DEVELOPMENT OF A FILTER FOR PHYCOCYANIN BIO-OPTICAL ESTIMATION

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ABSTRACT

Phycocyanin is a unique pigment for cyanobacteria in inland waters which has been identified by remote sensing. Several band ratio algorithms were developed to estimate and identify phycocyanin using its absorption spectral characteristics. However, other water column constituents influence the remote sensing reflectance measurements at the PC absorption wavelengths. To remove these interferences from the remote sensing reflectance spectra, we proposed a filter to calculate a new remote sensing reflectance for the target wavelengths. The filter showed a better performance for phytoplankton dominated environments enhancing its applicability for the quantification of phycocyanin during algal bloom conditions. This filter demonstrates to be useful because of the new Earth Observing Sensors which will include the phycocyanin absorption spectral bands such as the Ocean and Land Color Instrument (OLCI) from the European Space Agency and SABIA-MAR which is a project from two space programs from Brazil and Argentina.

Index Terms— Earth Observing System, Environmental monitoring, Water pollution, Geophysical signal processing, Lakes

1. INTRODUCTION

Phycocyanin (PC) is an accessory photosynthetic phycobilin pigment, which has been used as a proxy to estimate cyanobacteria concentration in inland waters [1]-[2]. Cyanobacteria, also known as blue-green algae (BG), under certain ecological and biological condition, produce toxins which have been affecting water quality of aquatic systems around the world [2]. Thus, the monitoring of Cyanobacterial Harmful Algal Blooms (CHABs) is needed particularly in the aquatic systems that have had a history of occurrence and are used for recreation and water supply for domestic use. However, traditional methods for monitoring CHABs consist of field sample collection, laboratory analysis, microscopic identification, and enumeration of phytoplankton, which are time-consuming and costly procedures [3]. Remote sensing techniques have been proved to be a valuable tool for this application. It uses the distinct optical characteristic of PC, i.e., absorption minima around 620 nm [4]-[6] as an indicator of CHABs.

So far, three different semi-empirical remote sensing reflectance (R_{rs}) band ratio models have been proposed to analyze the PC content in inland waters with dominance of chlorophyll-*a* (chl-*a*), total suspended solids (TSS), and colored dissolved organic matter (CDOM). These band ratios explored the PC absorption feature around 600 to 620 nm and the reflectance peak either at 650 nm or around 700 nm. These models are, (1) Schalles and Yacobi (SC00) [4] ($R_{rs}(650)/R_{rs}(624)$), (2) Simis et al (SI05) [5] ($R_{rs}(709)/R_{rs}(620)$), and (3) Mishra et al (MI09) [6] ($R_{rs}(700)/R_{rs}(600)$).

Mishra et al. [6] exploited the PC absorption at 600 nm instead of the minima at 620 nm, because of the reduced influence of chl-*a* at 600 nm. Ogashawara et al. [7] reviewed five PC algorithms and also noticed that MI09 was more sensitive to PC than the others algorithms, however, they also observed that 600 nm still have influence of others factors such as chl-*a* and TSS. In this research, we present a novel method to enhance the accuracy of PC bio-optical models by reducing the interference of chl-*a* and TSS on the PC absorption spectral region.

2. HYPOTHESIS

Our hypothesis is based on Mishra et al. [6] and Ogashawara et al. [7] observations of the influence of chl-*a* and TSS on the R_{rs} spectra at PC absorption region. To test our hypothesis, we ran a series of two dimensional (2D) color correlation plots of R_{rs} spectra from a tropical reservoir located between São Paulo and Rio de Janeiro States, Brazil - Funil Hydroeletric Reservoir (22º32' S and

