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Satellite estimates of chlorophyll-*a* concentration in the Brazilian Southeastern continental shelf and slope waters, Southwestern Atlantic

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ABSTRACT

Comparisons between *in situ* measurements of surface chlorophyll-*a* concentration (CHL) and ocean color remote sensing estimates were conducted in the Brazilian Southeast coast, Southwestern South Atlantic. *In situ* fluorometric data were acquired in four hydrographic cruises carried out during the austral summer and winter of 2001 and 2002. The satellite estimates of CHL were derived from SeaWiFS data recorded in HRPT mode by INPE's station with a nominal 1.1 km resolution. Four algorithms were used to estimate CHL: two empirical - Ocean Chlorophyll 4 bands (OC4v4), and 2 bands (OC2v4); one semi-analytical - Garver, Siegel, Maritorena (GSM01); and one based on neural network (NN). Comparisons of estimated and measured CHL were done within a temporal window of 12 hours from the *in situ* sampling time. SeaWiFS algorithms values are 5x5 pixel medians centered on the location of *in situ* sampling station. For the study area CHL was fairly well estimated by all the SeaWiFS algorithms. OC4 performed better (R^2 = 0.71; *rms* = 0.22) than the other algorithms (OC2, GSM01, and NN). The OC2 algorithm also showed a good performance with R^2 = 0.67 and *rms* = 0.23. The neural network algorithm performed better than the semi-analytical one (R^2 = 0.62 and 0.55, respectively), but with a higher *rms* (0.34 and 0.20, respectively). In general, the OC4, OC2, and NN algorithms showed a tendency for overestimating CHL at higher concentrations and underestimating at lower values. The semi-analytic GSM01 algorithm overestimated only the lower CHL, but underestimated most of the other values.

Keywords: Ocean color, Chlorophyll, SeaWiFS, Southwestern Atlantic

1. INTRODUCTION

The selective absorption of solar radiation in the blue and green wavelengths of the electromagnetic spectrum by the photosynthetic pigments, mainly by chlorophyll-*a*, allows the quantification of the oceanic phytoplankton biomass through satellite ocean color measurements[1,2]. In this context, the Sea-viewing Wide Field-of-view Sensor (SeaWiFS), launched in August, 1997, aims to provide quantitative data of the bio-optical properties of the oceans, examining the oceanic factors that affect climate global changes. The estimate of derived products, such as chlorophyll-*a* concentration, radiances and primary productivity obtained with the utilization of algorithms developed for ocean color remote sensing data, must be compared and validated in relation to *in situ* measurements. However, the bio-optical properties of the South Atlantic waters remain badly known, despite isolated efforts of some researchers[3,4,5,6].

The accuracy, precision and utility of the ocean color empirical algorithms to estimate the superficial chlorophyll-*a* distribution depends on the characteristics of these algorithms and on the *in situ* observations utilized on their respective developments. The ocean color semi-analytical algorithms have as their main advantage over the empirical band-ratios algorithms, the simultaneous derivation of various optical properties from a single spectrum of water leaving radiances. Nevertheless, the relative complexity of the semi-analytical algorithms has made difficult their development and operational implementation. The main advantages of an approach using neural networks to estimate sea surface chlorophyll-*a* concentration (CHL) are the association with non-linear complexities, the reduced sensitivity to noise, and an apparent more efficient filtering of residual errors of the atmospheric correction[7].

In this work, fluorometric *in situ* CHL measurements are compared against SeaWiFS estimates in the Brazilian Southeastern continental shelf and slope region, Southwestern South Atlantic. The accuracy of two empirical algorithms, one semi-analytical, and one by neural network applied to estimate CHL using satellite data are evaluated by the Pearson coefficient of determination (R^2) and the root mean square error (*rms*).

