MODELING CLOROPHYLL-A CONCENTRATION BASED ON SIMULATED OLCI/SENTINEL-3 AND MSI/SENTINEL-2 BANDS IN A TROPICAL WATER RESERVOIR

Carina Inácio Portela[1,2], Rejane de Souza Paulino[1,2], Lorena de Moura Joia[1], Evlyn Márcia Leão de Moraes Novo[1,2], Vitor Souza Martins[3] and Cláudio Clemente Faria Barbosa[1,2]

[1] Postgraduate Program in Remote Sensing – PGSER, Earth Observation and Geoinformatics Division - DIOTG, National Institute for Space Research - INPE, São José dos Campos 12227-010, SP, Brazil, carina.portela@inpe.br, rejane.paulino@inpe.br, lorena.gomes@inpe.br, evlyn.novo@inpe.br, claudio.barbosa@inpe.br; [2]Instrumentation Laboratory for Aquatic Systems (LabISA), Earth Observation Coordination of National Institute for Space Research (INPE), São José dos Campos 12227-010, SP, Brazil; [3]Department of Agricultural & Biological Engineering, Mississippi State University, Starkville, MS 39762, USA, vmartins@abe.msstate.edu.

ABSTRACT

Remote sensing is an essential tool for mapping the dynamics of the optical components in tropical water reservoirs, allowing the identification of eutrophic conditions and their influences. This study is based on in situ data collected at the Itaipu reservoir, located on the Brazil-Paraguay border, to analyze limnological data of chlorophyll-a (chl-a), employing remote sensing techniques, calibration, and validation of simulated bio-optical algorithms for the OLCI/Sentinel-3 and MSI/Sentinel-2 sensors. The empirical algorithm calibration and validation were based on Monte Carlo's simulation. The results showed that the second-order derivative effectively revealed the spectral features of chl-a presence in the water. Furthermore, the best model included the slope between the 673 and 681 simulated bands (R^2 ~0.64 and MAPE of ~35%) with a polynomial adjustment of degree two. The narrower spectral band of the OLCI sensor, compared to that of the MSI sensor, allowed a greater sensitivity to phytoplankton features, even at the low chl-a concentrations.

Key words — Remote sensing, chlorophyll-a, hyperspectral, water quality.

1. INTRODUCTION

The monitoring of water quality is an important management tool to guarantee the sustainability of aquatic systems [1] [2]. Different Optically Active Components (OACs) present in the water column (e.g., clorophyll-a) can be combined to remote sensing measurements to predict the water quality [3] [4]. For example, Phytoplankton is a primary food source for many existing aquatic organisms and fish communities, being an interesting indicator of the richness of aquatic environments [5]. These organisms are suitable indicators of water pollution, making the species composition and abundance important parameters for assessing the water quality and the ecological health of an aquatic system [6] [7].

Chlorophyll-a (chl-a) occurs as a photosynthetically active pigment in almost all types of phytoplankton species, influencing the backscatter intensity of water and other components [8]. According to [9] phytoplankton cells behave as strong absorbers of visible light, playing an important role in the absorption properties of natural waters. Knowing the spatial distribution of chl-a is fundamental, as it is related to in reservoirs' trophic state [10].

In this sense, this study aims to estimate the concentration of chlorophyll-a in the Itaipu reservoir using empirical algorithms. The Rrs from MSI/Sentinel-2 and OLCI/Sentinel-3 sensors were simulated using in situ hyperspectral reflectance (Rrs) measurements which were also submitted to first and second-order derivative analyses.

2. MATERIAL AND METHODS

This paper was divided into two steps: (i) derivative analysis of water reflectance spectra obtained *in situ* and (ii) calibration and validation of a bio-optical algorithm based on chlorophyll-a concentration and simulated Rsr for the OLCI/Sentinel-3 and MSI/Sentinel-2 sensors bands.

2.1. Study area

The Itaipu Reservoir is located on the Brazil-Paraguay border and belongs to the Paraná river drainage basin. The reservoir has a flooded area of 1350 km, 170 km of extension, and a maximum depth of 223.10 m upstream [11]. The hydroelectric plant Itaipu Binacional plays an important role in the Brazilian energy matrix, supplying 10.8% of the energy produced in Brazil. and 88.5% of all energy consumed in Paraguay [11]. Spectral measurements were collected at 19 sampling points distributed along the Itaipu reservoir (Figure 1).

