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Empirical and semi-empirical chlorophyll-*a* modeling for water quality assessment through river-lake transition in extreme Southern Brazil

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Abstract: Mirim lagoon is the second largest lacustrine water body in Southern Brazil, providing water for local communities. However, algae growth and water quality in the lagoon and in tributaries rivers is influenced by nutrient's increase. In this context, this study performs the empirical and semi-empirical chlorophyll-*a* (Chl-*a*) modeling using remote sensing and *in situ* data for water quality assessment. Water quality data were collected at 15 sample locations in the lagoon on the date of Sentinel-2 satellite overpass. Surface reflectance data were derived from the Sen2Cor atmospheric correction method and correlated with Chl-*a* concentration. The best model presented a Pearson's correlation coefficient = 0.81 and Mean Absolute Error = 0.13µg.L^{-1}. Low Chl-*a* concentration is observed at the Northern lagoon, possibly due to suspended solids presence. The same occurs in the left margin, being associated with the influence of land use for agriculture. High Chl-*a* concentrations are associated with shallower and lentic areas. The mean Chl-*a* concentration predicted by the model was 17.34µg.L^{-1}, similar to the observed value *in situ* (16.32µg.L^{-1}). Overall, the empirical model developed can be applied as a tool to reduce costs and efforts in fieldwork measures and to understand eutrophication in this river-lake transition ecosystem.

Key words: Eutrophication, Inland waters, Phytoplankton blooms, Sentinel-2, Water quality monitoring.

INTRODUCTION

Eutrophication is one of the major threats to inland water quality. It is caused by excessive nutrient loads in the water body, leading to algal growth and fish kills (Paerl et al. 2003, Yu et al. 2017). Excess of nutrients in water bodies can increase phytoplankton blooms, which are commonly measured in terms of chlorophyll-*a* (Chl-*a*) (Kosten et al. 2012). Chl-*a* concentration provides important information about water quality and its potential risks to human health, since some phytoplanktonic organisms, such as cyanobacteria, can produce toxic compounds (Lobo et al. 2009, Hanisch & Freire-Nordi 2015).

Mirim lagoon is an important water resource in the extreme south of the state of Rio Grande do Sul (Brazil) and the second-largest water body with lacustrine characteristics in Brazil (Tormam et al. 2017). The lagoon is connected to the Patos lagoon by the São Gonçalo channel, which has a length of 76 km (see Fig. 1). This connected system forms one of the main transboundary watersheds in South America with extreme environmental and economic importance for both the Rio Grande do Sul state (Brazil) and Uruguay (Oliveira et al. 2015). Moreover, the Patos-Mirim system is responsible for the drainage of an area of 200,000 km² and promotes strong impacts on the adjacent coastal area through

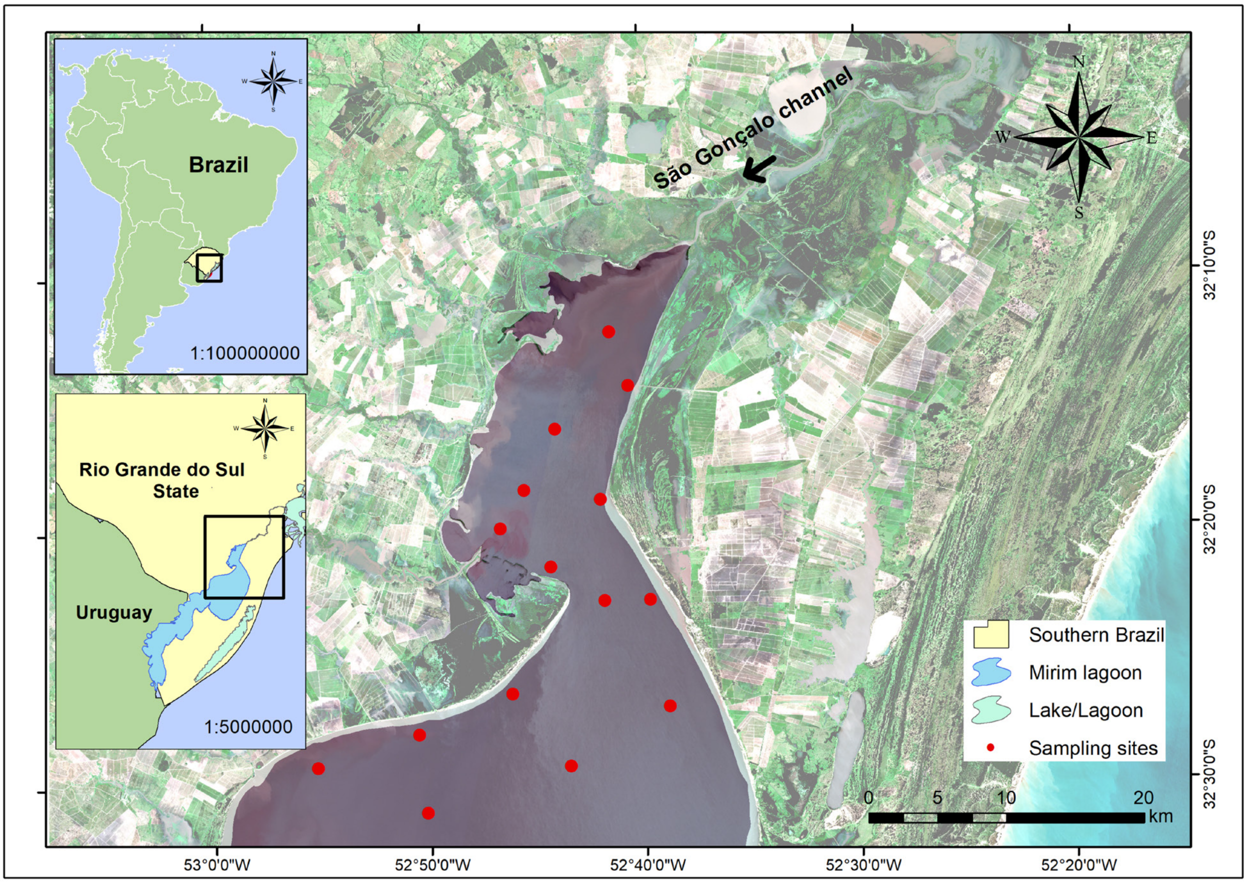

Figure 1. Location of the Mirim lagoon in Southern Brazil. R (4) G (3) B (2) composition of the Mirim lagoon image from the MSI sensor onboard the Sentinel-2 satellite acquired on October 15, 2018.

