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An improved algorithm for estimating chlorophyll-a in coastal waters of southern Brazil from multispectral satellite images

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ABSTRACT

Remote sensing chlorophyll-A (CLA) estimates from global models have been used to support decision making in southern Brazil, the most important bivalve mollusks production region (~9 thousand tons in 2022) in the country, and a recent study indicated that these estimates poorly represent the actual levels of CLA. The aim of the study was to develop an improved algorithm for estimating CLA in these coastal waters from multispectral images. A CLA database generated in situ between 2007 and 2009 was used to calibrate and validate algorithms based on spectral data from the Medium Resolution Imaging Spectrometer (MERIS) (ENVISAT satellite) (300m spatial resolution), including algorithms based on red and near-infrared bands: two bands (2B and M2B), three bands (3B) and the Normalized Difference Chlorophyll Index (NDCI and MNDCI). Outputs from the global models OC4ME and Neural Network were also evaluated. NIR-red algorithms outputs correlated significantly with the measured CLA, except for MNDCI. The best performing models during the calibration, those based on 2B and NDCI ($R^2 = 0.37$, residual standard error = 2.57 mg.m⁻³), were validated and fitted better the measured data ($R^2 \geq 0.22$) and showed lower RMSE values (around 2.5 mg.m⁻³) than the global models' outputs, which did not even correlate significantly ($p > 0.05$) with in situ CLA measurements. The developed models performed better than the global models evaluated nevertheless they have a limited prediction power when compared to regional algorithms developed elsewhere and this is probably linked to the low range of CLA measurements used to train the models.

Keywords: Remote sensing, Algae blooms, Monitoring, Cross validation.

Um algoritmo aprimorado para estimativa de clorofila-a em águas costeiras do Sul do Brasil a partir de imagens multiespectrais satelitares

RESUMO

Estimativas de sensoriamento remoto de clorofila-A (CLA) de modelos globais têm sido usadas para apoiar a tomada de decisões no sul do Brasil, a mais importante região de produção de moluscos bivalves (~9 mil toneladas em 2022) do país, e um estudo recente indicou que essas estimativas representam mal os níveis reais de CLA. O objetivo do estudo foi desenvolver um algoritmo aprimorado para estimar a clorofila-a nessas águas costeiras a partir de imagens multiespectrais. Um banco de dados CLA coletado in situ entre 2007 e 2009 foi utilizado para calibrar e validar algoritmos baseados em dados espectrais do Espectrômetro de Imagem de Média Resolução (MERIS) (satélite ENVISAT) (resolução espacial de 300m), incluindo algoritmos baseados em bandas vermelhas e infravermelhas próximas: duas bandas (2B e M2B), três bandas (3B) e o Índice de Clorofila por Diferença Normalizada (NDCI e MNDCI). Previsões dos modelos globais OC4ME e Rede Neural também foram avaliadas. Os resultados dos algoritmos NIR-red correlacionaram-se significativamente com o CLA medido, exceto para MNDCI. Os modelos com melhor desempenho durante a calibração, aqueles baseados em 2B e NDCI ($R^2 = 0,37$, erro padrão residual = 2,57 mg.m⁻³), foram validados e ajustaram-se melhor aos dados medidos ($R^2 \geq 0,22$) e apresentaram menores valores de RMSE (cerca de 2,5 mg.m⁻³) do que os resultados dos modelos globais, que nem sequer se correlacionaram significativamente ($p > 0,05$) com as medições in situ de CLA. Os modelos desenvolvidos tiveram um desempenho melhor do que os modelos globais avaliados, no entanto têm um poder de previsão limitado quando comparados com algoritmos regionais desenvolvidos noutros locais e isto está provavelmente ligado à baixa gama de medições de CLA utilizadas para treinar os modelos.

Palavras-chave: Sensoriamento remoto, Floração de algas, Monitoramento, Validação cruzada.

Introduction

Algal blooms are a natural phenomenon which have become increasingly prevalent in lakes, reservoirs, and oceans due to environmental changes promoted by human activities. These blooms pose significant threats to the environment and human health (XIAO et al., 2024). The emergence of this phenomenon is influenced by several environmental factors (Ninio et al., 2020), including the nutrient content of waters. Nutrients, such as nitrogen (N) and phosphorus (P), play a crucial role in determining the algal growth (Bonilla et al., 2023; Wang et al., 2022), influencing algal population dominance and gene expression.

In aquatic environments, these nutrients are commonly found in coastal regions. Coastal waters, especially those located near estuaries, are the most productive in the oceans because they are shallow, have high water temperatures, and high nutrient content brought by rivers (Pinto et al., 2019). Oceanic processes are also responsible for supplying nutrients to these regions, through ocean currents and upwelling events (Simões et al., 2021). Given these characteristics, coastal waters are susceptible to sudden and significant increases in microalgae concentrations and, when these events cause adverse impacts on the environment, they are called Harmful Algal Blooms (HAB) (Schramm and Proença, 2005). Among these impacts, toxins produced by some species of algae can accumulate in the food chain, causing fisheries closures, as well as disease or mortality of marine species and humans (Dai et al., 2023). Toxic syndromes caused by human consumption of bivalve shellfish that have ingested toxin-producing phytoplankton are a public health risk found worldwide.

