term field studies are quite scarce in the Argentine Sea, given the limited financial resources for oceanographic research, emphasizing the relevance of reliable Chl-*a* estimations derived

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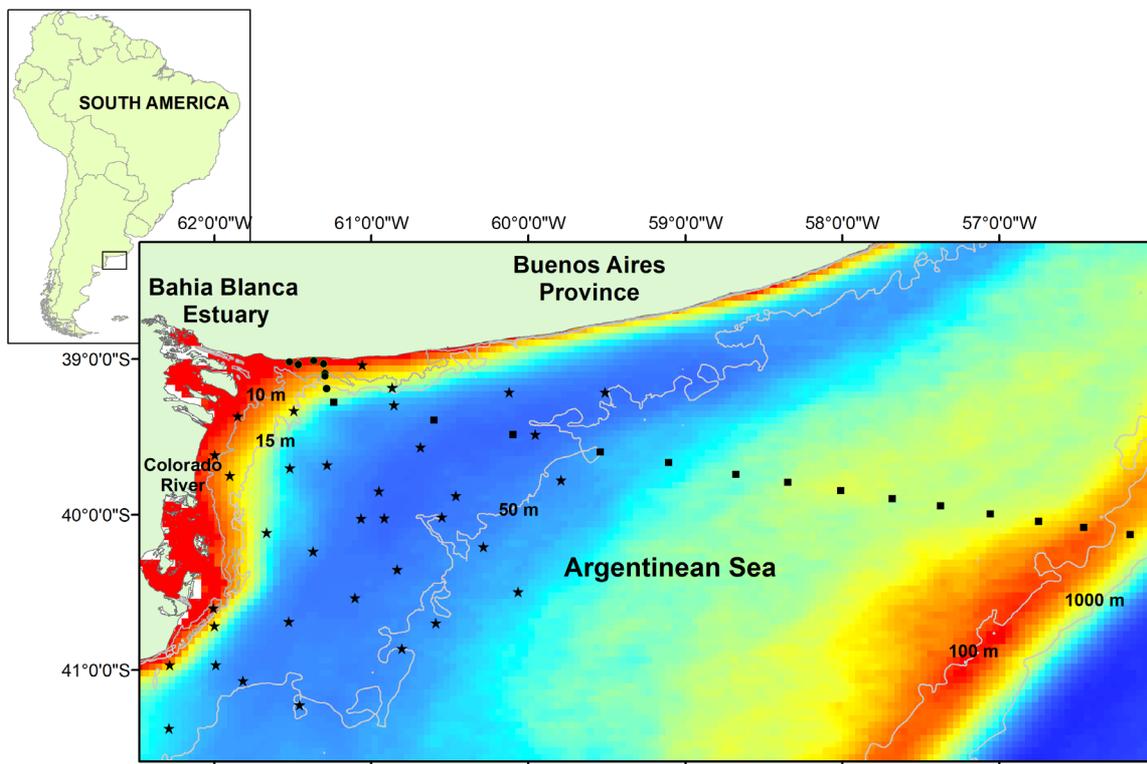


Figure 1. Location of study area in the northern Patagonian continental shelf and sampling sites. Black circles indicate sites sampled in the coastal area ($z < 15$ m, $N = 28$) collected between November 2013 and March 2017. Black stars are stations collected from the R/V Dr. Bernardo Houssay and ARA Puerto Deseado ($N = 49$) in October 2010, April 2012, April 2013 and black squares are sites collected in March 2019 on the PNA Dr. Bernardo Houssay ($N = 16$).

from satellite data. Therefore, the objective of the present study is to test, for the first time in this optically complex area, using multiple atmospheric corrections and algorithms, several different Chl-*a* products derived from the Moderate Resolution Imaging Spectroradiometer on board Aqua (MODIS-Aqua) and the Ocean and Land Color Instrument on board Sentinel 3 (OLCI-Sentinel 3) using in situ Chl-*a*.