the freshwater and nutrients input (Hirata et al. 2010). In this context, the transition between the river and the lagoon systems is a critical zone for water quality. Transition zones are regions where hydrological conditions switch from river-dominated to lake mixing processes (Thornton et al. 1990), and it is responsible for a series of environmental problems. Nutrients derived from the basin are responsible for a significant proportion of the lake's productivity, which is enhanced by anthropogenic inputs (Wang et al. 2019). Currently, the São Gonçalo channel has been impacting the water quality of the Mirim lagoon. Albertoni et al. (2017) showed that the São Gonçalo channel is eutrophic with a high probability of cyanobacterial bloom. Furthermore, Mirim lagoon also has several agricultural areas in its surroundings, increasing nutrient load in the water. Therefore, in periods of low rainfall, it is common to find algae accumulation at some specific points (Fernandes et al. 2007). In the estuary, agricultural activities contribute to the input of fertilizers (Tormam et al. 2017), nutrients (Grutzmacher et al. 2008), chemicals and organic phosphates fertilizers in the Mirim lagoon (Fia et al. 2009).

While traditional water sampling supports the understanding of biophysical factors that control algae blooms, there is a lack in understanding its spatial dynamics in this large lagoon (3,739 km^2). Thus, optical remote sensing has become an alternative to support inland water studies (Gholizadeh et al. 2016). Due to the wide range of imaging and high frequency of data acquisition, optical sensors constitute a continuous monitoring tool, having the potential to complement conventional *in situ* monitoring approaches (Palmer et al. 2015, Fassoni-Andrade et al. 2017). Algae pigments are Optically Active Components (OAC) and absorb electromagnetic radiation in specific wavelengths (Kirk 1994, Lobo et al. 2009). In the last decades, remote sensing techniques have enabled the bio-optical characterization of aquatic environments and the estimation of water constituents (Bukata et al. 1981, Mertes et al. 1993, Dekker et al. 1996, Gitelson et al. 2003, Mishra & Misha 2012, Li et al. 2015, Watanabe et al. 2018, Martins et al. 2019). Inland waters and lakes are optical complex environments, which make them a challenging environment to retrieve accurate information about biogeochemical parameters using remote sensing techniques (Pierson & Strombeck 2000).

Algorithms to determine Chl-*a* using remote sensing were first created for open ocean waters, where the phytoplankton and its byproducts control the optical properties (Palmer et al. 2015). Therefore, when employed in waters that are influenced by other OAC, such as coastal and turbid inland waters, these algorithms tend to not perform as well as expected (Matthews 2011, Palmer et al. 2015). In recent years, algorithms based on remote sensing were developed to estimate Chl-*a* concentration in turbid and nutrient-laden waters, typical of inland waters (Yacobi et al. 2011, Beck et al. 2016). Among these algorithms, empirical and semi-empirical methods have been developed (Le et al. 2009, Gilerson et al. 2010, Yacobi et al. 2011, Vazyulya et al. 2014). The empirical algorithms represent effective data optimization but they are limited in terms of generalization in time and space (Odermatt et al. 2012). Empirical and semi-empirical algorithms were developed using statistical regressions comparing reflectance satellite data with *in situ* data of limnological parameters (Ogashawara 2015). However, empirical algorithms are typically developed with different spectral bands and limnological data without prior knowledge, while the semi-empirical algorithm uses bio-optical information for modelling the best relationship between radiometric and limnologic data (Ogashawara 2015). These algorithms were developed and/or applied in shallow lakes (Palmer et al. 2015), reservoir (Randolph et al. 2008), inland, estuarine and coastal waters (Moses et al. 2009), lakes (Gilerson et al. 2010), gulfs (Vazyulya et al. 2014) and estuary (Fassoni-Andrade et al. 2017).

Augusto-Silva et al. (2014) investigated remote sensing based algorithms to estimate Chl-*a* concentrations in tropical inland reservoirs. The authors found that the spectral resolution of MEdium Resolution Imaging Spectrometer (MERIS) was successful to estmate Chl-*a* when combining them with empirical calibration. Similarly, empirical algorithms were developed by Fassoni-Andrade et al. (2017) in the Patos Lagoon estuary. The authors developed suspended solids (SS) and Chl-*a* models for Landsat-8 Operational Land Imager (OLI) sensor data, applying Linear Spectral Mixing Model. The proposed empirical models were developed using simple and multiple linear regressions between *in situ* and radiometric data. The standard bio-optical algorithms from satellite radiometric measures are often limited to the region's characteristics of which they were developed or also for a specific optical water type. Therefore, when applied to different and dynamics environments, they can cause errors in the estimation of the parameters. Therefore, develop local empirical algorithms with data measured *in situ* are necessary (Vazyulya et al. 2014). According to Palmer et al. (2015), the advances in optical orbital sensors offers a scientific prospect regarding inland water research. This new generation of sensors includes the Multispectral Imager (MSI), onboard the Sentinel-2 satellite, which has spatial and spectral resolutions suitable for studying inland waters, presenting a opportunity for the study of small lakes due to these sensor resolutions (Toming et al. 2016).