HAB surveillance programs have been implemented worldwide with the goal of protecting public health by monitoring and providing early warning of toxic HABs. Essentially, these programs involve periodical field sampling (You et al., 2022) to measure the concentration of toxic cells in water samples (You et al., 2022, Ruiz-Villarreal et al., 2022) and toxin levels in shellfish tissue. Additional parameters are commonly recorded to correlate phytoplankton fluctuations with secondary variables such as total phytoplankton density and chlorophyll-A (CLA) concentration (Nazeer et al., 2017). Generating these data can be expensive and laborious. Toxic cell counts or total phytoplankton density typically require analysis under a microscope in a laboratory. The probes can read the CLA spectrum present in phytoplankton in situ and in real time, due to the

interaction of light with photosynthetic pigments, such as CLA, the main pigment of microalgae (Kirk, 2011). However, the required equipment can be expensive and maintaining these probes in the water at all monitoring points required by a HAB surveillance program can be challenging.

In this scenery, the use of CLA estimates generated by remote sensing to help detect and determine the extent of HAB has become a relevant research topic (Bresciani et al., 2018). This type of data offers advantages such as low cost, constant availability, and its synoptic vision, which allows analyzing large areas in the same image (Hunter et al., 2008). With advances in computer technology, modeling techniques, and data acquisition methods, water quality and algal bloom prediction models have progressed rapidly (XIAO et al., 2024). New models and techniques have emerged in recent years, and improvements have been made to existing models to achieve more accurate prediction and early warning of blooms (Zhou et al., 2023). By utilizing remote sensing techniques, image data can provide spectral information, and vegetation indices of water bodies, enabling monitoring and identification of the quantity, spatial distribution, and types of algae (Qi and Hu, 2021). Airborne or satellite platforms are typically used to acquire remote sensing image data (Ruiz-Villarreal et al., 2022).

There are also drawbacks related to remote sensing. Uncertainties in the estimates of CLA by this method especially in coastal waters can be generated by factors such as the water depth, atmospheric correction issues, interference of compounds of different colors and the presence of suspended material and colored dissolved organic matter (Silva and Garcia, 2021; Watanabe et al., 2018). Especially in coastal and estuarine waters, which present complex and variable optical characteristics, the accuracy of CLA estimates through remote sensing strongly depends on specific algorithms. These algorithms must be adjusted to minimize interference from other constituents and adapt to regional environmental conditions (Lins et al., 2017). Algorithms have been designed to estimate the concentration of CLA in such waters by adopting different combinations of spectral bands (Watanabe et al., 2018) and the red and near-infrared (NIR) bands are used to reduce interference from other optically active constituents (Gilerson et al., 2010). Three NIR-red algorithms stand out for CLA estimation in coastal waters: the two-band algorithm (2B), the three-band algorithm (3B) and the Normalized Difference Chlorophyll Index (NDCI) algorithm

(Watanabe et al., 2018). Data from different sensors are used to estimate CLA concentration, including the Medium Resolution Imaging Spectrometer (MERIS) (ENVISAT satellite) that has already been used for oceanic and coastal waters (Watanabe et al., 2018). This sensor has favorable characteristics for CLA estimation in coastal waters (Mishra et al., 2014), including its temporal (3 days), spatial (300 m) and spectral (visible and near infrared spectrum) resolutions.

There are also the standard algorithms, or global algorithms, for estimating CLA. These are expected to be versatile, since they are generated from a large amount of in situ data, in a wide range of CLA concentrations, and in different regions of the globe. However, they often show poor accuracy in regional studies, thus requiring adjustments or the development of complementary regional algorithms. Independently of the algorithm adopted to estimate CLA based on remote sensors, the validation of the estimates with the help of in situ data is highly recommended, and the needed data is restricted in many cases.

Santa Catarina (SC) is a state in southern Brazil contributing the largest production of cultivated bivalve mollusks, responsible for >90 % of the national production (Souza and Santos, 2021). In 2022, 2,067 tons of oysters and 7,076 tons of mussels were produced by 356 marine farms located in this state (<https://www.observatorioagro.sc.gov.br/areas-tematicas/producao-agropecuaria/paineis/>). The first initiatives of HAB monitoring started in 1997, and an official HAB surveillance program encompassing all shellfish production zones along the coast of SC has been running since 2012. The results of these efforts evidence that coastal aquaculture in Santa Catarina is affected by HAB on a regular basis and that these events are an important issue, both in terms of public health and economy (Vianna et al., 2023). In an attempt to explain the occurrence of HAB along the coast of SC, remote sensing chlorophyll estimates have been used as a proxy of HAB (Vianna et al., 2016). However, a recent study suggest that the estimates of CHL generated by global algorithms are poorly correlated with algal blooms on the coast of SC and the study authors claim that remote sensing studies are needed “for the development of algorithms aimed at estimating CHL, phytoplankton and toxic phytoplankton in SC based on data generated locally and thus adapted to the predominant algal species, as well as specific oceanographic and

coastal conditions of the region” (Vianna et al., 2023).