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2. DATA AND METHODS

2.1 *In situ* data

In situ CHL were measured during four oceanographic cruises conducted in the Brazilian Southeastern coast during austral summer and winter of 2001 and 2002 (Figure 1). The study area embraces the continental shelf and slope waters between Cape Sao Tome (22°S), State of Rio de Janeiro, and the Sao Sebastiao Island (23°50'S), State of Sao Paulo. The mesoscale cruises were held from 7 – 13, February 2002 (M1); 12 – 19, July 2001 (M2); 5 – 24, January 2002 (M3); 3 – 21, August 2002 (M4). The phytoplankton abundance was estimated from 250 mL of surface water samples filtered onto 25 mm Whatman GF/F filters. These were kept in liquid nitrogen until laboratory analyses using Turner 10-AU-005 fluorometer were performed. Chlorophyll was extracted in 90% acetone solution using the non-acidification method[8].

2.2 Remote sensing

Ocean color remote sensing images from SeaWiFS sensor were acquired at the same periods of the oceanographic cruises and processed as CHL fields with the application of empirical, semi-analytical and neural network algorithms. The SeaWiFS sensor has 8 spectral bands with a nominal spatial resolution of 1.1 km at nadir and a daily revisit time.

SeaWiFS images were acquired locally in high resolution mode at INPE's receiving station, in Sao Jose dos Campos, Brazil. The digital processing of the images was accomplished using SeaDAS software. Raw data was radiometrically calibrated to generate normalized water leaving radiances. The images considered of interest were selected according to the study area. Each image passed through atmospheric correction algorithms[9] before the calculation of CHL values.

The empirical algorithms Ocean Chlorophyll 4 bands – OC4, and Ocean Chlorophyll 2 bands – OC2[10] were applied to the SeaWiFS data, as well as the semi-analytical algorithm Garver, Siegel, Maritorena version 01 – GSM01[11], and the neural network algorithm NN[7] to estimate CHL. The OC2 algorithm estimates CHL based on a band ratio of $R_{RS}(490)/R_{RS}(555)$ using a modified cubic polynomial function (MCP). The OC4 algorithm also relates a band ratio with CHL using a polynomial function, but is based on the maximum band ratio (MBR) determined as the highest ratio (R_{max}) between the values of $R_{RS}(443)/R_{RS}(555)$, $R_{RS}(490)/R_{RS}(555)$, and $R_{RS}(510)/R_{RS}(555)$. O'Reilly et al.[10] presented a review of the OC2 and OC4 algorithms based in a wider and more representative data set from different oligotrophic and eutrophic biogeochemical provinces. The latest versions of the OC2 and OC4 algorithms were used in the present work to estimate CHL. The fourth order polynomial of the OC4 version 4 algorithm is defined as:

$$CHL = 10^{(0,366-3,067\,R_{4S}+1,930\,R_{4S}^2+0,649\,R_{4S}^3-1,532\,R_{4S}^4)} \tag{1}$$

where $R_{4S} = \log_{10}(R_{max})$. The modified cubic polynomial equation for the OC2 version 4 algorithm is defined as:

$$CHL = 10,0^{(0,319-2,336\,R_{2S}+0,879\,R_{2S}^2-0,135\,R_{2S}^3)}-0,071 \tag{2}$$

where $R_{2S} = \log_{10}\left(R_{555}^{490}\right)$.

Maritorena et al.[11] presented a protocol to improve the semi-analytical model initially proposed by Garver and Siegel[12], for global applications. The complete formulation of the model can be expressed as the following:

$$L_{WN}(\lambda) = \frac{tF_0(\lambda)}{n_w^2}\sum_{i=1}^{2} g_i\left\{\frac{b_{bw}(\lambda)+b_{bp}(\lambda_0)(\lambda/\lambda_0)^{-\eta}}{b_{bw}(\lambda)+b_{bp}(\lambda_0)(\lambda/\lambda_0)^{-\eta}+a_w(\lambda)+Chl_{ph}^*(\lambda)+a_{cdm}(\lambda_0)\exp[-S(\lambda-\lambda_0)]}\right\} \tag{3}$$