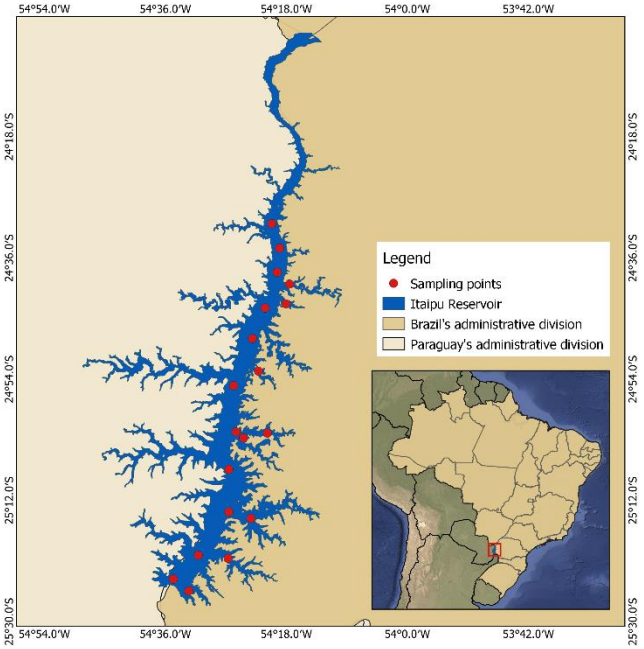


Figure 1. Study area location and sampling points.

2.2. *In situ* data

Limnologic (chlorophyll-a concentration, total suspended solids, and Secchi disk depth) and radiometric data were obtained in March 2013. Radiometric measurements above water were obtained using three intercalibrated TriOS-RAMSES spectroradiometers, following the protocol of Mobley [12] to compute the remote sensing reflectance (Rsr), in the spectral range between 400 nm and 950 nm (spectral resolution of 1 nm). The Rsr was calculated as shown in equation 1:

$$R_{rs} = \frac{L_t(\theta,\phi,\lambda) - \rho(\theta,\phi)L_{sky}(\theta',\phi,\lambda)}{E_d} \quad (1)$$

Where L_t is the total radiance, L_{sky} the sky radiance, $\rho(\theta,\phi)$ the reflectance of the air-water interface and E_d the downward irradiance. The limnological parameters determined in the Itaipu reservoir indicates low concentrations of chlorophyll, total suspended matter (TSM) and Secchi depth (Table 1).

	Chl-a (µ/L)	TSM (mg/L)	Secchi (m)
Minimum	0.59	0.63	0.80
Maximum	4.81	4.00	1.70
Mean	1.43	1.87	1.30
Standard deviation	1.14	0.91	0.23

Table 1. Synthesis of *in situ* limnological data.

2.3. Spectral derivative analysis

In this research, a derivative analysis was applied to assess from chlorophyll-a absorption features in the Rrs spectra. Rrs spectra were initially smoothed using a functional data analysis method (b-spline function), available in the FDA package in R [14]. Then, first and second-order derivatives were performed at the smoothed spectra [15].

2.4. Calibration and validation of bio-optical algorithms

OLCI/Sentinel-3 and MSI/Sentinel-2 bands were simulated using the Rrs data and the spectral response function of each sensor [16]. Useful algorithms for estimating the chlorophyll-a concentration in Brazilian reservoirs were identified and applied in this study. Namely: (i) ratio of two bands, (ii) three bands [17], (iii) slope [18], and (iv) NDCI (Normalized Difference Index for Chlorophyll) [19].

To calibrate and validate the algorithms, a Monte Carlo simulation was performed, with 1000 iterations. At each iteration, the dataset was split into 70% for calibration and 30% for validation. Algorithms' performance assessment used the following metrics: R^2 (determination coefficient) and MAPE (Mean Absolute Error in Percentage). Finally, the selection criteria to select the best model was based on the smallest error and the median of the results generated in the Monte Carlo simulation.

3. RESULTS AND DISCUSSION

In the 1st order derivative (Figure 2b), the region between 400 nm and 500 nm showed small positive variations, possibly associated with the scattering by the inorganic fraction, and the absorption caused by organic matter and chlorophyll-a. The positive and negative features near 560 nm and 665 nm indicate the presence of chlorophyll-a, but they are also regions influenced by the scattering of suspended solids. The region above 700 nm presents a negative variation, resulting from the expressive decrease in reflectance in this range (Figure 2a), related to the strong absorption of radiation by the water [20].

