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A COMPARISON BETWEEN SEMI-ANALYTICAL AND EMPIRICAL REFLECTANCE MODEL IN THE CASE OF A HIGH OCEANIC PHYTOPLANKTON BLOOM IN THE SOUTH WESTERN ATLANTIC OCEAN

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1: INTRODUCTION

Semi-analytical (SA) and empirical ocean color algorithms are routinely used to monitor global chlorophyll biomass in the oceans. SA models are particularly attracting since they relate inherent optical properties of the seawater to apparent optical properties like remote sensing reflectance. In addition to this, SA models have the capacity to derive various bio-optical parameters from a single set of remote sensing reflectance data. Empirical algorithms make no use of optical theory and are derived from statistical relationships between remote sensing reflectance ratios and chlorophyll a concentration. Maritorena *et. al* (2002) used model parameters which were derived through a "statistical optimization procedure" to maximize the algorithm performance for the global ocean. Remote sensing reflectance at five wavebands are used as model input, combined with IOP parameters that vary depending on water optical characteristics: spectral phytoplankton specific absorption coefficients, the spectral slopes of colored dissolved and detrital material and the power law exponents for spectral variability of particle backscattering. The resulting SA model, called GSM01, is now routinely used by SeaDAS software.

Empirical algorithms are regularly up dated as the SeaBASS global ocean color database increases although high chlorophyll data from case 1 waters are not sufficiently represented. In November 2004 during an oceanographic cruise (PATEX I) along the Patagonian shelf break, bio-optical data were collected within a large phytoplankton bloom dominated by diatoms and dinoflagellates (Garcia *et al.,* 2006). The dataset consists of radiometric measurements and chlorophyll concentration data at 18 stations along the shelf break.

A SA reflectance model, based on the GSM01 was used to retrieve chlorophyll concentration as well as particle backscattering and colored dissolved organic matter (CDOM) absorption. The results from this model were then compared with the global ocean color empirical algorithms OC2v4 and OC4v4. In addition, comparison between the GSM01 and empirical models based on SeaWifs images was carried in the same region.

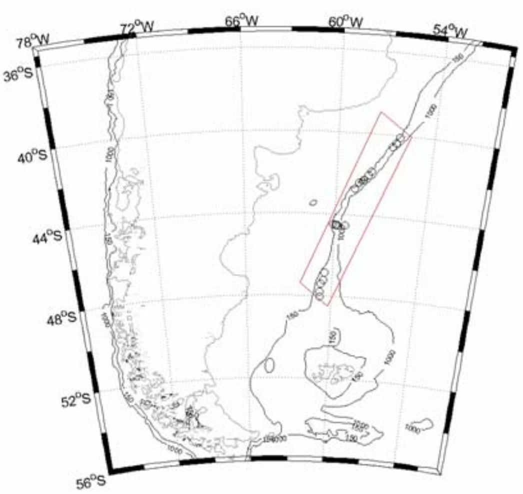

Figure 1: Map showing the Patagonian Shelf break. The black circles represent the sampling stations during PATEX I cruise. The red box represents the area selected for satellite data retrieval.

2: Ocean color algorithms

2.1. Semi-Analytical reflectance model

A second order Gordon reflectance model (Equation 1, Gordon *et. al*., 1988) was used with the parameters found in the literature.

$$R_{rs}(\lambda)=\sum_{i=1}^{2} l_i\left[\frac{b_b(\lambda)}{a(\lambda)+b_b(\lambda)}\right]^i$$