This study hypothesizes that chlorophyll-a (CLA) estimation algorithms adapted to the specific environmental conditions of the Santa Catarina (SC) coast will provide greater accuracy in the detection and quantification of harmful algal blooms (HAB) when compared to global and generic remote sensing algorithms. This hypothesis is based on the premise that environmental characteristics and predominant phytoplankton species in SC can affect the accuracy of CLA estimates obtained through remote sensing.

The hypothesis will be tested by developing new models or tuning previously developed ones based on a locally generated CLA database and by comparing the performance of the generated algorithms with previously developed global algorithms. The study specific objectives were: i) to use CLA data measured in situ between 2007 and 2009 to develop new models and to tune previously developed models for CLA estimation based on bands 6, 7, 9 and 10 MERIS sensor images; we hope to be able to achieve a model with higher accuracy and lower uncertainty; ii) to compare the performance of global algorithms for CLA estimation with the models developed by the present study; we expect to observe a superior performance of the models developed by the present study.

Materials and methods

Figure 1 describes the methods adopted in the present study. In summary, regression techniques were used to develop algorithms to predict CLA levels in coast of SC by correlating in situ CLA measurements with: 1 - data from bands 6 (620 NM), 7 (665 NM), 9 (708.75 NM) and 10 (753.75 NM) of MERIS; 2 - outputs from previously developed NIR-red algorithms; and 3 - outputs of global algorithms for CLA. Finally, part of CLA database was used to validate the best performing alternatives under the environmental conditions of SC.