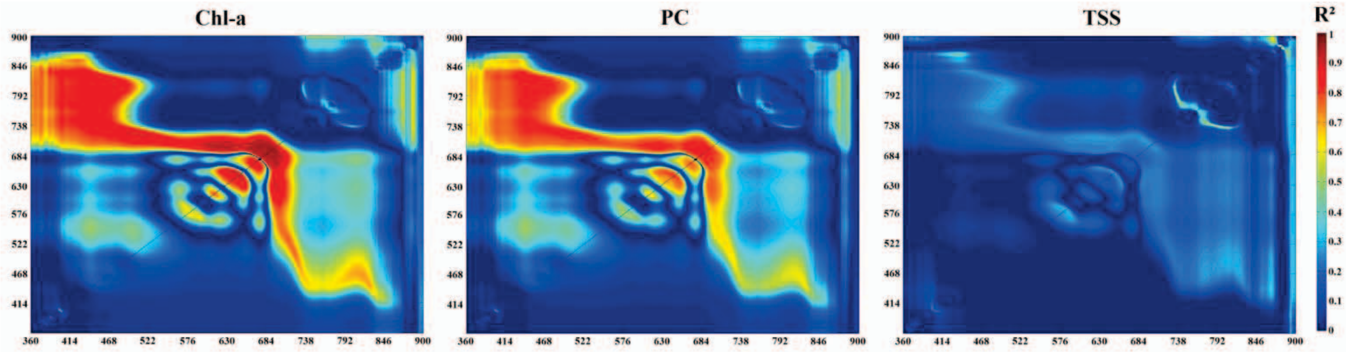

Fig 1 - Two dimensional color correlograms of R_{rs} band ratios and concentration of chl-*a*, PC and TSS.

44º45' W). Each 2D color correlation plot correlates 292681 band ratios values from the R_{rs} spectra to each limnological concentration (Figure 1). Concentrations of chl-*a,* PC, and TSS were measured from water samples using the methods described in Ogashawara [7].

2D color correlation plot analysis confirmed the observations made by Mishra et al. [6] and Ogashawara et al. [7] by producing the highest R^2 (0.93) between chl-*a* concentrations and MI09, while SC00 and SI05 showed a R^2 of 0.88 and 0.90 respectively. These results also showed that PC algorithms are very sensitive to chl-*a*. For PC concentrations prediction, SC00 and SI05produced a R^2 of 0.77 and 0.78 respectively, while MI09 showed a R^2 of 0.82; proving that MI09 is the most sensitive to PC as well. However, all algorithms showed more sensitivity to chl-*a* than PC. For the TSS 2D color correlation plot, SC00 produced a R2 of 0.18 (p= 0.41), while SI05 and MI09 showed a R^2 of 0.26 (p= <0.001) and 0.24 (p= 0.019) respectively, indicating some influence of TSS at the PC absorption feature.

3. FILTER DEVELOPMENT

To develop the filter we used two different study sites: the Funil Reservoir (Brazil) and Catfish Ponds (Stoneville, MS, USA) [7]. Figure 2 shows ternary plots of the normalized absorption coefficients of phytoplankton, non-algal particles and CDOM at 620 nm which is a typical PC absorption band. These ternary plots show that for the Funil Reservoir (Fig. 2A) the CDOM absorption is higher while for the catfish ponds the phytoplankton absorption coefficient was higher than the others.

In order to reduce the influence of these constituents at the PC absorption spectral region, we developed a filter using the inverse R_{rs} values. The R_{rs} values were used due to the fact that it could act as a proxy to spectral absorption. These values were used to isolate the PC absorption signal at 600, 620, and 625 nm from the composite absorption signal at those spectral regions due to the influence of OCAs the absorption of non PC constituents. R_{rs}^{-1} at 575 nm was used in this PC absorption isolation procedure with an assumption that inverse reflectance at 575 nm could be related to the absorption of chl-*a* and reflectance of TSS. R_{rs}^{-1} (575 nm) value was subtracted from the reflectance value at 600, 620, and 625 nm and then inverted again (Eq. 1). The filtered value of R_{rs} was then used in the band ratios.

$$R_{rs}(\lambda_0) = \left[R_{rs}{}^{-1}(\lambda_0) - R_{rs}{}^{-1}(575)\right]^{-1} \quad (01)$$

where: λ0 is the target wavelength.