Successive differentiation in the spectrum measured over a water body allows the removal of the background effect caused by certain COAs [21]. The application of the 2nd order derivative more effectively revealed chlorophyll-a absorption features, even considering its small concentration in the reservoir. The spectral response in the range between 400 nm and 550 nm is commonly influenced by the scattering of inorganic particles in moderately turbid waters [22] and by the absorption of other COAs, was extinguished. The effect of water absorption predominant in the near-infrared region was also nullified.

The significant spectral features of the chlorophyll-a pigment revealed by the 2nd derivative are expressed by the peak of maximum reflectance in the green region (~570 nm), the absorption point in the red range (~675 nm), and

the other peak of reflectance at ~685 nm, related to phytoplankton fluorescence (Figure 2c). For MSI/Sentinel-2, due to the bandwidth centered at 665 nm, there was a loss of information since it includes the absorption band at ~675 nm and the fluorescence peak at ~685 nm. In contrast, the OLCI/Sentinel-3 simulated bands allowed greater sensitivity of the absorption and scattering features associated to the phytoplankton (Figure 2e), due to its finer spectral resolution in the red region (bands 665/ 673/681 nm).

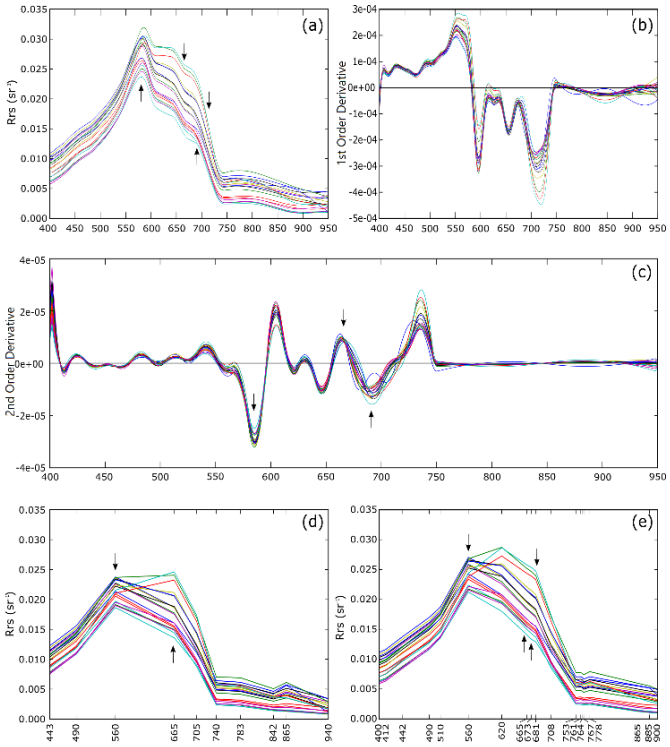


Figure 2. (a) Field spectrum, (b) 1st order derivative, (c) 2nd order derivative, bands simulation for (d) MSI/Sentinel-2 sensor and for (e) OLCI/Sentinel- 3. Arrows indicate regions of the chl-a pigment interactions with electromagnetic radiation.

The correlation analysis between the concentration of chlorophyll-a and MSI/Sentinel-2 data presented the best adjustment for the slope between the bands centered in the wavelengths of 665 nm and 705 nm. In this case, it showed R^2 of ~0.46 and MAPE of ~44.70%, for the median model with degree 2 polynomial. The linear fit for the same composition presented metric values close to the polynomial fit, with R^2 of ~0.45 and MAPE of ~50%. For the OLCI/Sentinel-3 sensor, the best models were the composition of 3 bands 665,681,708 nm (median model with R^2 ~0.61 and MAPE of ~38%) and the slope between the 665/673 nm bands (R^2 ~0.84 and MAPE of ~36%) and 673/681 (R^2 ~0.64 and MAPE of ~35%), all with degree 2 polynomial adjustment.