Sampling was performed either from fishing boats or during dedicated oceanographic cruises, collecting a total of 93 surface samples. From November 2013 to March 2017, 28 samples were collected in the permanent sampling area located in the coastal zone (39°S – 62.5°W ; 41.5°S – 60°W) from local artisanal fishing boats (red dots in Figure 1). During four oceanographic cruises, 65 samples were collected in October 2010, April 2012, April 2013 and March 2019 from the R/V Dr. Bernardo Houssay and ARA Puerto Deseado on the continental shelf (Figure 1, black and

green stars). Field Chl-*a* was estimated after filtering between 100 and 200 ml of seawater through Whatman GF/F filters, depending on water turbidity. Immediately after filtration, the filters were wrapped in aluminum foil and stored in an ultra-low freezer at -80°C until laboratory analysis. Photosynthetic pigments were extracted with 90% acetone for 24 h in the darkness at -20°C . Chl-*a* was determined by fluorimetry after Holm-Hansen et al. (1965) with a Shimadzu RF-5301 spectrofluorophotometer using the excitation and emission bands centered at 460 and 671 nm, respectively.

Daily MODIS-Aqua level 1A data at 1.1 km spatial resolution for the sampling dates were downloaded from the Ocean Color web site (<http://oceancolor.gsfc.nasa.gov>) and were processed using SeaDAS 7.4 software to obtain L2 Chl-*a* product using the OC3M algorithm (O'Reilly et al., 2000) and a switching atmospheric correction (AC) algorithm that uses the

near infrared (NIR) or the short-wave infrared (SWIR) bands (NIR/SWIR-OC3M). Following the good results obtained by Delgado et al. (2019) in this study area, the NASA standard AC algorithm that uses NIR bands (Stumpf et al., 2003; Bailey et al., 2010) was applied to stations located offshore (> 10 km from the coast), while the alternative AC algorithm that uses SWIR bands was applied to pixels located less than 10 km from the coast (Wang and Shi, 2005). Given the presence of turbid waters in the region, the high total radiance mask (HILT) was not applied and the cloud-masking was performed using the Rayleigh-corrected reflectance (dimensionless) at 2130 nm with a threshold of 0.018.

Daily OLCI-Sentinel 3A and B level 2 (L2-WFR) images for the sampling dates at 300 m spatial resolution were downloaded from the Eumetsat web page (<https://coda.eumetsat.int/>) and the chl_OC4Me and chl_nn Chl-*a* products were evaluated. The chl_OC4Me product, developed for Case-1 waters, is calculated using a combination of the baseline and the bright pixel (Antoine and Morel, 1999, Moore et al. 1999) atmospheric correction combination (BAC/BPAC) and the Chl-*a* semi-analytical maximum band ratio OC4Me algorithm, originally designed for the MERIS sensor (Morel et al., 2007). The chl_nn alternative product for Case-2 waters is calculated using an alternative AC developed for complex waters (AAC) based on an artificial neural network (Doerffer and Schiller, 2007) from which Chl-*a* concentration is derived through an Inverse Modelling Technique.

The match-up procedure consisted of extracting a box of 3 x 3 pixels centered at the location of the in situ measurements. A match-up was accepted only if more than 6 out of 9 pixels of the box were valid considering the standard flags. Then, a spatial uniformity criterion was applied based on the coefficient of variation (cv), the ratio of the standard deviation to the mean pixel value of the box, where match-ups with $cv > 0.3$ were discarded. A time difference window of ± 6 h between the satellite overpass and the in situ measurements was considered for the mid-shelf region (not influenced by tidal forces), while for coastal stations (< 10 km from the coast) a time difference window of ± 2 h was used to avoid the possible influence of the tide.

To compare the performance of the different Chl-*a* products, linear regressions were performed; the slope, intercept, and coefficient of determination (R^2)

were computed on log-transformed satellite and in situ Chl-*a* data, because bio-optical data is known to have a log-normal distribution (Campbell et al., 1995). After analysis, the results were back transformed to linear space for interpretation (Seegers et al., 2018). The statistical errors considered were the root-mean-square error (RMSE) (Equation 1), bias (Equation 2), and the percentage error (PE) (Equation 3), defined as follows:

$$RMSE = 10 \sqrt{\frac{1}{n} \sum [\log y - \log x]^2} \quad (1)$$

$$bias = 10 \frac{1}{n} \sum (\log y - \log x) \quad (2)$$

$$PE = \frac{1}{n} \sum (|y - x|) * 100 \quad (3)$$

where x is the in situ measured value, y the satellite estimated value and n the number of match-ups.