The Mirim lagoon provides socio-economic and ecological activities in Southern Brazil (Fernandes et al. 2007), but this lagoon is still poorly monitored, especially in the case of Chl-*a* concentration. This study evaluates the Chl-*a* modeling in the Mirim Lagoon using Sentinel-2 MSI image and provides the preliminary assessment of Sao Gonçalo channel influence on the water quality of the lagoon. In addition, this paper presents the procedure for Chl-*a* modeling by combining Sentinel-2 MSI reflectance data and *in situ* measurements in the Northern Mirim lagoon, in order to understand the spatial variability of Chl-*a*. This mapping of Chl-*a* may help in the management, evaluation, monitoring and inspection actions in the Mirim lagoon.

MATERIALS AND METHODS

Sentinel-2 MSI image data

The MSI sensor, onboard the Sentinel-2 satellite, provides 12-bit radiometric resolution, 10m, 20m, and 60m spatial resolutions and 13-band spectral resolution, with widths ranging from 15nm to 180nm (Drusch et al. 2012). Sentinel-2 MSI image of the study area was obtained on October 15, 2018 (Fig. 1). Data is available from the European Space Agency (ESA) (https://scihub.copernicus.eu/). The image is delivered in Level-1C, on Top-Of-Atmosphere (TOA) reflectance. For accomplishing OACs analyzis, it was necessary to pre-process the image, performing an atmospheric correction (AC), converting it from TOA reflectance to Bottom-Of-Atmosphere (BOA) reflectance. The AC algorithm used was Sen2Cor, and is accessible on SNAP (Sentinel Application Platform) software. This algorithm was specially developed for the processing and analyzis of Sentinel's mission products (STEP, 2018). Sen2Cor uses auxiliary data such as look-up tables and atmospheric radiative transfer models to classify the image in 12 different classes (e.g. water, vegetation, clouds, cirrus). The output of the algorithm is an image in BOA reflectance and Quality Indicators of the correction (Ansper & Alikas 2018).

Sen2Cor has been showing good results for being a practical method, tested in several validation studies in different regions of the world with different water types (Toming et al. 2016, Ruescas et al. 2016, Martins et al. 2017, Main-Knorn et al. 2017, Sola et al. 2018, Warren et al. 2019). Warren et al. (2019) tested six AC algorithms over 13 inland water bodies, showing that none of the models performed well over the entire band set (444 to 865 nm). Despite that Sen2Cor was not the best one AC method tested, results were satisfactory for inland waters. Ruescas et al. (2016) compared Sen2Cor with other AC methods in lakes (Spain and Peru-Bolivia) and demonstrated that the method was consistent for inland waters. Our study is the first application of Sen2Cor algorithm in lagoons over Southern Brazil. Once *in situ* reflectance measurements were not available, we were not able to compare and evaluate the performance of Sen2Cor algorithm. However, to demonstrate that the AC performed well, we compared Sen2Cor results with the results from another AC method, the Image correction for atmospheric effects (iCOR). The iCOR algorithm is an AC tool that can process satellite data collected over coastal, inland or transitional waters and land, and supports the inter-comparison of AC approaches. More details of the algorithm can be found on De Keukelaere et al. (2018). The algorithm was validated for coastal and inland waters by De Keukelaere et al. (2018), where the assessment of iCOR for inland and coastal waters showed reasonable results for Landsat-8 and Sentinel-2 satellites. After the AC, the reflectance at each pixel corresponding to the *in situ* collection point were selected from different MSI/Sentinel-2 sensor bands based on single pixel extraction, allowing to correlate these data with the concentrations found on field.

Data collection and laboratory analyzis

In situ data was collected on October 16th, 2018, period considered of high rainfall rates in the region (Souza 2015). Fifteen points were sampled over the Northest Mirim lagoon (Fig. 1), area directly affected by the São Gonçalo channel. The coordinates of the points were measured using a GARMIN GPS navigation model GPSmap 60CSx. For the Chl-*a*, at each point, 1 liter of surface water at a depth of 0.30m was collected. It was placed in amber glass, to avoid contact with sunlight, and kept under refrigeration. The average wind speed remained relatively low during the collection period, being of approximately 13.5km.h^{-1} (AGROMET 2018), which reduces the possible variability of the constituent's concentration since the moment of the image acquisition. The sample analyzis was performed in the Water Laboratory of the Chemical Engineering Course of the Federal Institute of Education, Science and Technology Sul-rio-grandense/IFSul - Campus Pelotas. The method used for determining Chl-*a* concentration in the phytoplankton was the spectrophotometric, according to the methodology described in APHA (2005), and Eq. 1 was used to calculate Chl-*a* concentration. In addition to the Chl-*a* concentration, pH, through a pH meter, and phosphorus, by the Molybdovanadate method, were also estimated. All the parameters evaluated in this study were analyzed using descriptive statistics: mean, median, minimum and maximum values, standard deviation and coefficient of variation (CV).

$$Chl\text{-}a\left(\mu g.L^{-1}\right) = 26,7 * \left(A_{664} - A_{750}\right) * \frac{1000 * V}{S} \quad (1)$$

where, (A_{664} - A_{750}) is the difference in absorbances read at 664nm and 750nm; V is the volume of the extract in mL; and S is the volume of the filtered sample in mL.