The analyses of the standardized errors of the dispersion for the three best models explaining chl-a concentration indicated that the combination of the bands 665,681,708 nm resulted in biased residue, indicating that the second-degree polynomial transformation was not suitable for adjusting this variable (Figure 3c). Despite the lack of a trend, the residue dispersions in the slope models were clustered around chlorophyll-a concentration below 2.0 µg/L, indicating that these algorithms are unsuitable for estimating higher concentration values.

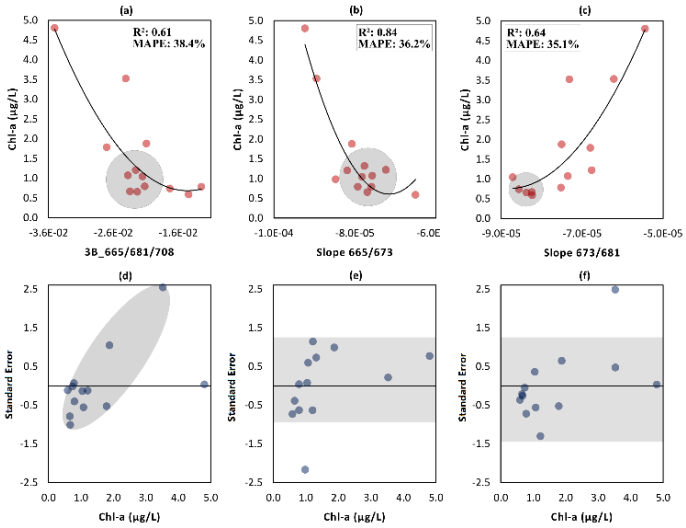


Figure 3. Regression of the median models generated in the Monte Carlo simulation: (a) 3 bands 665/681/708 nm, (b) slope 665/673 and (c) slope 673/681, and the respective standard errors in (d), (e) and (f).

Furthermore, the well-defined concavity of the slope model between the 665/673 nm bands (Figure 3b), suggests a level of confusion for the estimation of chlorophyll-a concentration values lower than ~0.80 µg/L, since for the same concentration estimate there are two slope values associated.

Many of the models used to estimate chl-a concentration over inland waters use chl-a absorption bands in the red (~675 nm) and NIR (near-infrared) (~710 nm) ranges, related to phytoplankton scattering [23][24][16]. However, these models are based on ranges of high chl-a concentration. This way, there is a shift of the reflectance peak towards the regions of ~705 nm and ~740 nm, what is not observed at low Chl-a concentrations [20]. In these cases, the spectra shape in the NIR is explained much more by the absorption of water than by the scattering of phytoplankton, which makes it difficult to use the bands in this region for generating models that estimate chl-a concentrations.

5. CONCLUSIONS

Based on the results presented, we conclude that the OLCI/Sentinel-3 sensor showed good potential for monitoring this variable, especially for reservoirs with a low concentration of chlorophyll-a. Without the predominance of the optical component chlorophyll-a, it was possible to define an empirical algorithm to estimate the concentration of this parameter in water. The good performance of the OLCI

sensor in comparison to the MSI sensor was due to the fine spectral resolution, which allowed the subtle spectral response of Rsr in the absorption (~675 nm) and fluorescence region (~685 nm). Although three models for the OLCI sensor presented a good design, taking as reference the statistics values, the slope 673,681 model was the most coherent based on the standardized error distribution and the shape of the estimated curve. Note that the proposed model estimates values in a small range of chlorophyll concentration (0.60 - 4.80 µg/L) which may represent a limitation of the model.

6. REFERENCES

[1] R. Altenburger et al. Future water quality monitoring—Adapting tools to deal with mixtures of pollutants in water resource management. *Science of the total environment*, 512 (v.): 540-551 (pp.), 2015.

[2] S. Behmel et al. Water quality monitoring strategies—A review and future perspectives. *Science of the Total Environment*, 571 (v.): 1312-1329 (pp.), 2016.

[3] M. H. Gholizadeh, A. M. Melesse, L. Reddi. A comprehensive review on water quality parameters estimation using remote sensing techniques. *Sensors*, 16 (v.): 8(n.): 1298 (pp.), 2016.

[4] J. C. Ritbhie, P. V. Zimba, J. H. Everitt. Remote sensing techniques to assess water quality. *Photogrammetric engineering & remote sensing*, 69 (v.): 6 (n.): 695-704 (pp.), 2003.