For the analyzed period measured, Chl-*a* values varied between 0.22 and 7.03 mg m⁻³ with a mean value of 1.64 mg m⁻³. From the total of 93 samples collected for the whole study area, only 41 remained as valid match-ups after applying the exclusion criteria previously described. Considering all match-ups ($N=41$), the MODIS-Aqua NIR/SWIR-OC3M product showed a poor correlation with in situ data ($R^2 = 0.39$; black line and equation in Figure 2A). Even though the slope is close to 1, large errors indicate a poor performance of the algorithm with high scatter ($RMSE = 1.65$, $PE = 118\%$) and a clear tendency to overestimate in situ data, as indicated by the bias (1.18). This result is expected as more than half of the samples were collected within the coastal zone ($z < 15$ m; $N=23$; $R^2 = 0.21$, red symbols in Figure 2A), characterized by turbid waters (Delgado et al., 2017; 2019), where Chl-*a* empirical algorithms usually tend to fail (O'Reilly et al., 2000). Within this coastal zone ($z < 15$ m), SPM concentrations varied between 30-100 mg l⁻¹ (Delgado et al. 2019) and the composition of the phytoplankton community was highly variable. It was dominated by large chain-forming diatoms (40-80 % of total abundance), with a relatively low specific absorption coefficient (mean 0.032 (m² mg Chl-*a*)⁻¹) due to the packaging effect (Delgado et al., 2019). This zone is also characterized by the regular presence of coccolithophorid species *Gephyrocapsa oceanica* (Delgado et al., 2019, Guinder et al., 2018),

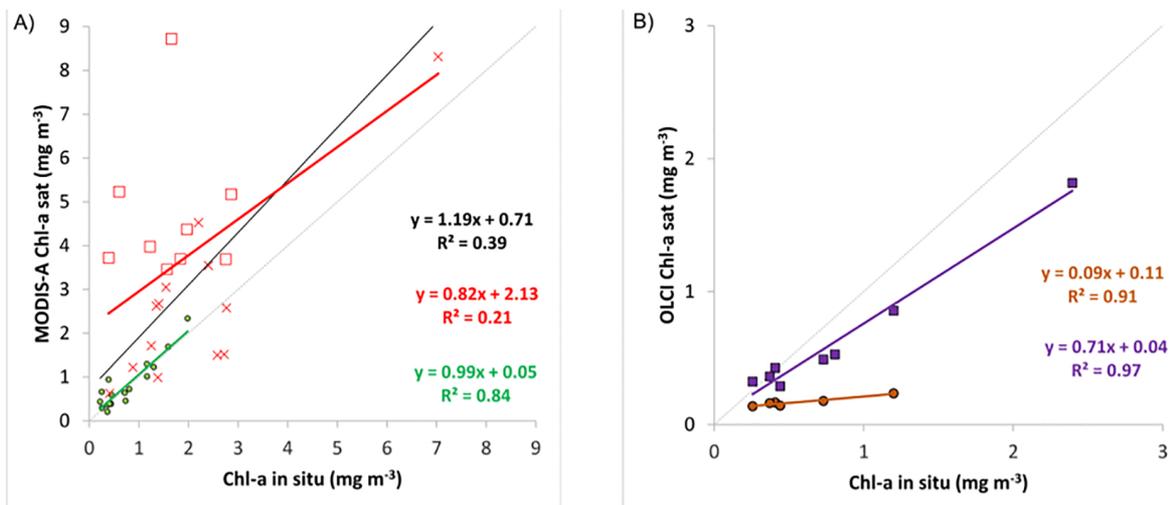


Figure 2. Comparison between in situ and satellite-derived Chl-*a* on the Northern Patagonian continental shelf. A) MODIS-Aqua NIR/SWIR-OC3M product linear regression considering all data (black line and equation); Color coded symbols indicate stations located deeper than 15 m depth (green) and coastal stations (red). For the coastal stations, squares indicate stations located less than 10 km from the coast (SWIR AC). Crosses indicate stations located > 10 km from the coast (NIR AC). B) OLCI-Sentinel 3 Chl-*a* chl_nn (orange) and chl_OC4Me (purple) products at offshore stations (> 15 m). The coefficient of determination (R^2) is shown.