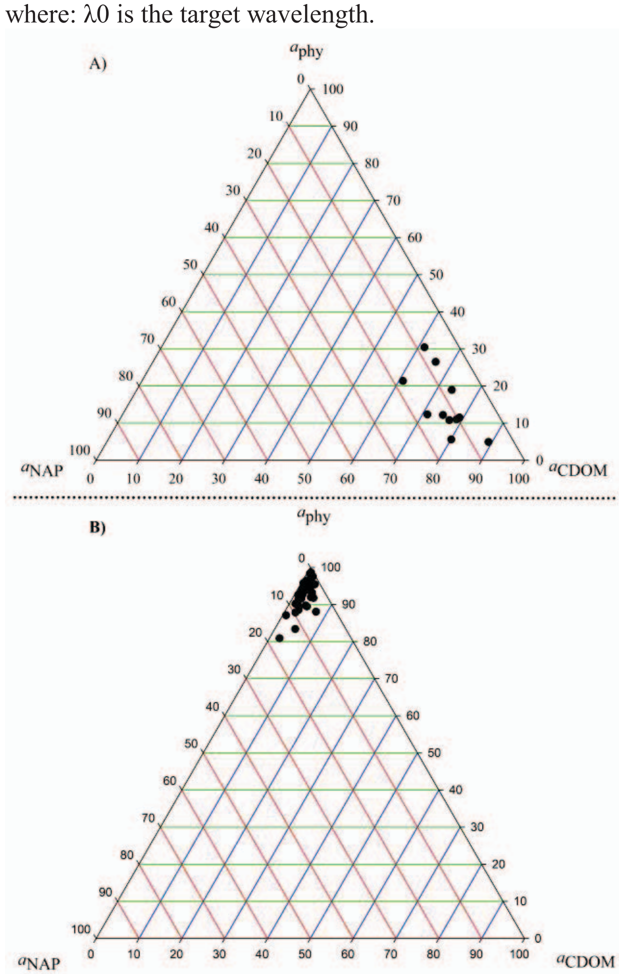

Fig. 2. Ternary plot from A) Funil Reservoir (CDOM dominated water) and B) Catfish ponds (phytoplankton dominated water).

To perform the evaluation of the filter we conducted a cross calibration and validation procedure using the mixed dataset of Funil Reservoir and catfish ponds datasets presented in Ogashawara et al. [7] and a performance comparison analysis of the band ratios before (Raw) and after the filtering process (Filter). The Normalized Root Mean Square Error (NRMSE) was calculated during validation for the calibration procedure that involved mixed dataset from Funil Reservoir (Brazil) and Catfish Ponds (Stoneville, MS, USA) [7].

4. RESULTS AND DISCUSSIONS

Linear calibrations for three bio-optical models and their filtered version were realized using the Mixed Dataset from Funil Reservoir and catfish ponds [7]. Table 1 shows the results including R^2, adjusted R^2, slope (X_1) and p-value. It was noticed that after the application of the filter, the R^2 increased in all cases when compared to the Raw algorithm.

Table 1 - Calibration Parameters from Mixed Dataset

Model	Filter	R^2	Adj. R^2	X_1	*p*-value
SC00	Raw	0.499	0.476	-1614.55	0.000166
SC00	Filtered	0.705	0.691	1320.626	$p < 0.0001$
SI05	Raw	0.684	0.67	132.365	$p < 0.0001$
SI05	Filtered	0.784	0.774	327.53	$p < 0.0001$
MI09	Raw	0.546	0.525	198.107	$p < 0.0001$
MI09	Filtered	0.7	0.685	728.147	$p < 0.0001$

To evaluate the improvement of each approach we calculated (Table 2) the NRMSE (%) between the estimated and measured PC concentration, after the application of the calibration described in Table 1. This analysis shows that for the mixed dataset, the filtered procedure produced the lowest errors for all three algorithms with a NRMSE(%) of 12.69, 9.67, and 18.49 for SC00, SI05, and MI09 respectively; while using the raw values the NRMSE(%) were 56.42, 16.04, and 23.40% for SC00, SI05, and MI09 respectively. For Funil Reservoir dataset, the lowest NRMSE(%) was found in the filtered version of MI09, with an NRMSE (%) of 75.28, however, the filtered application of SC00 algorithm showed the most significant improvement among all models. In the catfish ponds datasets, the use of our filter was the most successful because of the significantly higher PC concentrations in that water body. It is important to note that, MI09 did not show a significant improvement in all three datasets before and after the filter procedure, proving once again that it is least sensitive to chl-*a* and TSS and most sensitive to PC.