Equation 1

In this equation, the absorption coefficient a(λ) is written as

$$a(\lambda)=a_w(\lambda)+a_{phyto}(\lambda)+a_{cdom}(\lambda)$$

Equation 2

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where $a_w(\lambda)$, $a_{phyto}(\lambda)$, and $a_{cdom}(\lambda)$ are the spectral absorption coefficient of pure water, phytoplankton cells and colored dissolved organic material, respectively. Similarly, $b_b(\lambda)$ can be written as

$$b_b(\lambda)=b_{bsw}(\lambda)+b_{bp}(\lambda)$$

Equation 3

where $b_{bsw}(\lambda)$ and $b_{bp}(\lambda)$ are the backscattering coefficients of pure seawater and particulate matter respectively. Among these five components of total absorption and total scattering, $a_w(\lambda)$ and $b_{bsw}(\lambda)$ are known. $a_{phyto}(\lambda)$, $a_{cdom}(\lambda)$ and $b_{bp}(\lambda)$ change as a function of phytoplankton, CDOM and particulate matter concentrations. They are modeled as

$$\begin{aligned}
a_{phyto}(\lambda)&=a^*_{phyto}(\lambda)*[Chl]\\
a_{cdom}(\lambda)&=a_{cdom}(\lambda_0)*\exp(-S(\lambda-\lambda_0))\\
b_{bp}(\lambda)&=b_{bp}(\lambda_0)\left(\frac{\lambda}{\lambda_0}\right)^{-\eta}
\end{aligned}$$

Equation 4

where a^*_{phyto} is the chlorophyll *a* specific absorption coefficient (taken from Maritorena *et. al.,* 2002), [Chl] is the chlorophyll *a* concentration, $a_{cdom}(\lambda_0)$ and $b_{bp}(\lambda_0)$ are the CDOM absorption coefficient and particulate backscattering coefficient at the reference wavelength λ_0, S is the spectral decay constant for CDOM absorption and η is the power law exponent for particulate backscattering coefficient. Both S and η where also taken from the work of Maritorena *et. al.* (2002).

Using this parameterization Equation 1 can be rewritten:

$$R_{rs}(\lambda)=\sum_{i=1}^{2} l_i\left[\frac{b_{bsw}(\lambda)+b_{bp}(\lambda_0)\left(\frac{\lambda}{\lambda_0}\right)^{-\eta}}{a_w(\lambda)+a^*_{phyto}(\lambda)*[Chl]+a_{cdom}(\lambda_0)*\exp(-S(\lambda-\lambda_0))+b_{bsw}(\lambda)+b_{bp}(\lambda_0)\left(\frac{\lambda}{\lambda_0}\right)^{-\eta}}\right]^i$$

Equation 5

$$MSD=\frac{1}{(N_\lambda-1)}\sum_{i=1}^{N_\lambda}\left[R_{rs_{\text{modelled}}}(\lambda_i, Chla, a_{cdom}(\lambda_0), b_{bp}(\lambda_0))-R_{rs_{\exp}}(\lambda_i)\right]^2$$

Equation 6

which is a function of three variables: Chl a, $a_{cdom}(\lambda_0)$, $b_{bp}(\lambda_0)$.

The three variables (Chl a, a_{cdom}, b_{bp}) were retrieved by minimizing the mean square difference MSD (Equation 6). In this equation, $Rrs_{modeled}$ and Rrs_{exp} refer to modeled (calculated) and experimental (measured) remote sensing reflectance. The MSD equation was solved using the Levenberg-Marquardt nonlinear method.

2.2. Empirical models

Two empirical algorithms were used in this work: The NASA OC2v4 and OC4v4. Both are based upon reflectance band ratios and are defined as follow

$$[Chl\_OC4_{v4}]=10^{\left(A_0+A_1R+A_2R^2+A_3R^3+A_4R^4\right)}$$

Equation 7

$$[Chl\_OC2_{v4}]=10^{\left(A_0+A_1R+A_2R^2+A_3R^3\right)}+A_4$$

Equation 8

where the coefficients A_i are listed in Table 1.

Table 1: Pamareters of the empirical algorithms

	Coefficients				
Model	**A_0**	**A_1**	**A_2**	**A_3**	**A_4**
OC2v4	*0.319*	*-2.336*	*0.879*	*-0.135*	*-0.071*
OC4v4	*0.366*	*-3.067*	*1.930*	*0.649*	*-1.532*

R is either the reflectance ratio Rrs(490)/Rrs(555) in the case of the OC2v4 or is the maximum band ration of Rrs(443)/Rrs(555), Rrs(490)/Rrs(555) and Rrs(510)/Rrs(555) in the case of the OC4v4.