[5] P. CHAUHAN et al. Surface phytoplankton (chl-a) estimation in the Arabian Sea using IRS-P4 Ocean Color Monitor (OCM) satellite data. *International Journal of Remote Sensing*, 23 (v.): 8 (n.): 1663-1676 (pp.), 2002.

[6] E. Willén. Phytoplankton in water quality assessment–an indicator concept. *Hydrological and limnological aspects of lake monitoring*, 2 (v.): 58-80 (pp.), 2000.

[7] Z. H. Yusuf. Phytoplankton as bioindicators of water quality in Nasarawa reservoir, Katsina State Nigeria. *Acta Limnologica Brasiliensia*, 32 (v.), 2020.

[8] S. Balzano et al. Seasonal changes in phytoplankton on the north-eastern shelf of Kangaroo Island (South Australia) in 2012 and 2013. *Oceanologia*, 57 (v.): 3 (n.): 251-262 (pp.), 2015.

[9] C. C. F. BARBOSA, E. M. L. M. NOVO, V. S. MARTINS (Ed.). *Introdução ao sensoriamento remoto de sistemas aquáticos: princípios e aplicações*. Instituto Nacional de Pesquisas Espaciais, São José dos Campos, 2019.

[10] H. Lopes et al. Análise espaço-temporal da clorofila-a no reservatório de Itaparica por meio de imagens Landsat-TM. *Anais XVI Simpósio Brasileiro de Sensoriamento Remoto*, 6628-6635 (pp.), 2013.

[11] Itaipu Binacional. Reservatório. Available at: <https://www.itaipu.gov.br/energia/reservatorio>.

[12] C. D. Mobley. Estimation of the remote-sensing reflectance from above surface measurements. *Applied Optics*, 38 (v.): 36 (n.): 7442 (pp.), 1999.

[14] A. J. O. Ramsay, H. Wickham, S. Graves. Fda: Functional data analysis. 2022. Available at: <https://cran.r-project.org/web/packages/fda/fda.pdf>.

[15] F. Tsai, W. Philpot. Derivative Analysis of Hyperspectral Data. *Remote Sens. Environ*., 66 (v.): 41–51 (pp.), 1998.

[16] C. Cairo et al. Hybrid Chlorophyll-a Algorithm for Assessing Trophic States of a Tropical Brazilian Reservoir Based on MSI/Sentinel-2 Data. *Remote Sens.*, 12 (v.): 40 (pp.), 2020.

[17] A. Gitelson et al. Estimation of chlorophyll-a concentration in productive turbid waters using a Hyperspectral Imager for the Coastal Ocean: The Azov Sea case study. *Environ. Res. Lett.* 6 (v.): 1-6 (pp.), 2011.

[18] D. R. Mishra, S. Mishra. Plume and bloom: Effect of the Mississippi River diversion on the water quality of Lake Pontchartrain. *Geocarto Int.*, 25 (v.): 555–568 (pp.), 2010.

[19] S. Mishra, D. R. Mishra. Normalized Difference Chlorophyll Index: A novel model for remote estimation of chlorophyll-a concentration in turbid productive waters. *Remote Sens. Environ.*, 177 (v.): 394-406 (pp.), 2012.

[20] J. T. O. Kirk. *Light and photosynthesis in aquatic ecosystems*. Cambridge University Press, Cambridge, 2010.

[21] D. G. Goodin et al. Analysis of Suspended Solids in Water using Remotely Sensed High Resolution Derivative Spectra. *Photogramm. Engineering Remote Sensing*, 59 (v.): 4 (n.): 505–510 (pp.), 1993.

[22] D. Doxaran et al. Spectral Signature of Highly Turbid Waters Application with SPOT Data to Quantify Suspend Particulate Matter Concentrations. *Remote Sensing of Environment*, 81 (v.): 1 (n.): 149-161 (pp.), 2002.

[23] B. P. Page, A. Kumar, D. R. Mishra. A novel cross-satellite based assessment of the spatio-temporal development of a cyanobacterial harmful algal bloom. *Int. Journal Appl. Earth Obs. Geoinformation*, 66 (v.): 69-81 (pp.), 2018.

[24] F.S.Y. Watanabe, E. Alcântara, J. L. Stech. High performance of chlorophyll-a prediction algorithms based on simulated OLCI Sentinel-3A bands in cyanobacteria-dominated inland waters. *Advances in Space Research*, 2018.