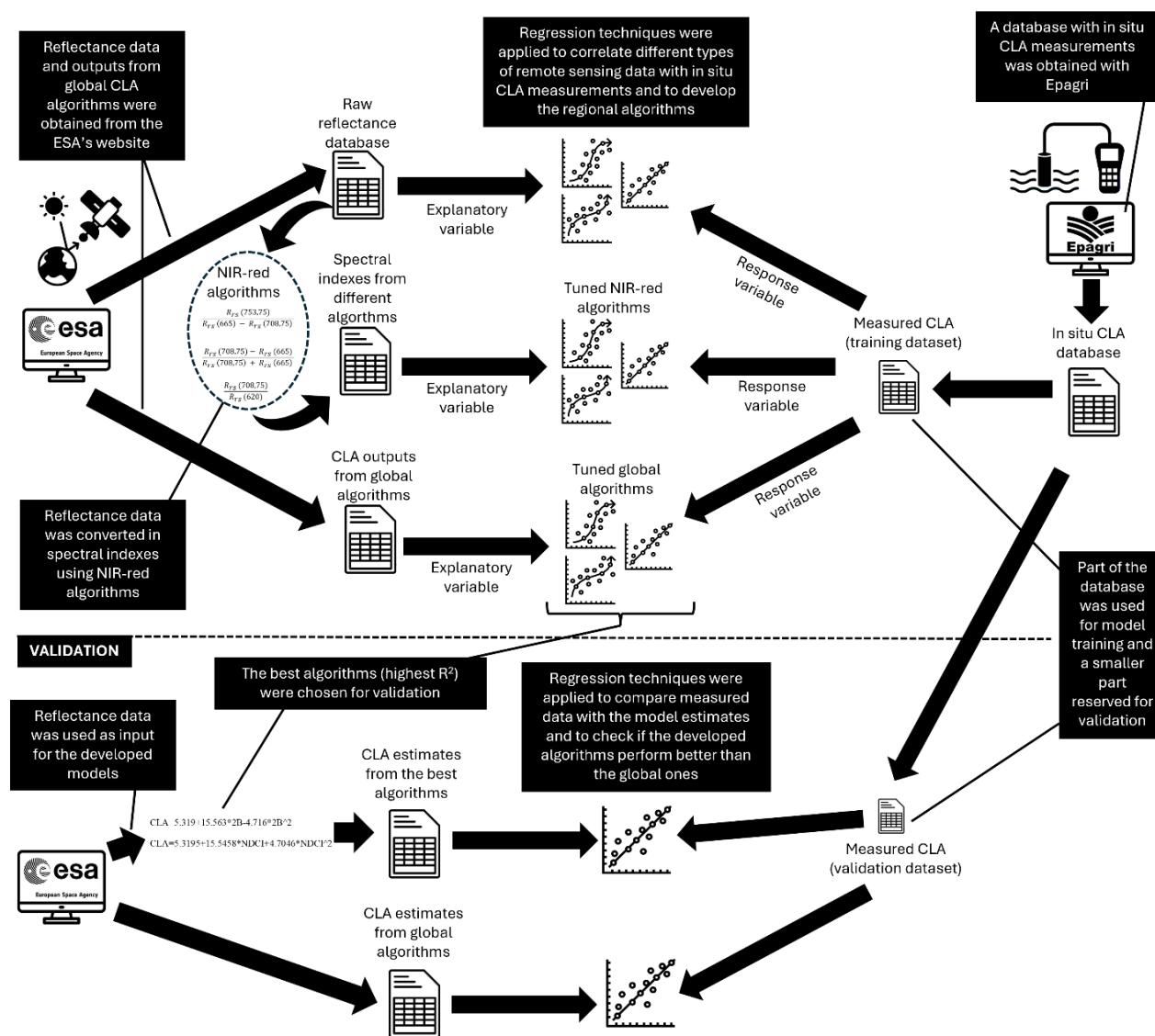


Figure 1. Scheme of the methods adopted in the present study.

Study area

Santa Catarina is a state in southern Brazil (95,736 km² - 1.12% of the country's total territory) with a 561-km coastline formed by sheltered bays and numerous islands (Resgalla Jr. 2011; Suplicy et al., 2015). The nearshore waters of SC have complex circulation patterns and receive freshwater inputs from various river systems (Resgalla Jr., 2011). During summer, the prevailing winds in the region blow from the northeast, while in winter they come from the south/southeast (Freire et al., 2017). On the continental shelf, the Brazil current stands out as the predominant current, responsible for transporting the masses of Tropical Water (TW) and South Atlantic Central Water (SACW) (Freire et al., 2017). TW is characterized by warmer temperatures, reaching around 20°C, and flows in a

south-southwest direction. On the other hand, the SACW presents colder temperatures, varying between 6 °C and 18 °C. Both currents follow a similar course, close to the edge of the continental shelf (Mascarenhas Jr and Ikeda, 1994). Coastal Waters (CW) are composed of a mixture of waters from the mainland and the South Atlantic and have an average salinity of less than 33.7 ppm. Marine farms are spread along the SC coast at a minimum distance of 200 m from sandy beaches and 80 m from rocky shores, but, generally, not farther than one kilometer from the coast (Suplicy, 2019). They are located in zones with depths ranging from 1.9 to 8.8 m (Souza et al., 2017) and are mostly small-scaled, 80% of them covering areas smaller than two hectares.

Data obtaining and processing

The in situ CLA database was provided by Epagri (www.epagri.sc.gov.br) and contains measurements by a probe (YSI 660) obtained fortnightly, from 2007 to 2009, in 30 monitoring points within marine farms along the coast of SC. For this study, data from 27 of these locations were used due to the availability of data coinciding with the passage of the satellite (Figure 2).

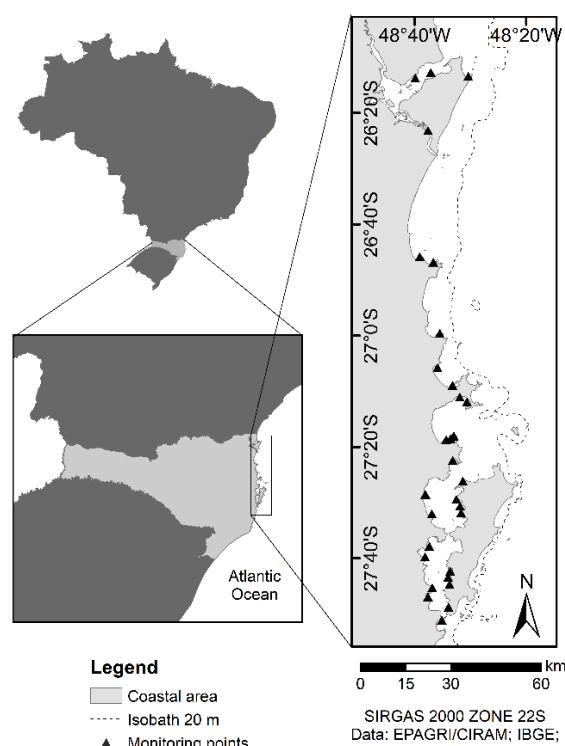


Figure 2. Indication of chlorophyll-a monitoring points located within the limits of marine farms along the coast of Santa Catarina.

Table 1 – NIR-red algorithms which combine different NIR-red spectral bands to reduce interference from other optically active constituents on the CLA estimates. The values between parentheses correspond to the spectral bands centers (nm).