where L_{WN} is the normalized water leaving radiance, t is the air-sea transmission factor; $F_0(\lambda)$ is the extra-terrestrial solar irradiance; n_w is the refraction index of water; $g_1 = 0.0949$ sr^{-1} and $g_2 = 0.0794$ sr^{-1}; $bb_w(\lambda)$ is the backscattering of water; $a_w(\lambda)$ is the absorption by water; $bb_p(\lambda)$ is the backscattering by particles; Chl_{ph}^* is the chlorophyll-*a* specific absorption coefficient; S is the spectral decay for the dissolved matter and detritus absorption (*cdm*); η is the exponent of the power law for the particulate backscattering coefficient; λ_0 is the wavelength 443 nm wavelength.

The neural network model (NN) proposed by Gross et al.[7] was also applied in the present work. The authors[7] proposed the utilization of a multi-layer perceptron network to estimate CHL from the SeaWiFS reflectances. The perceptron is a simple form of a neural network used to classify a special type of pattern denominated as linearly separable, i.e. when the patterns stay in opposite sides of a hyperplane[13]. Rumelhart et al.[14] developed a back-propagation training algorithm, demonstrating that it is possible to train with efficiency networks with intermediate layers. This resulted in the most utilized model of neural networks, known as MLP.
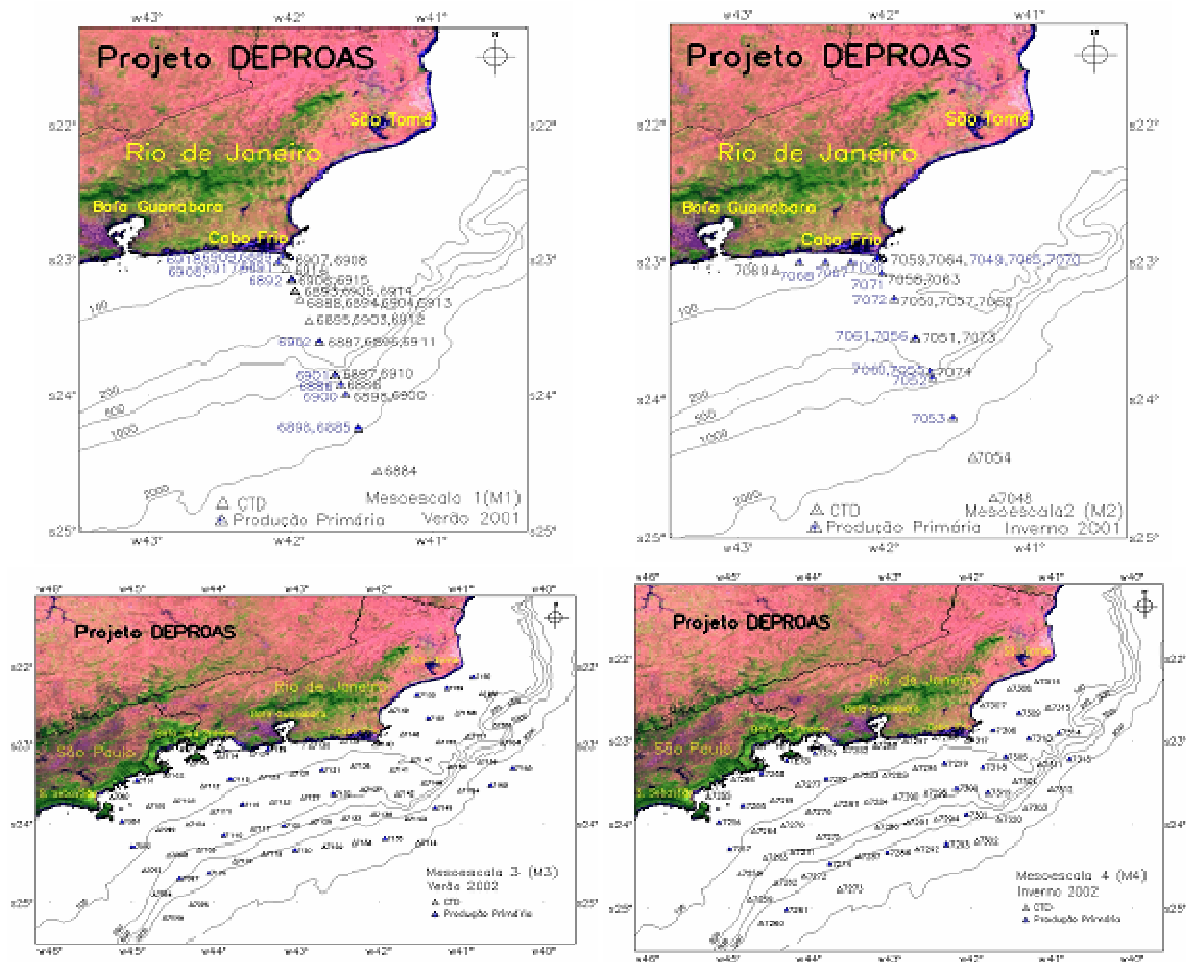