Empirical and semi-empirical model for Chl-*a* estimation

As mentioned, a wide range of algorithms for Chl-*a* retrieval have been developed. Mishra & Mishra (2012) developed a normalized difference chlorophyll index (NDCI) in order to predict the concentrations of Chl-*a* in turbid productive estuarine and coastal waters using remote sensing data. Accurate correlations between Chl-*a* concentrations and two (2BDA) and three-band (3BDA) combinations in the near red and infrared regions have been reported by Moses et al. (2009) and Dall'Olmo & Gitelson (2005), respectively. Therefore, before generating an empirical model for Chl-*a* estimation in the Mirim lagoon, we tested these three semi-empirical algorithms that are based in the red or near-infrared (NIR) reflectance and are well known in the literature, which are presented in Table I. These algorithms were developed for sensors other than MSI. So, in order to apply the algorithms with the Sentinel-2 images, we had to make small adaptations to the bands: the band centered at 708nm was replaced by the band at 705nm and the band centered at 753nm was replaced by the band at 740nm.

The presence of phytoplankton in water will imply strong absorption in the blue (wavelength range from 430 at 450nm) and in the red (630 at 675nm) spectral regions, and higher reflectance

Table I. Semi-empirical algorithms to estimate Chl-*a* concentration.

Semi-empirical algorithm	Equation	Reference
NDCI	$\mathrm{Chl-a} \sim \frac{R(708)-R(665)}{R(708)+R(665)}$	Mishra & Mishra (2012)
3BDA	$\mathrm{Chl-a} \sim R_{665}^{-1} - R_{708}^{-1})^{*}R_{753}$	Gitelson et al. (2003)
2BDA	$\mathrm{Chl-a} \sim R_{665}^{-1})^{*}R_{708}$	Dall'Olmo & Gitelson (2005)

in the green spectral region, around wavelength 550nm, and in the NIR region, around wavelength 715nm, which is related to the scattering caused by phytoplankton cells (Curran & Novo 1988, Augusto-Silva et al. 2014). Thus, Chl-*a* can be detected using the spectral bands located in the blue, green, red or NIR regions of the reflectance spectrum (Blondeau-Patissier et al. 2014). In this way, two approaches for the empirical modeling were tested, single band and ratio bands, which were chosen based on other studies (Moses et al. 2009, Gilerson et al. 2010, Gurlin et al. 2011, Watanabe et al. 2015, Fassoni-Andrade et al. 2017, Gholizadeh & Melesse 2017). The single bands from Sentinel-2 MSI image used were those which Chl-*a* has strong absorption, in the spectral region of blue (B2) and red (B4), and where it has a peak of reflectance, green (B3) and NIR (B8). The band ratio was applied between the single bands tested, and aims to normalize (reduce) the effects of other variables, such as the ratio red-NIR, which tends to reduce the reflection od sediment effects (Matthews 2011). The reflectance at each pixel corresponding to the *in situ* collection point was selected from the different Sentinel-2 MSI sensor bands, allowing to correlate these data with the concentrations found on the fieldwork.

The verification of the data normality was performed through the Kolmogorov-Smirnov (KS) non-parametric test. After checking the normality of the data, Pearson's correlation coefficient (R) was used to verify the significant correlations ($p < 0.05$). From significant correlations, multiple regression was applied to establish empirical models. In the multiple regression analyzis, the "enter" method was used to include the independent variables in the model. Chl-*a* was used as the dependent variable, while the reflectance of single bands and band ratios that presented a significant correlation with the parameter were used as independent variables, generating an empirical model for Chl-*a* estimation. The final model selected was based on the best combination of statistical parameters and minor errors. The adjusted coefficient of determination (adjusted R^2), the F-Test of significance ($p < 0.05$), the Root-Mean-Square Error (RMSE) and the Mean Absolute Error (MAE) (Dill Hinnah et al. 2014), were used to evaluate the performance of the generated models (Fassoni-Andrade et al. 2017).

RESULTS AND DISCUSSION

Inter-comparison of atmospheric correction methods

Fig. 2(a) shows the comparative assessment of surface reflectance values (ρ_w) from the Sen2Cor and iCOR AC methods. This cross-validation aims to ensure that the results obtained by Sen2Cor are consistently comparable with