Algorithm	Formula (MERIS)	Authors
2B	$\frac{R_{rs}(708,75)}{R_{rs}(665)}$	Dekker, 1993
3B	$\frac{R_{rs}(753,75)}{R_{rs}(665) - R_{rs}(708,75)}$	Dall'Olmo et al., 2003
NDCI	$\frac{R_{rs}(708,75) - R_{rs}(665)}{R_{rs}(708,75) + R_{rs}(665)}$	Mishra and Mishra, 2012

Reflectance data at surface level, with atmospheric correction, from bands 6, 7, 9 and 10 of the MERIS (ESA, 2006) was obtained from the ESA platform (<https://earth.esa.int/eogateway/catalog>). MERIS was mounted on the ENVISAT satellite, of the European Space Agency (ESA) which was launched in 2002 and deactivated in 2012. A total of 36 scenes with cloud coverage of up to 10% captured on the same day of in situ CLA measurements were selected. The Sentinel Application Platform (SNAP) (SNAP-ESA, 2022) was used to reproject and crop the images (Limits: -27.136 N; -28.094 S; -48.619 W; and -48.103 E) and to extract the data from the pixels corresponding to the coordinates of each monitoring point.

The reflectance data obtained for different spectral bands obtained from MERIS were converted in spectral indexes using the NIR-red algorithms described on Table 1. The 2B (Dekker, 1993) and the NDCI (Mishra and Mishra, 2012) algorithms were also tested with a different band composition, as proposed by Watanabe et al. (2018), which will be called here M2B and MNDCI (M stands for “modified”), respectively. We also used the 3B (Dall'Olmo et al., 2003) algorithm to calculate spectral indexes.

M2B	$\frac{R_{rs}(708,75)}{R_{rs}(620)}$	Watanabe et al., 2018
MNDCI	$\frac{R_{rs}(708,75) - R_{rs}(620)}{R_{rs}(708,75) + R_{rs}(620)}$	Watanabe; Alcântara; Stech, 2018

R_{rs} stands for remote sensing reflectance.

CLA estimates (mg.m^{-3}) generated by the global algorithms Neural Network (NN) and OC4ME were also obtained on the ESA platform for the monitoring points and dates in the database. The NN algorithm estimates the CLA concentration through the Inverse Modeling Technique, with the application of a Neural

Network model of Inverse Radiative Transfer (IRTM-NN) (ESA, 2006), using the surface reflectance of MERIS spectral bands 2, 7 and 9 (ESA, 2006). The OC4ME algorithm CLA outputs are computed applying the equation below to MERIS spectral data (Morel et al., 2007):

$$\log_{10}[Cla] = a_0 + \sum_{i=1}^4 \left(a_i \cdot \left(\log_{10} \left(\frac{Rrs(\lambda_{azul})}{Rrs(\lambda_{verde})} \right) \right)^i \right)$$

Where $\log_{10}[Cla]$ = base 10 logarithm of CLA concentration, $Rrs(\lambda_{blue})$ = blue reflectance band ($R_{560}^{443} > R_{560}^{490} > R_{560}^{510}$), $Rrs(\lambda_{green})$ = green reflectance band, and for the MERIS sensor, the coefficients at 0 = 0.3255, at 1 = -2.7677, at 2 = 2.4409, at 3 = -1.1288 and at 4 = -0.4990.

Model calibration and validation

When all the obtained data was combined (for different dates and monitoring points), it was possible to obtain a total of 100 observations for each of the studied parameters (measured CLA, reflectance, reflectance indexes and CLA outputs from global models). This database was randomly separated in a training set and a validation set (68/32). The models were developed using the training dataset through simple linear and polynomial regression, having in situ CLA data (mg.m^{-3}) as the response variable and the different parameters as the explanatory ones. The models were compared based on the goodness of fit (R^2) and Residual Standard Error (RSE) and those with the best performances during the training were used to estimate the CLA concentration based on the validation dataset. The outputs from the global CLA models obtained from the ESA website (without any processing/transformation) were also compared with the measured CLA data in the validation database. Different parameters were used for the validation procedures and comparison

between the models: goodness of fit (R^2) and RSE of linear models comparing measured and modeled CLA concentrations and RMSE.

Results

Model fitting

The measured CLA concentrations ranged from 0.6 to 15.3 mg.m^{-3} for the analyzed period. When analyzed individually, none of the spectral bands correlated significantly ($p > 0.05$) with measured CLA (Table 2). Global algorithms outputs did not correlate significantly ($p > 0.05$) with the measured data either (Table 2). On the other hand, the studied NIR-red algorithms correlated significantly with the measured CLA, with the exception of MNDCI. The highest levels of explained variance, 37%, and the lowest residual standard errors, 2.57 mg.m^{-3} , were obtained for both models having 2B and NDCI algorithms as the explanatory variables. The lack of significant correlations discarded the possibility of developing models based on single spectral bands or models to tune the global model outputs. Therefore, only the 2B and NDCI were chosen to be used in the validation procedures and will be referred to as tuned 2B and tuned NDCI algorithms (Figure 3).

Table 2 - Results of linear regression having the CLA in situ (mg.m^{-3}) measurements as the response variable and different remote sensing parameters and CLA global model estimates as explanatory variables.