Fig. 1. Sampling grid of the mesoscale cruises 1 and 2 (summer and winter 2001), and 3 and 4 (summer and winter 2002), along the Brazilian Southeastern continental shelf and slope. Isobaths are in meters. Land mask is a SPOT 5 vegetation image.

The comparisons obtained between the *in situ* CHL and those estimated with SeaWiFS data were calculated inside a 12 hours window from the *in situ* sampling. The pairs of data were composed between the CHL_{insitu} and the median value of a 5 x 5 pixels (25 km^2) centered on the geographical position of the sampling station in the corresponding satellite image. The fluorometric data were statistically compared to the satellite estimates through linear regression analysis and root mean square error.

3. RESULTS AND DISCUSSION

For illustration, examples of SeaWiFS images processed using the 4 algorithms tested in this work are shown (Figure 2). In the 07/17/2002 the oligotrophic waters of the BC are observed offshore, over the slope region, in dark blue colors. An

intrusion of chlorophyll richer waters coming from the South can be observed over the inner shelf with CHL values > 2,0 mgm^{-3} around the Island of Sao Sebastiao (23°53'S-45°15'W). A surface signature of a mesoscale eddy with a mean diameter of ~70 km was identified in front of Cape Sao Tome between 22.50°S - 22.80°S, and 40.50°W - 41.50°W. Richer waters from the shelf (CHL>2.0 mgm^{-3}) appear being entrapped to the interior of this eddy. Another eddy with a mean diameter of ~75 km was observed around 23.30°S-41.50°W over the shelf break. Similar structures, but with smaller dimensions, were noted over the shelf, between Cape Sao Tome (22.00°S) and Cape Frio (23.00°S), with CHL values ranging between 2.0-2.7 mgm^{-3}. Patches of relatively higher phytoplankton biomass (CHL>2.0 mgm^{-3}) were observed in the coastal zone between Cape Frio and Vitória (20.50°S).
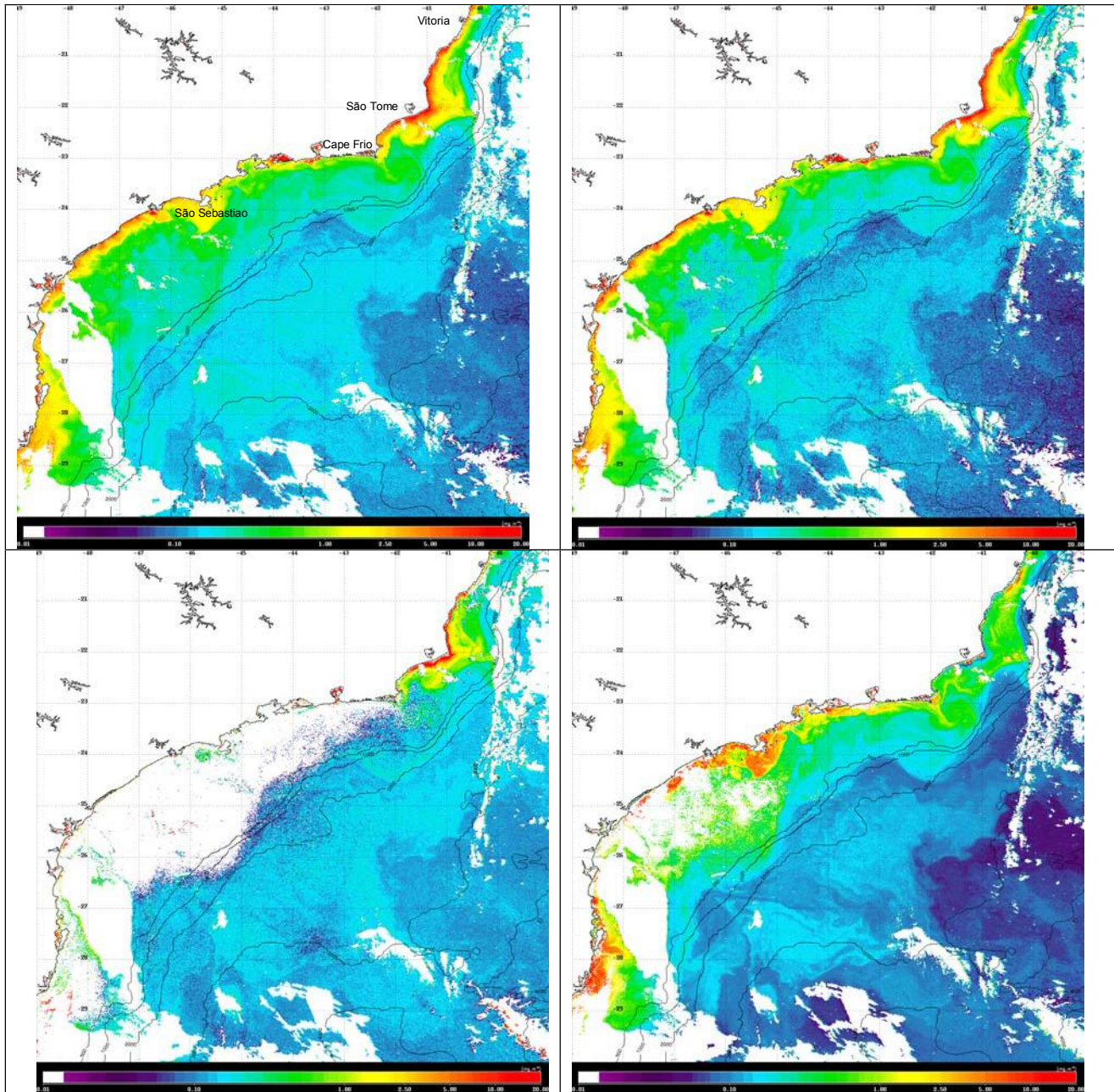

Fig. 2. Surface distributions of chlorophyll concentration estimated with OC4 (upper left), OC2 (upper rigth), GSM01 (lower left), and NN (lower right) algorithms applied to SeaWiFS data acquired on 07/17/2002 (see text for details). Isobaths in meters. Color table in logarithmic scale. Land and clouds are masked in white.