which could cause high back-scattering on satellite imagery due to their calcified cell structure (Brown and Yoder, 1994). In turn, when only stations located offshore from the 15 m isobath were considered, the OC3M algorithm showed the best performance (Figure 2A green symbols). For these stations, waters have typically lower SPM concentrations (< 6 mg l⁻¹; Delgado et al., 2019) and low CDOM absorption values (443) (0.06 – 0.13 m⁻¹; unpublished results Maximiliano Arena). Phytoplankton communities in these stations were dominated by dinoflagellates, smaller cells corresponding to the nanoplankton size class (Guinder et al., 2018). In the offshore waters, match-ups showed a better fit ($R^2 = 0.84$) and lower errors (bias = 1.09 and PE = 16 %) than those observed in the coastal zone alone or for all the data pooled together (Figure 2A, Table1), with estimates closer to the 1:1 line. The AC performance could not be evaluated at this study due to the lack of radiometric measurements; nevertheless, based on previous results (Delgado et al., 2019), showing good performances in offshore waters and high errors in coastal waters (disregarding the bands used for the AC: NIR or SWIR), we can infer that AC is not a major issue. On the other hand, high SPM values, variations in pigment packaging, species composition, and variable CDOM concentrations (not

reported here) relative to phytoplankton biomass, seem to be the main causes of the poor performance of Chl-*a* estimation in the near-coastal area using the standard empirical algorithm leading to a general overestimation of the measured Chl-*a*.

Sentinel 3 images are available since November 2017, thus OLCI derived Chl-*a* products were only tested using in situ Chl-*a* determinations obtained during the oceanographic cruise on board the R/V Dr. Bernardo Houssay in March 2019 with offshore data ($z > 15$ m, Figure 1, green stars). The Case-2 water neural network Chl-*a* product (chl_nn) rendered a good fit ($R^2 = 0.91$) and low scatter around the regression line, but it largely underestimated Chl-*a* values (PE = 39 %), not representing well the measured Chl-*a* range (Figure 2B, orange). In turn, the standard Case-1 water OLCI OC4Me product presented the best fit ($R^2 = 0.97$) and the lowest errors (PE = 21 %), with predicted values closer to the 1:1 line (Figure 2B, purple). A slight underestimation of the in situ data can be observed, which may result from the reported tendency of OLCI L2 products to underestimate the water-leaving radiance (Zibordi et al., 2018).

It can be concluded that the standard MODIS-Aqua (OC3M) and OLCI (OC4Me) Case-1 waters products are reliable in the inner shelf and mid-shelf ($z > 15$ m) of the Southwestern Buenos Aires Province (Figure 1).

Table 1. Statistical results of the performance of MODIS-Aqua and OLCI-Sentinel 3 Chl-*a* products evaluated on the northern Patagonian Shelf. R^2 = coefficient of determination; RMSE = root mean square error; PE = percentage error; N = number of match ups; z = depth (m).

Depth (m)	MODIS-Aqua			OLCI-Sentinel 3	
	NIR/SWIR-OC3M			chl_nn	chl_OC4Me
	All data	z < 15	z > 15	z > 15	z > 15
R^2	0.39	0.21	0.84	0.91	0.97
Slope	1.19	2.13	0.99	0.097	0.71
Intercept	0.71	0.82	0.05	0.11	0.04
bias	1.18	1.52	1.09	0.39	0.8
RMSE	1.65	2.31	1.51	3.14	1.36
PE (%)	118	203	16	39	21
N	41	23	18	6	8

Environmental or monitoring studies can be performed considering this highly valuable data with confidence knowing there is only a slight underestimation of Chl-*a* in situ values for concentrations above 1 mg m⁻³. For the coastal zone located in shallow waters (z < 15 m), the Case-1 water MODIS-Aqua OC3M Chl-*a* product completely fails to reproduce the in situ fluorometric Chl-*a* (mg m⁻³) values, evidence of the need to develop specific algorithms in these turbid and optically complex waters.

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AUTHOR CONTRIBUTIONS

AA.L.D.: Conceptualization; Investigation; Writing original draft; Writing - review & editing.

P.D.P.: Funding Acquisition; Writing - review & editing.

A.D.: Conceptualization; Writing - review & editing.

M.A.: Investigation; Writing - review & editing.

C.C.: Writing - review & editing.

J.E.G.C.: Investigation; Writing - review & editing.

A.M.: Investigation; Writing - review & editing.

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