3: Results and Discussion

3.1. In situ Measurements

The radiometric measurements were carried out with a Satlantic TSRB and include spectral surface downwelling irradiance and subsurface spectral upwelling radiance measurements from which remote sensing reflectances at five wavelengths (412, 443, 490, 510 and 555 nm) were calculated. The chlorophyll analysis where performed using the fluorimetric method. The chlorophyll a concentrations measured during PatEx I experiment range from 1.8 to 19.9 mg.m^{-3}. The SA model however highly overestimated one *in situ* chlorophyll value (output of the SA model was 150.7mg.m^{-3} for an *in situ* concentration of 6.4mg.m^{-3}). This station was removed from the dataset for the regression calculation of both SA and empirical models. Such high overestimations were also observed using the SA and empirical models with satellite data. Figure 2 shows the performance of the chlorophyll algorithms used in this work. The coefficients of determination (r^2) were 0.90, 0.85 and 0.70 for the OC4, OC2 and SA algorithms respectively (Table 2). The limited *in situ* dataset available would not allow final conclusion about the superiority of one model. The encouraging observation is that the three models remained fairly consistent even at very high chlorophyll concentration, with the NASA operational model (OC4v4) showing better consistency.

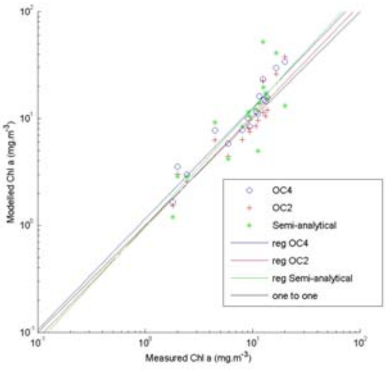

Figure 2: Regression of empirical and SA models versus *in situ* chlorophyll for the PatEx I dataset.

Table 2: Regression parameters of empirical and SA models with *in situ* data.

	Patex N=17		
	OC2v4	**OC4v4**	**SA**
r^2	0.8529	0.8974	0.6996
Slope	1.0410	1.0389	1.0936
Intercept	-0.0161	0.0607	-0.0042

3.2. Chlorophyll derived from SeaWiFS

In order to test these models with a more extended dataset, a comparison between SA and empirical models was carried out based on chlorophyll concentration retrieved from one kilometer resolution SeaWiFS images from October 2003 to February 2004. One image per month was selected: 19th Oct 17th Nov 14th Dec, 16th Jan and 7th Feb (the selected region corresponds to the PatEx I sampling area - Figure 1). The calculated chlorophyll concentration as measured from satellite data were filtered to remove values above 100mg.m^{-3} (Table 3).

Table 3: Data removed by filtration process (number of pixels).

	SeaWiFS data removed				
	Oct.	**Nov.**	**Dec.**	**Jan.**	**Feb.**
All data	78108	71786	89517	82715	64505
OC2v4	48	20	93	96	133
OC4v4	16	4	1	9	3
GSM01	2	0	1	0	0
Filtered data	78059	71763	89424	82618	64491

Firstly, as was observed from *in situ* measurements in November 2004, very high chlorophyll concentrations were observed by SeaWiFS sensor (Figure 3 and Figure 4). The three models (OC4v4, OC2v4 and GSM01) where in good agreement as shown in Table 4 and Table 5 except for October. Overall, the coefficients of determination were better with satellite data than with *in situ* data, probably due to the larger dataset. The maximum chlorophyll values were observed in December, with a concentration of about 40 mg.m^{-3} as calculated with the OC4v4. The maximum value estimated by both OC2v4 and GSM01 algorithms reached almost 100 mg.m^{-3} for the same month, suggesting that both tended to overestimate high chlorophyll concentration.