Explanatory variable	R ²	p	RSE	Model
Band 6	0.03	0.2702	3.20	
Band 7	0.08	0.0653	3.11	
Band 9	0.01	0.5528	3.23	
Band 10	0.01	0.9826	3.23	
2B algorithm	0.37	0.0000	2.57	$\text{CLA} = 5.319 + 15.563 \cdot 2B - 4.716 \cdot 2B^2$
3B algorithm	0.16	0.0340	2.98	$\text{CLA} = 5.3195 - 6.4494 \cdot 3B + 8.3590 \cdot 3B^2$
NDCI algorithm	0.37	0.0000	2.57	$\text{CLA} = 5.3195 + 15.5458 \cdot \text{NDCI} + 4.7046 \cdot \text{NDCI}^2$
M2B algorithm	0.14	0.0241	3.02	$\text{CLA} = 5.3195 + 6.9685 \cdot \text{M2B} + 6.8717 \cdot \text{M2B}^2$
MNDCI algorithm	0.11	0.1719	3.06	
OC4ME	0.03	0.3233	3.09	
NN	0.01	0.6507	3.16	

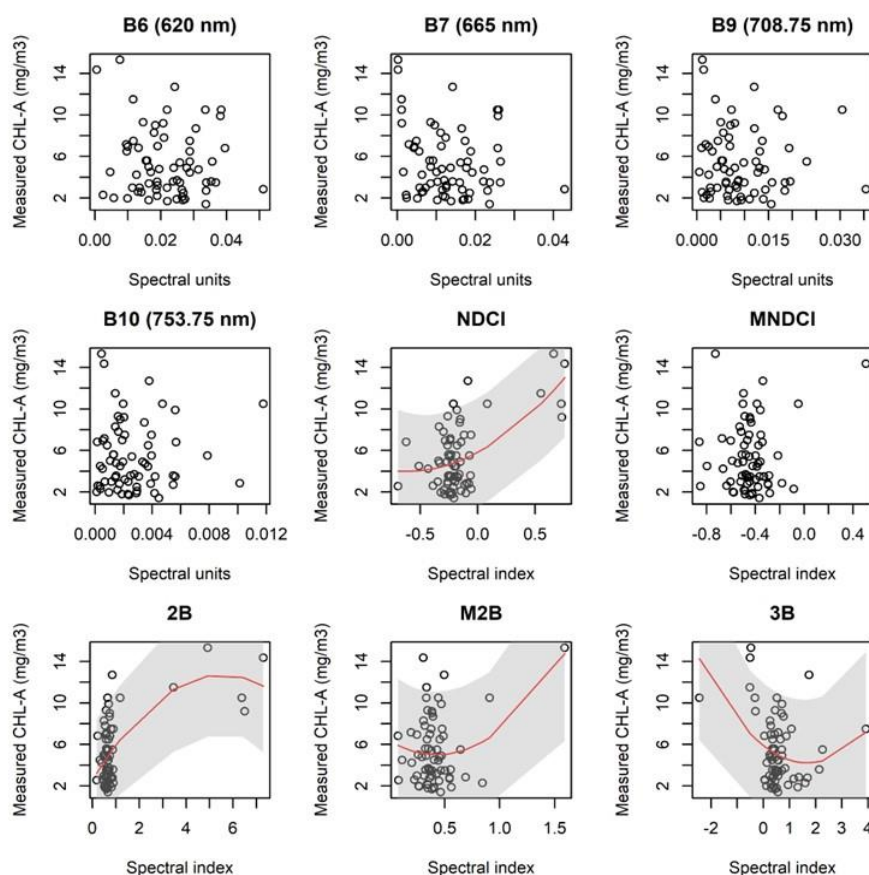


Figure 3. Scatterplot describing the relation between CLA in situ (mg.m^{-3}) measurements and different remote sensing parameters. The red lines represent second-order polynomial models for parameters correlating significantly with the in situ CLA measurements. The gray hatches represent the confidence interval at the 95% confidence interval.

Model validation

The comparison of measured versus modeled results showed that the tuned NDCI and tuned 2B algorithms performed better than the global models. The tuned models' outputs fitted better the measured data ($R^2 \geq 0.22$) and showed lower RMSE values than the global models'

outputs. The error of the tuned models ranged around 2.5 mg.m^{-3} . As previously observed for the training database, the global models' outputs did not correlate significantly with the measured CLA levels available in the validation database either and, when compared with the models developed by the present study, showed higher errors (Table 3, Figure 4).

Table 3 - Validation parameters of models aimed at estimating CLA based on remote sensing algorithms.