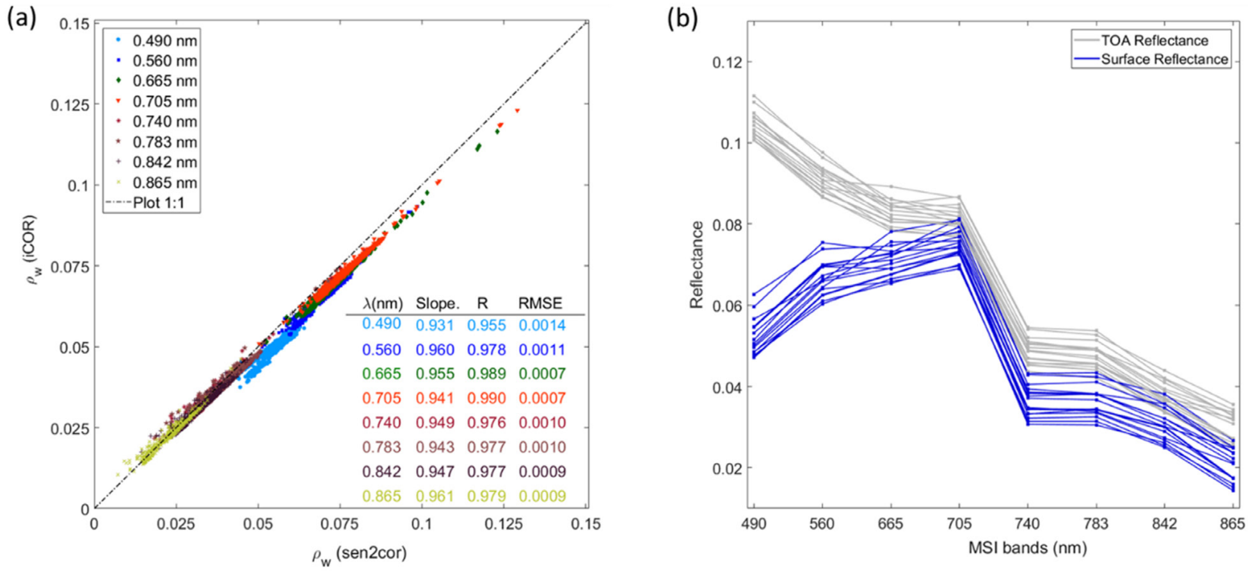

Figure 2. (a) Comparison of surface reflectance (ρw) between Sen2Cor and iCOR products across the lagoon; (b) Comparison between Sen2Cor surface reflectance and Top-of-Atmosphere (TOA) reflectance.

another methods, in this case iCOR, which is an AC tool that was developed to process, besides others, inland waters and land (De Keukelaere et al. 2018). From Fig. 2(a), it can be observed that the Sen2Cor results are almost similar to iCOR for all bands tested, which is a positive measure for our study (R > 0.955 and RMSE < 0.0014). Warren et al. (2019) showed that both processors showed improved performance when comparing to coastal and inland waters, and they suggested that these algorithms are better suited for AC over inland water. Fig. 2(b) shows the water spectrum in the 15 sampled points, comparing the TOA reflectance and surface reflectance after the Sen2Cor AC. The shape and magnitude after applying Sen2Cor AC coincides with the spectrum of typical water, with no scattering effect in blue band. As the image did not have high changes in Chl-*a*, such as flowering events, this signal at 660nm was not so evident. Also, the infrared bands show a low reflectance, which is reasonable and consistent for water.

Water Quality Parameters

The pH values were classified within the range required by Brazilian legislation (Brasil 2005) for "Class 2" (6 ≤ pH ≤ 9), which is the Mirim lagoon classification. Samples ranged from 7.00 to 8.00 (Table II) , presenting neutral and slightly alkaline values. Determining the pH values is important since it interferes with the chemical phenomena of water and with the metabolism of aquatic organisms. The photosynthetic activities carried out by algae communities consume and remove carbon dioxide to produce oxygen, increasing the hydroxide levels in water and consequently, pH values (Sharip et al. 2014). According to Vieira (2011), pH values can reach 9.0 in periods of high sunshine, which is related to algae photosynthetic activity in lakes and reservoirs with a high density of phytoplankton. Souza (2015) found similar pH values for the São Gonçalo channel, 6.8 for the high rainfall period (spring). This shows a similarity between the water quality of the São Gonçalo channel and the Northern Mirim lagoon. Chl-*a* concentrations in the lagoon varied considerably between the points sampled, with a CV of 0.83. The

Table II. **Descriptive statistics of the data obtained in the study.**

	pH	Chl-*a* ($\mu g.L^{-1}$)	Phosphorus ($mg.L^{-1}$)
Mean	7.71	16.32	0.12
Minimum	7.00	3.56	0.03
Median	7.80	11.57	0.10
Maximum	8.00	56.07	0.34
Standard deviation	0.30	13.48	0.08
Coefficient of variation (CV)	0.04	0.83	0.68

minimum concentration of Chl-*a* was 3.56µg. L^{-1}, while the maximum was 56.07µg.L^{-1} (Table II). This variation can be justified by the distance between the sampling points, resulting in distinct concentrations due to the different environmental characteristics of the lagoon. Overall, the values were high, but still within the range required by Brazilian legislation (< 30µg.L^{-1}). In an estuary near Mirim lagoon, Fassoni-Andrade et al. (2017) found low values of Chl-*a* in the winter period for the Patos lagoon (~ 2.93µg.L^{-1}). An increase in concentrations is expected as summer approaches, where there is a greater algae bloom due to the higher water temperature. The mean value for phosphorus was 0.12 mg.L^{-1} (Table II), higher than the acceptable limit established by Brazilian legislation (0.050 mg.L^{-1}). High phosphorus values may be related to a high Chl-*a* concentration, since it is one of the nutrients that support the increase in primary productivity, resulting in the growth of algae. Fia et al. (2009) also found very high phosphorus values in Mirim lagoon and its tributaries, characterizing these watercourses as hypereutrophic due to high concentrations of organic matter and nutrients (Lamparelli 2004, CETESB 2007). Nutrients such as phosphorus bioavailable form are an important factor to affect water quality (Şener et al. 2013), playing an important role in eutrophication processes on shallow waters (Soulsby et al. 2001).

The Northern Mirim lagoon is connected to the São Gonçalo channel, a fact that directly influences the water quality dynamics in this region. The channel is a natural outlet from Mirim lagoon waters, yet in some conditions (precipitation, water volume in the lagoons, wind speed, and direction) the flow direction may become reverse, flowing from the Patos lagoon to the Mirim lagoon (Souza 2015). This transition zone has an impact on water quality. The high Chl-*a* and phosphorus concentrations found at some points in this study indicate the eutrophication potential of these waters. Both water bodies (São Gonçalo channel and Mirim lagoon) are surrounded by agricultural areas which entail nutrient enrichment in the water, provoking algae blooms. The water dynamics in this region are complex, with an exchange of water from the channel to the lagoon in some cases, but the main direction being from the lagoon to the channel. Souza (2015) analyzed a variety of water quality parameters in the São Gonçalo channel and observed that in the region near to the connection with the Mirim lagoon the quality was worse. These findings contribute to the understanding that water quality of these two watercourses have a direct influence on one another.