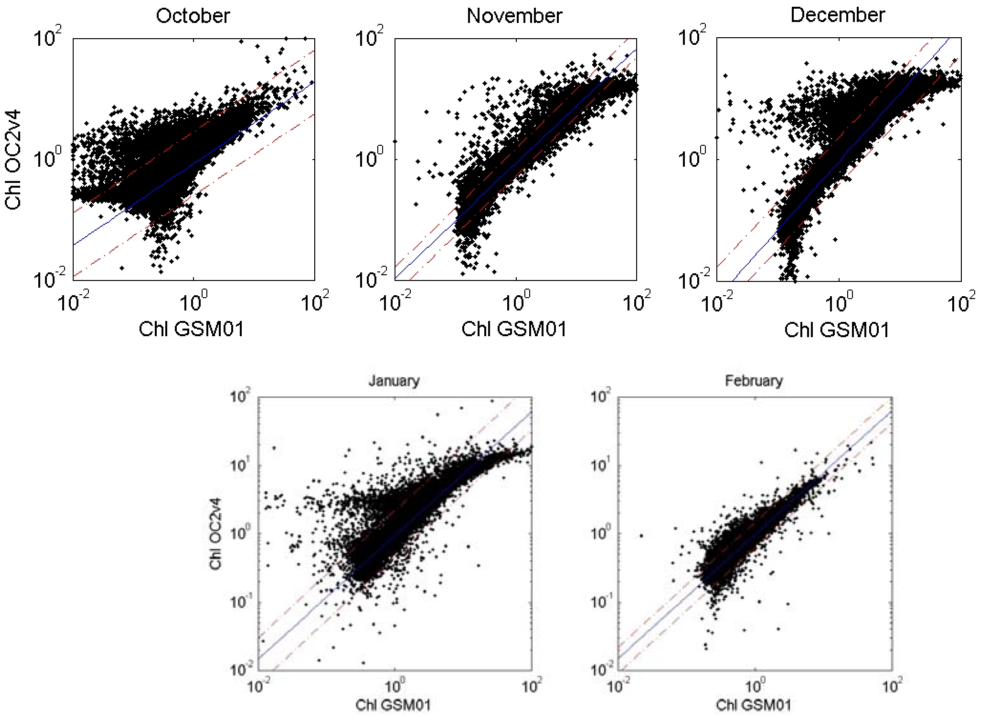

Figure 3: Regression of OC2v4 versus SA model for Summer 2003/2004. Solid line is the regression line, the two dash dotted lines represent the 95% confidence bounds of the regression.