The empirical algorithm OC4 presented the best performance during the summer (R^2=0.87) even although with a higher *rms* when compared with OC2 (0.22 and 0.20, respectively). The other algorithms tested – GSM01 and NN, also presented a good performance. The relative performance of the algorithms was similar during the winter, but with lower coefficients of determination (Figure 3). Considering the whole data set (Figure 4), the NN algorithm presented a higher coefficient of determination than with GSM01. The OC4 algorithm presented the best performance (R^2=0.71, *rms*=0.22). In general, the OC4 algorithm underestimated the lowest CHL values, and overestimated the highest concentrations.
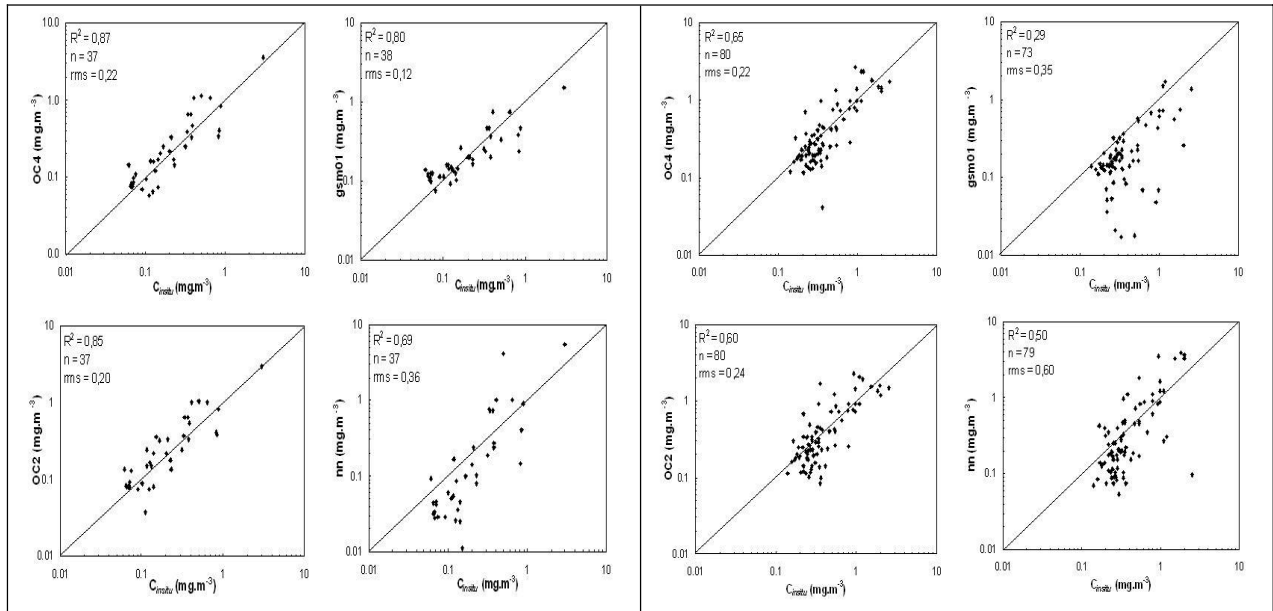

Fig. 3. Comparisons between SeaWiFS CHL estimates and *in situ* values: Scatter plots of SeaWiFS OC4, OC2, GSM01, and NN (see text) against C_{insitu} obtained during summer (left) and winter (right).
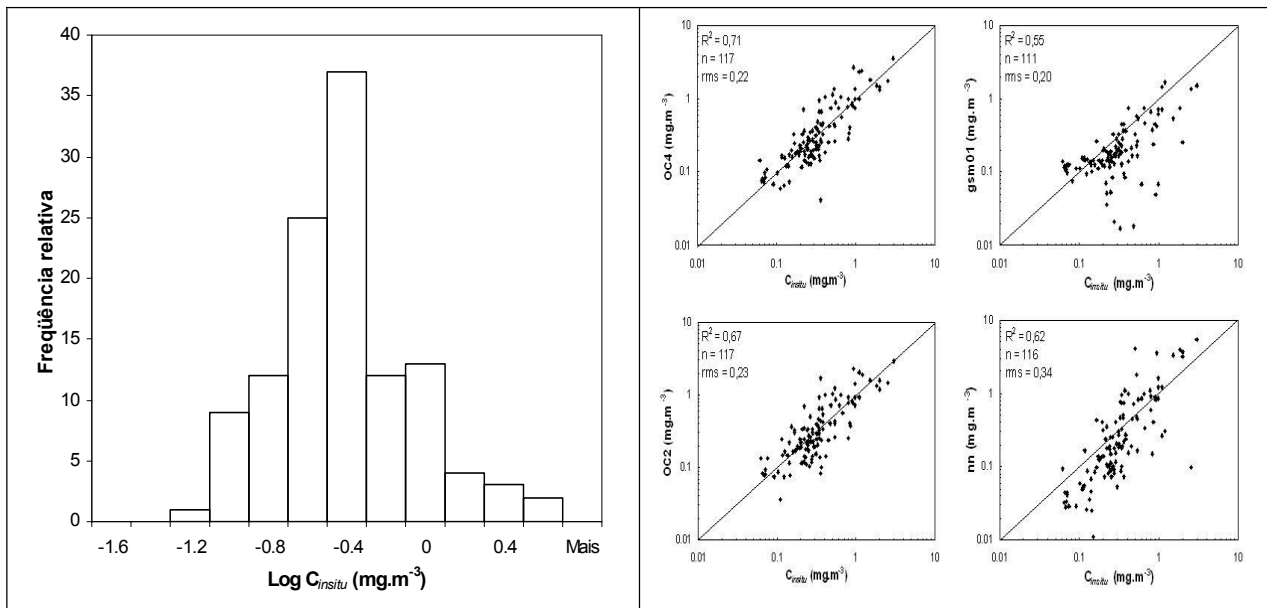