Correlation between Chl-*a* and Sentinel-2 MSI data

In situ concentrations of Chl-*a*, band reflectance and band ratio were tested for normality by the Kolmogorov-Smirnov test. Bands B2, B3 and B4, and the ratio bands B3/B2, B8/B4, B4/B8, B8/B3 e B3/B8 presented normal distribution ($p > 0.025$). Table III shows the correlations between the Chl-*a* data collected *in situ* in Mirim lagoon and the reflectance of the spectral bands. Chl-*a* concentration presented a significant correlation ($p < 0.05$) with the B2, a spectral region with high absorption of this component (R = 0.61). Tebbs et al. (2013), using images from the Landsat ETM+ sensor, also found a reasonable correlation with the blue band (R = 0.40), a high correlation with the NIR region (R = 0.92) and a moderate correlation with the green band (R = 0.58). Zhang et al. (2011), using MODIS sensor data, found a poor correlation between Chl-*a* concentration and the reflectance in the visible region (R = -0.027 for the red band; R = 0.182 for the blue band; R = 0.195 for the green band; R = 0.468 for the NIR band).

Band ratios are used with the purpose of generating a greater amplitude in the effect of Chl-*a*. Chlorophyll recovery algorithms for turbid eutrophic waters often use bands at the wavelengths of red and NIR, capturing the reflectance limit of red, which is associated with the proliferation of dense surface algae (Gower et al. 2008, Gilerson et al. 2010). The ratio between the bands B4 and B8 showed a significant correlation with the concentrations of Chl-*a* (B4/B8 = -0.54 e B8/B4 = 0.56). Tebbs et al. (2013) evaluated that the B8/B4 ratio was the best correlation with Chl-*a* (R = 0.90). A significant correlation (R = -0.52) was also found between Chl-*a* and the B3/B8 ratio, wavelengths at which Chl-*a* has high reflectance. The B3/B2 presented the highest significant correlation with Chl-*a* (R = -0.75). This ratio highlights the differences between the two bands, increasing sensitivity to Chl-*a* and decreasing to SS, since Chl-*a* has an absorption region at the wavelength of blue and a maximum reflectance in green (Yacobi et al. 2011). This spectral relationship has already been used in other studies that performed the same type of analyzis. Fassoni-Andrade et al. (2017) found a R = 0.86 between the Chl-*a* data and the B3/B2 ratio using Landsat-8 OLI sensor for the Patos lagoon. Brezonik et al. (2009) analyzed the correlation of Lansat-5 TM sensor bands with Chl-*a* data in a Northern US lake, finding that the best adjustments were for B2 (R = 0.76) and B3 (R = 0.73). Gholizadeh & Melesse (2017)

Table III. Pearson's correlation coefficient (R) between the Chl-*a* data analyzed in the Mirim lagoon and the reflectance of the spectral bands.

Parameter	Band	R
Chl-*a* ($\mu g.L^{-1}$)	B2 (blue)	0.61*
	B3 (green)	0.29
	B4 (red)	0.47
	B3/B2	-0.75*
	B8 (NIR)/B4	0.56*
	B4/B8	-0.54*
	B8/B3	0.51
	B3/B8	-0.52*

*** The correlation is significant at the 0.05 level (2 extremities).**

analyzed the correlation between Landsat-8 OLI sensor bands and Chl-*a* concentration in the Bay of Florida, and found values ranging from R = -0.52 (B2/B8) to R = 0.60 (B8/B2) in the dry season, and R = -0.64 (B4/B8) to R = 0.65 (B2/B3) in the rainy season.

Modeling and mapping of Chl-*a*

Table IV shows the semi-empirical algorithms tested was very low (R between 0.042 and 0.052) for all models tested. This can be explained by the fact that these algorithms were created for different lakes in other regions and also using other sensors. Mishra & Mishra (2012) proposed the NDCI to estimate the concentration of Chl-*a* using MERIS images in estuarine and coastal turbid productive waters. Another justification would be the not so high values of Chl-*a* found in Mirim lagoon, which may have contributed to a low correlation, since the semi-empirical algorithms were generated for very productive waters. With the low correlation by the semi-empirical algorithms, the regression analyzis of multiple variables to establish an empirical model of estimation of Chl-*a* in Mirim lagoon was used, considering the significant correlations in Table III. Different independent variables (reflectance and ratios between Sentinel-2 MSI sensor bands) were combined to choose the best prediction model (Table V). All the different combinations obtained a high R, showing that there is a strong correlation between the dependent variable and the independent variables. This demonstrates that the models are efficient in predicting Chl-*a* from the selected independent variables. Model 2 showed the lowest RMSE and MAE values compared to the other models generated. Despite not presenting the highest adjusted R^2 it was chosen because it presented a satisfactory correlation (R = 0.81 and R^2 = 0.65) and the smallest errors.

Fig. 3 presents the multiple regression and the equation for the chosen model. All band values varying from 0 to 1. Chl-*a* was mapped satisfactorily across the study area (Fig. 4) using the empirical model generated. Low concentrations of Chl-*a* were observed both in the Northern end as well as in the lowest left margin (red ellipses). The low concentration mapped in the Northern end of the lagoon may be related to a significant higher concentration of SS in this region (Albertoni et al. 2017), especially because of its high turbidity and eutrophic waters, which dominate the spectral signal, preventing the detection of Chl-*a* in the images (Härmä et al. 2001). The same factor can be associated to the low concentration predicted in the left margin, mainly due to the influence of land use and occupation in this region (agriculture) which promotes sediments input in this area. Yellow ellipses (Fig. 4) show high concentrations of Chl-*a* (from 15 to 40µg.L^{-1}) representing shallower areas which average 3m deep (Munar et al. 2018), providing less water circulation and increasing primary productivity (Baumgarten et al. 1995). The highest concentration predicted by the model was 153.2µg.L^{-1}, a value high above the maximum concentration found *in situ*

Table IV. Pearson's correlation coefficient (R) between semi-empirical algorithms and Chl-*a in situ* data.