Source	RMSE	R^2 measured vs modeled	p measured vs modeled	RSE measured vs modeled
Tuned 2B algorithm	2.52	0.22	0.008	1.52
Tuned NDCI algorithm	2.49	0.24	0.006	1.37
OC4ME	8.15	0.05	0.300	5.89
NN	4.51	0.08	0.140	4.31

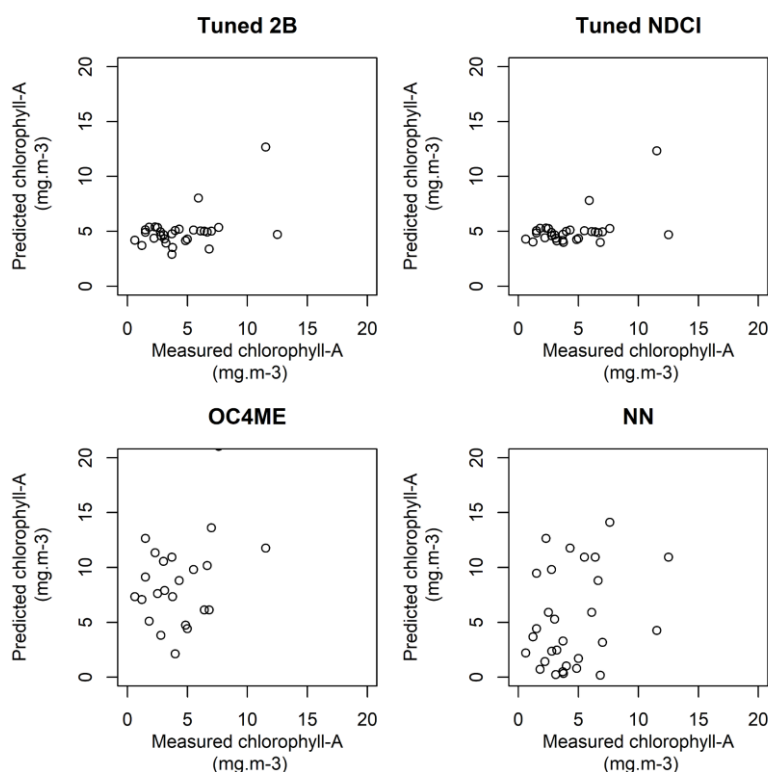


Figure 4. Scatterplots describing the relationship between in situ CLA measurements and estimates from different remote sensing algorithms.

Discussion

Remote sensing estimates of CLA can be a useful tool to support decision making in coastal zones (Moraes et al., 2023) and have been used by authorities responsible for HAB surveillance programs around the globe (NCCOS, 2023). These experiences have shown the importance of tuning/recalibrating global algorithms aimed at estimating CLA, to make them more representative on a regional level. Previous studies report poor performance of global algorithms in regions across the globe (Moore et al., 2009), e.g. on the North Coast of the Brazilian State of São Paulo (Valério, 2013) and in the Southwest and South Atlantic Ocean (Garcia et al., 2005). Specifically in SC, a recent study suggests that global algorithms for CLA prediction perform poorly (Vianna et al., 2023). Our results corroborate that finding and advances the knowledge by evidencing that the CLA estimates from global algorithms, such as OC4ME and NN, do not even correlate significantly with data measured in situ on the coast of SC. This finding indicates that global models' outputs cannot properly represent the levels of CLA in SC and evidence the risks of decision-making based on them.

This study was aimed at developing improved algorithms for estimating chlorophyll-a in coastal waters of southern Brazil from multispectral images. Among the tested approaches, it was not possible to develop algorithms based on isolated spectral bands nor to tune the global models given the lack of correlation of these with the measured CLA levels. On the other hand, tuning the NIR-red algorithms based on CLA data measured in situ in SC allowed the development of two algorithms that perform better than the tested alternatives (OC4ME and NN). During the calibration phase, our two best models (based on 2B and NDCI) showed similar levels of explained variance around 37% and also similar RSE of 2.57 mg.m⁻³. Generally, in these more complex water environments, models that use the NIR and red bands tend to perform better (Flores-Anderson et al., 2020).

Other studies succeeded in developing regionally optimized models based on NIR-red algorithms. In general, the performance of our algorithms during the calibration phase were not as high as those reported by previous studies. In relation to CLA prediction algorithms based on NDCI, levels of explained variance (R²) higher than 0.7 are obtained in most cases: 0.72 to 0.95

(chl-a range: 1 – 60 mg.m⁻³) for Mississippi River Delta, Chesapeake Bay, Delaware Bay, and Mississippi Sound/Mobile Bay (Mishra and Mishra, 2012); 0.98 (CLA range: 2.33 - 208.68 mg.m⁻³) in a freshwater reservoir in Southeastern Brazil (Funil hydroelectric reservoir) (Watanabe et al., 2018); 0.90 and 0.96 (CLA range: ~4 - ~14 g.m⁻³) in the northern Gulf of Mexico (Mishra et al., 2014); 0.77 and 0.76 in the northern and southern subareas of the coast of Peru (Escudeiro et al., 2024); 0.79 in global continental and coastal aquatic systems (Neil et al., 2020).

These studies did not use exactly the same type of functions, sensors or spectral bands as the present research. For instance, Mishra and Mishra (2012) used a quadratic function and Watanabe et al. (2018) obtained their best results using data from the OLCI sensor from Sentinel-3 and Mishra et al. (2014) used images from the Hyperspectral Imager for the Coastal Ocean (HICO).