Fig. 4. Comparisons between SeaWiFS CHL estimates and *in situ* values: frequency distribution of log(C_{insitu}) (left); scatter plots of SeaWiFS OC4, OC2, GSM01, and NN (see text) versus C_{insitu} (right).

Comparison between *in situ* chlorophyll measurements and satellite remote sensing estimates are scarce in Brazilian waters. Omachi and Garcia[4] analyzed SeaWiFS empirical algorithms to estimate CHL in the Southwestern-South Atlantic and concluded that a band ratio of 2 bands (490 and 555 nm) obtains better results (R^2=0.90) than an approach using 4 bands. Garcia et al.[6] show that the NASA's OC4v4 algorithm for extracting chlorophyll-*a* data in the Southwestern Atlantic would result in an error margin of at least 42% in waters without strong influence of continental discharge (from La Plata River or Patos Lagoon). A derived regional algorithm improved the error margin to some extent (32%), and significantly reduced the bias. The authors also concluded that in coastal waters affected by river runoff, the OC4v4 algorithm highly overestimates chlorophyll values.

The data set utilized in the present study includes samples from Case 1 and Case 2 waters. The NASA's algorithms are adjusted to a heterogeneous and representative data set, but mainly for Case 1 waters. Nevertheless, frequent and well distributed *in situ* measurements in the Southwestern Atlantic are scarce which requests the adjustment of regional algorithms. When *in situ* chlorophyll measurements are compared with satellite estimates other methodological aspects of the data processing dominates in relation to the bio-optical algorithms itself. An efficient atmospheric correction is fundamental for good performance of those algorithms. Since in the visible part of the electromagnetic spectrum most of the radiance measured by an orbital sensor in the top of the atmosphere is originated in the atmosphere itself and not in the ocean[15], small errors during the atmospheric correction scheme can result in significant deviations from the marine bio-optical properties.

4. CONCLUSIONS

In the present work, comparisons between *in situ* chlorophyll concentrations and ocean color remote sensing estimates were accomplished over the shelf and slope waters of the Brazilian Southeastern coast, Southwestern South Atlantic region. The chlorophyll concentrations were reasonably well estimated with the use of SeaWiFS algorithms during the analyzed period. The NASA's OC4v4 algorithm presented the best performance among the 4 algorithms tested, in relation to the *in situ* fluorometric measurements. In general, the OC4 algorithm underestimates lower chlorophyll values and overestimates the higher concentrations.

The OC2v4 algorithm also presented a good performance. The neural network algorithm (NN) performed relatively better than the semi-analytical one (GSM01), but with a higher residual. The OC2 and NN algorithms showed a tendency to overestimate the higher chlorophyll concentrations and to underestimate the lower values. The GSM01 algorithm tended to overestimate the lower chlorophyll concentrations and to underestimate most of the other values.

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