To evaluate the differences observed on the errors estimators for the catfish ponds (Table 2), we performed a Monte Carlo Simulation (MCS) to calculate the R^2 between the PC concentration and the models values (before and after the filtering process). The R^2 values were from eight random sampling points; this action was repeated 10000 times finalizing with a number of 10000 R^2 values for each PC bio-optical model (raw and filtered).of the calibration of according to the number of R^2 values higher than 0.8 from each bio-optical model. We also performed the Mann-Whitney Rank Sum Test to evaluate if the two samples of R^2 values (n=10000) were statistically different.

Table 3 – MCS analysis

Model	Type	Number of Values (R^2) > 0.8	Rank Sum Test
MI09	Filtered	6704	
Phytoplankton dominated system (n= 10000)			
SC00	Raw	856	p = <0.001
SC00	Filtered	8146	
SI05	Raw	591	p = <0.001
SI05	Filtered	6151	
MI09	Raw	185	p = <0.001
MI09	Filtered	1364	

These results were summarized on Table 3 in which we

Table 2 - Error Analysis

Model	Filter	NRMSE (%)	Model	Filter	NRMSE (%)	Model	Filter	NRMSE (%)
Mixed dataset			Funil dataset			Catfish Ponds dataset		
SC00	Raw	56.42	SC00	Raw	410.147	SC00	Raw	73.73
SC00	Filtered	12.694	*SC00*	Filtered	170.516	*SC00*	Filtered	22.382
SI05	Raw	16.044	*SI05*	Raw	102.798	*SI05*	Raw	18.414
SI05	Filtered	9.67	*SI05*	Filtered	88.12	*SI05*	Filtered	12.873
MI09	Raw	23.401	*MI09*	Raw	79.804	*MI09*	Raw	25.25
MI09	Filtered	18.493	*MI09*	Filtered	75.282	*MI09*	Filtered	20.197

observed the increase on the number of R^2 values higher than 0.8 in all the bio-optical models. For the phytoplankton dominated waters the SC00 also showed the largest increase in the number of R^2 values higher than 0.8 (7290 values).

Table 4 summarizes the statistical results of MCS. For the phytoplankton dominated waters, the absorption of chl-*a* seems to be the main water component affecting the PC bio-optical models. We also observed that SC00 showed the highest improvement for both filters and in both study sites. We attributed this performance to the removal of chl-a effect which was enhanced by Mishra et al. [6] as the main problem by using the PC reflectance peak around 650 nm band.

Table 4 – Summary of the statistical results of MCS.

Model	Type	Mean R^2	Median	Std. Dev.
Phytoplankton dominated system (n= 10000)				
SC00	Raw	0.40	0.39	0.27
SC00	Filtered	0.85	0.94	0.21
SI05	Raw	0.27	0.19	0.25
SI05	Filtered	0.75	0.86	0.27
MI09	Raw	0.27	0.19	0.25
MI09	Filtered	0.58	0.60	0.20

5. FINAL CONSIDERATIONS

We presented a filter to improve PC estimation from band ratios of R_{rs}. We applied the improved bio-optical model to three PC band ratio algorithms which were calibrated and validated with a mixed dataset containing observations from field campaigns in two significantly different study sites. Calibration and validation results show that the improved models have the ability to accurately predict PC concentrations, while reducing the influence of chl-*a* and TSS at PC absorption spectral region, in natural environments with mixed species of algae. Our results also show that it is possible to enhance the accuracy of PC bio-optical models up to 77% in some cases. This improvement is important not only for semi-empirical algorithms but also for semi-analytical ones which typically use band ratio as an estimator of PC. These improved models can be applied to the upcoming satellite multispectral sensors such as the Ocean and Land Color Instrument (OLCI) from European Space Agency, which will have a spectral band centered at 620 nm.

6. ACKNOWLEDGMENT

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