In the present study, when in situ CLA measurements were compared with the model estimates (validation), R² of 0.22 and 0.24 and RMSE of 2.52 and 2.49 were obtained for our best models which were based on 2B and NDCI, respectively. The studies previously mentioned report similar levels of error, however the fitting between measured and predicted results is, in general, better than ours: RMSE ranging from 1.43 to 4.83 mg.m⁻³ and R² from 0.34 to 0.94 reported by Mishra and Mishra (2012); NRMSE of 9.30% and R² of 0.98 reported by Watanabe et al. (2018); RMSE ranging from 1.64 to 4.98 µg/L and R² from 0.11 to 0.74 reported by Mishra et al. (2014); RMSE reported by Neil et al (2020).

The comparison of our model based on 2B with similar models generated for other geographical areas also evidenced that our predictions did not fit as well the measured data, despite the errors having similar levels. Oliveira et al. (2016) obtained an R² of 0.71 during the calibration of a 2B algorithm to estimate CLA levels (CLA range: 1.0 to 974.0 mg.m⁻³) in a coastal bay in southeastern Brazil (Baía de Guanabara) using multispectral MERIS images. Different from our study, they used the ratio of red (665 nm) and green (560 nm) bands. Gurlin et al. (2011) investigated the performance NIR-red bands for the remote estimation of CLA in turbid productive waters (CLA range: 0 - 100 mg.m⁻³) from Fremont Lakes State Recreation Area in Nebraska, USA, using data from MERIS and MODIS. Their 2B model with MERIS data estimated CLA more accurately than the other

models, with average absolute errors of 2.3 mg.m⁻³. Lins et al. (2017) obtained an R²>0.80 for measured versus predicted results using three-band NIR-Red models. The authors still obtained good results with the 2B algorithm for Sentinel-2/MSI and Sentinel-3/OLCI data.

The limited performance of our models in relation to similar studies carried out elsewhere may be related to different factors. The CLA measurements used in our study ranged from 0.4 mg.m⁻³ to 15.3 mg.m⁻³. A sensitivity analysis performed by Ruddick et al. (2001) on two near-infrared (NIR) and red band ratio algorithms revealed that the relative error in CLA estimates tends to be more significant specifically at CLA concentrations lower than 10 mg.m⁻³, a range in which 91% of the observations in the used database are within. Other studies previously mentioned which obtained better fitting between measured and estimated data used databases with much higher CLA values to train the models, e.g.: 1 to 60 mg.m⁻³ - Mishra and Mishra (2012); 2.33 to 208.68 mg.m⁻³ - Watanabe et al. (2018); 1.0 to 974.0 mg.m⁻³ - Oliveira et al. (2016); 0 - 100 mg.m⁻³ - Gurlin et al. (2011); 1 - 100 mg.m⁻³ - Aranha e al. (2022). Therefore, the overall low levels of CLA in the used database is the most probable cause of the lower performance of the models generated in the present research. Furthermore, concentrations above 15.3 mg.m⁻³ may not be well represented by the models developed by the present study given the limited range of the database used to train the models. The limited spatial resolution (300 m) of the MERIS image might also have negatively impacted the performance of the developed models, since the large pixels may not precisely represent the levels of CLA in the monitoring stations. This problem could be overcome by using data from sensors with higher resolutions, such as the MSI sensor (Sentinel-2) which has a 20 m resolution. We could not test this given the absence of CLA measured data available for the period of operation of the MSI sensor. Future studies aimed at developing algorithms for CLA prediction in SC might benefit from databases including higher CLA values and for periods when remote sensing data with higher spatial resolution are available.

Conclusions

The results confirmed the hypothesis that chlorophyll-a (CLA) estimation algorithms adapted to the specific environmental conditions of the Santa Catarina (SC) coast provide greater accuracy when compared to global generic

algorithms. The CLA estimates from global algorithms, such as OC4ME and NN, did not even correlated significantly with in situ data collected along the SC coast. This finding highlights the risks of making decisions related to algal blooms based on the outputs of these models. Among the alternative algorithms developed by the present study, the tuned 2B and tuned NDCI provided the best results, with predictions showing significant correlation with measured data. Therefore, these algorithms can be currently considered the best available option for estimating CLA (up to 15.3 mg.m⁻³) in the coastal waters of Santa Catarina, based on remote sensing data.

However, it is important to note that these models (tuned 2B and tuned NDCI) have limited predictive power when compared to regional algorithms developed elsewhere. This limitation is probably linked to the narrow range of CLA measurements used to train the models and the limited spatial resolution of the MERIS sensor. Future studies aiming to develop CLA prediction algorithms for the SC coast would benefit from databases that include higher CLA values and data collected during periods when higher spatial resolution remote sensing, such as from MSI (Sentinel-2), is available.

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