Semi-empirical algorithm	Reference	R
NDCI	Mishra & Mishra (2012)	0.042
3BDA	Gitelson et al. (2003)	0.052
2BDA	Dall'Olmo & Gitelson (2005)	0.043

(56.07µg.L^{-1}). This value, though, refers to only one pixel in the image, being the other values within the average observed in fieldwork data. The mean value predicted by the model was 17.34µg.L^{-1}, which is close to the field data actual mean value (16.32µg.L^{-1}). Matthews et al. (2012) classify waters with Chl-*a* concentration < 20 µg.L^{-1} from oligotrophic to mesotrophic waters. Thus, Mirim lagoon waters can be classified as mesotrophic, with moderate concentration of phytoplankton.

One of the phytoplankton functions is to regulate the primary productivity rate in aquatic ecosystems (Kosten et al. 2012). Changes in phytoplankton concentration interfere at all levels of the ecosystem food chain, altering the ecological balance and the water quality (Ferreira et al. 2017). A growing number of studies have been showing the importance of understanding Chl-*a* dynamics in water bodies, being a crucial parameter for water quality (Gücker et al. 2009, Cardoso et al. 2012, Katsiapi et al. 2012, Carneiro et al. 2014). Mirim lagoon is a water source for human supply, agriculture, livestock and recreation, but Chl-*a* is still poorly investigated in the region. Understanding Chl-*a* spatial distribution is essential to comprehend its variation throughout the lagoon in order to identify critical zones that demands more attention. Mapping of Chl-*a* concentration is also important to understand the impact of land use and occupation. We observed that different water constituents mapped from satellite images interfere in Chl-*a* concentration. This is accentuated in the transition zone from Mirim lagoon to São Gonçalo channel and in the lagoon margins, probably due to agricultural activities. It is also important to notice that climate changes in South America are expected to increase extreme events occurrence, which may also raise nutrient input from terrestrial to aquatic systems (Roland et al. 2012, Carneiro et al. 2014). Therefore, the model developed to map Chl-*a* in Mirim lagoon may work as a tool to support decision-making in the region, not only in the case of adaptation for climate change, but also in order to better understand the influence of changes in land use and occupation on water quality.

Some studies have explored water quality in the Mirim lagoon and its tributaries, including the São Gonçalo channel (Grutzmacher et al. 2008, Coradi et al. 2009, Fia et al. 2009, Souza 2015, Tormam et al. 2017), demonstrating a high potential of these waters for eutrophication due to nutrient enrichment. Despite being a proxy for phytoplankton and a eutrophication-related variable, Chl-*a* is still poorly understood in this region. This research focused on understanding Chl-*a* spatialization in the Northern Mirim lagoon, contributing to the comprehension of this variable and its effects on the region. Therefore, it may be used as a tool for water quality monitoring. Over the last years, remote sensing of inland has undergone significant advances (Palmer et al. 2015). However, some

Table V. Statistics of Chl-*a* estimation models.

Model	Independent variable	R	R^2	Adjusted R^2	p-value (F-Test)	RMSE*	MAE*
1	B2, B3/B2, B8/B4, B4/B8, B3/B8	0.82	0.67	0.49	0.04	7.84	0.40
2	**B2, B3/B2, B4/B8, B3/B8**	**0.81**	**0.65**	**0.51**	**0.02**	**7.79**	**0.13**
3	B2, B3/B2, B4/B8	0.80	0.65	0.55	0.008	7.80	0.14

*** Unit of the variables in µg.L^{-1}.**

challenges have still to be overcome, regarding mainly to AC accuracy and the understament of adjacent effects in tributaries (Ruddick et al. 2006). Moreover, this study was conducted using a single image. In water quality studies using remote sensing, ideally the use of more images to generate the empirical model and validate it is recommended. However, the literature presents satisfactory results of correlation between field and modelled data using only a single image (Alcântara et al. 2009, Fassoni-Andrade et al. 2017). Thus, it is important to point that the modelled Chl-a obtained in this study does not account for environmental changes in the lagoon, which can affect in situ conditions. On the other hand, the mapping of Chl-*a* concentration in the studied region is an important tool that allows to understand Chl-*a* dynamics and its relations to land use and occupation. It also allows understanding the drivers that impact water quality in different regions of the lagoon, being an important tool to water monitoring and to support decision-making. The developed empirical model allows the prediction of Chl-*a* without fieldwork measurements, utilizing satellite data. This is an important factor for the studied region since the Mirim lagoon is a large waterbody.

CONCLUSIONS

Mirim lagoon is extremely important for the Southern of Brazil and for its neighbor country, Uruguay, since it is linked to the Patos lagoon for the São Gonçalo channel. Thus, understanding the water quality situation and dynamics is essential to a better management of these water bodies. From the Chl-*a* data measured *in situ* and reflectance data from different spectral bands of the MSI sensor onboard the Sentinel-2 satellite, it was possible to generate an empirical model to estimate the concentration of Chl-*a* for the Northern Mirim lagoon. The performance of the generated model was satisfactory, which allows the spatialization of these parameters over the entire studied region.