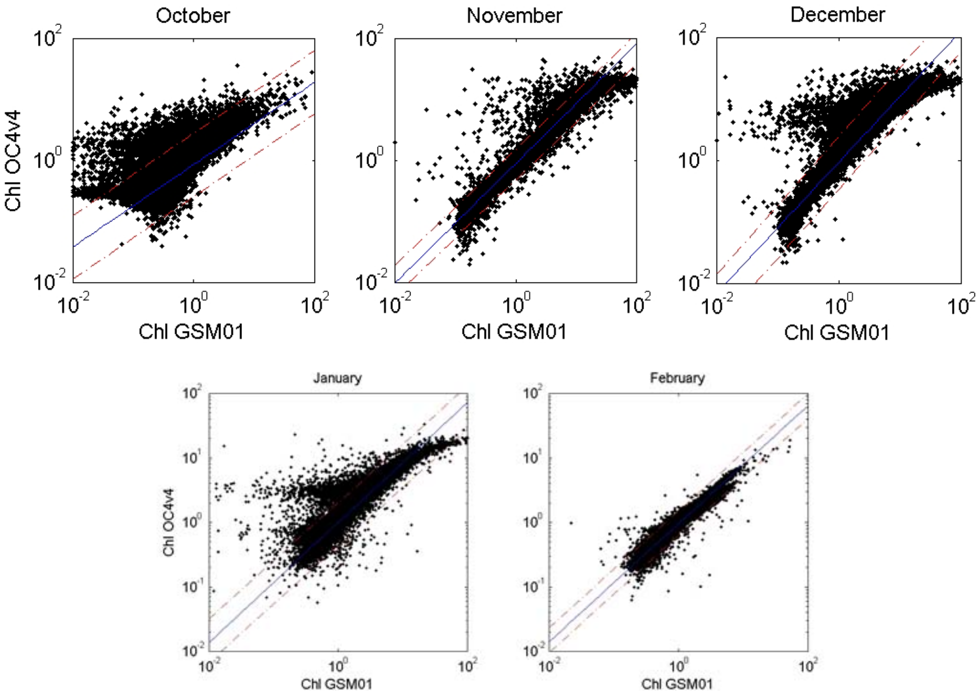

Figure 4: Regression of OC4v4 versus SA model for Summer 2003/2004. Solid line is the regression line, the two dash dotted lines represent the 95% confidence bounds of the regression.

Generally, the SA model was better correlated to the OC4v4 except for the month of October (Table 4 and Table 5). The tendency of the SA model was to overestimate the chlorophyll concentration at very high values (Figure 3 and Figure 4), mainly for November, December and January. For these three months and at different ranges of chlorophyll concentration, a significant proportion of the data points were overestimated by the empirical in comparison to the GSM01 algorithm. This is particularly noticeable for October. As shown with the 95% confidence bounds of the regression (dash dotted line), the data showing these deviations do not represent an important proportion. Nonetheless, this behavior will need further investigations especially because they seem to append on a fairly large range of chlorophyll concentrations. This trend actually appeared for all sampled months although with variable intensity. Chlorophyll concentration derived by both OC4v4 and GSM01 algorithms from Oct 2003 to Feb 2004 suggest a monthly variability in their agreement.

Table 4: Monthly regression for summer 2003/2004 on PatEx I sampling site, OC4v4 versus SA model. N indicates the number of data points.

OC4v4 vs SA	**Patagonian Shelf Summer - 2003/2004**				
	Oct.	**Nov.**	**Dec.**	**Jan.**	**Feb.**
N	78059	71766	89424	82618	64491
r^2	0.502	**0.969**	**0.944**	**0.887**	**0.940**
Slope	0.676	1.031	1.067	0.931	0.914
Intercept	-0.063	-0.052	-0.027	-0.001	-0.023

Table 5: Monthly regression for summer 2003/2004 on PatEx I sampling site, OC2v4 versus SA model. N indicates the number of data points.

OC2v4 vs SA	**Patagonian Shelf Summer - 2003/2004**				
	Oct.	**Nov.**	**Dec.**	**Jan.**	**Feb.**
N	78059	71766	89424	82618	64491
r^2	**0.51**	0.967	0.938	0.883	0.937
Slope	0.678	0.993	1.121	0.904	0.906
Intercept	-0.067	-0.087	-0.040	-0.025	-0.016

4: Conclusion

We have compared the performances of semi analytical and empirical ocean color algorithms to retrieve chlorophyll concentration in the Southwestern Atlantic Ocean. Based on *in situ* measurements of chlorophyll concentration gathered during PATEX I experiment, we observed that empirical algorithms can perform better than SA models. However, an encouraging result was that when compared with in situ chlorophyll data, both types of algorithms remains consistent even at high chlorophyll concentration.

When using satellite reflectance data, the algorithms still produced comparable values at high [Chla] although a tendency to overestimate chlorophyll concentration was observed for the SA model. The reliability of very high [Chla] estimated by satellite data still needs to be validated with *in situ* measurements.

An important point to be addressed in a further work is the seasonal variability of the relationship between OC4v4 and SA algorithms. The deviation from the one-to-one relationship was observed both at low and high chlorophyll concentration and this will need further investigation.

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