This study shows the capability of an empirical model to estimate Chl-*a* concentration

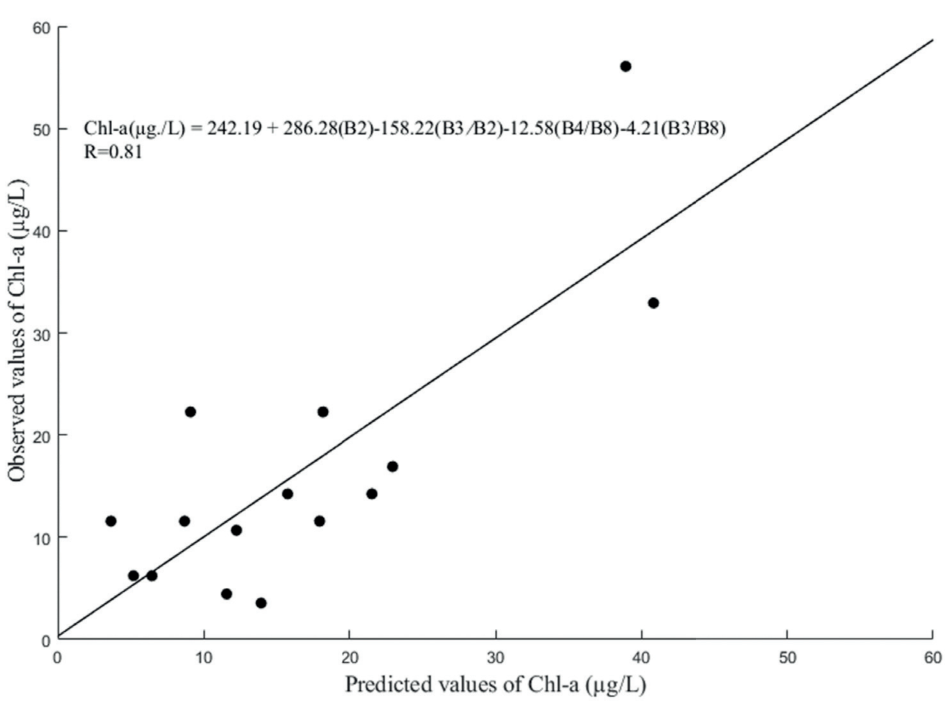

Figure 3. Predicted and observed values of Chl-a in the Northern Mirim lagoon.

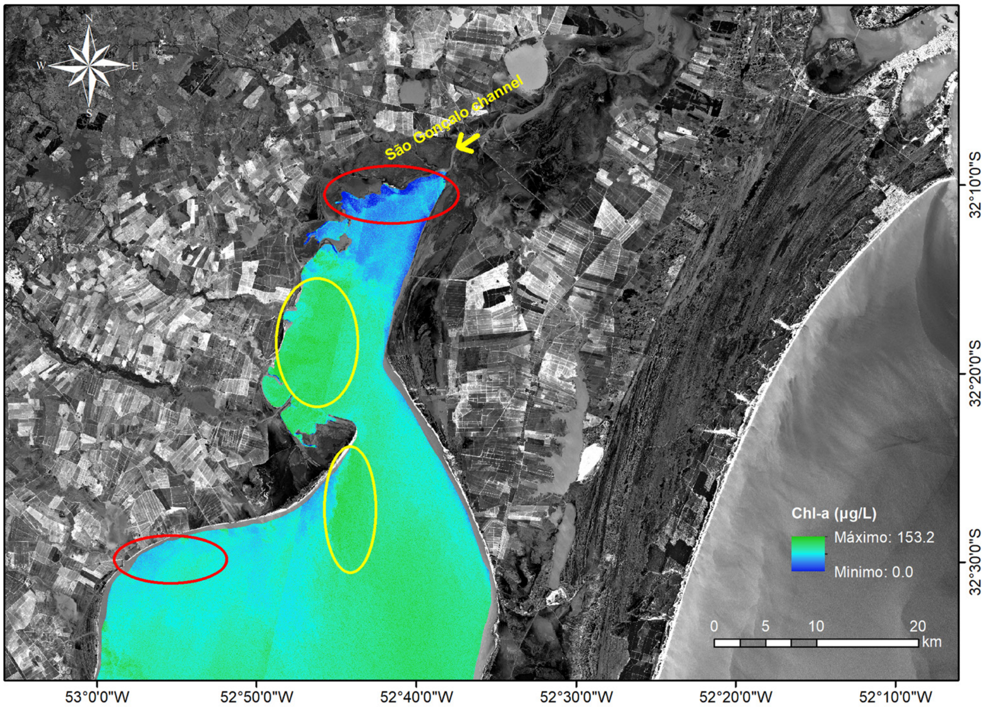

Figure 4. Mapping of Chl-a concentration (µg.L-1) in Mirim lagoon. Yellow ellipses represent higher concentrations and red ellipses smaller ones.

in the Mirim lagoon, even with limited *in situ* data. With this study, it is possible to analyze the spatial-temporal water dynamics much more efficiently, allowing public managers and surveillance agents to have a view of what happens around the lagoon, assisting inspection and mitigation actions.

For future studies, we recommend new *in situ* collection data to understand Chl-*a* dynamics in all the extension of the lagoon, combining fieldwork campaigns for validation of results in different periods of the year. Spectral *in situ* data collection would be recommended to test the AC as well. In general, the empirical model developed can be applied as a cost-effective tool to reduce the fieldwork measurements, as well as it can be used as a data source of Chl-*a* to understand eutrophication in this ecosystem.

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Cassia Brocca Caballero is the main author of the article, which is part of her dissertation research. Hugo Alexandre Soares Guedes is the supervisor of the research, being responsible for the multiple regression analysis and text revision. Alice César Fassoni-Andrade helped in the application of the LSMM and with text revision. Vitor Souza Martins was responsible for the logistic planning of field activities and helped with manipulation of Sentinel-2 image and text revision. Rosiméri da Silva Fraga helped in field activities and data manipulation, as well as text revision. And Karen Gularte Peres Mendes was responsible for water quality analysis and helped in text revision.