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Relationship between chlorophyll-a concentration and cyanobacteria cell density in São Paulo reservoirs: a statistical and remote sensing approach

Relação da concentração de clorofila a e densidade de células de cianobactérias de reservatórios paulistas: uma abordagem estatística e por sensoriamento remoto

Felipe dos Santos Coelho[*], Viviane Moschini-Carlos[**], Marcelo Pompêo[***]

[*] Departamento de Engenharia Ambiental, Universidade Estadual Paulista (UNESP), fs.coelho@unesp.br
[**] Departamento de Engenharia Ambiental, Universidade Estadual Paulista (UNESP), viviane.moschini@unesp.br
[***] Departamento de Ecologia, Universidade de São Paulo, mpompeo@ib.usp.br

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Abstract

Cyanobacterial blooms pose a significant threat to the quality and availability of water in São Paulo's public supply reservoirs. These organisms hold medical importance, and their monitoring is mandatory and regulated by specific legislation. Given that existing monitoring programs lack sufficient coverage in terms of frequency and spatial extent across the entire state, this study developed models to estimate cyanobacteria cell density from chlorophyll-a concentration data. The models provided instantaneous results through developed algorithms. Two algorithms were created: the General model and the Hyper ESH model. Both models demonstrated good fit, indicated by R^2 values of 0.82 and 0.85, respectively. Nevertheless, adjustments are required to enhance the robustness of these estimates. The primary necessary adjustment relates to establishing a method to effectively isolate cyanobacteria cell density data from other algal groups presented in CETESB's Water Quality Reports.

Keywords:
Algorithm, Cyanobacteria, Estimation, Models, Monitoring.

Resumo

Florações de cianobactérias constituem uma grave ameaça a qualidade e disponibilidade hídrica para os reservatórios de abastecimento público paulistas. Estes organismos são considerados de importância médica, e o monitoramento é obrigatório e disciplinado por legislação específica. Tendo em vista que os programas de monitoramento existentes não são capazes de abranger todo território estadual em número e frequência adequados, neste trabalho foram desenvolvidos modelos de estimativa de densidade de células de cianobactérias utilizando dados da concentração de clorofila-a que permitissem obter resultados de maneira instantânea através de algoritmos.

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Foram gerados dois algoritmos, um denominado de modelo geral, e o outro de modelo Hiper (ESH) e ambos apresentaram bom ajuste dos modelos aos dados, com R^2 de 0,82 e 0,85 respectivamente, no entanto requerem ajustes para que possam realizar estimativas robustas, o principal deles é o relacionado ao estabelecimento de um método que possibilita isolar melhor os dados das densidades de células de cianobactérias dos demais grupos algais dos Relatórios de Qualidade da Água da CETESB.
Palavras-chave:
Algoritmo, Cianobactérias, Estimativa, Modelos, Monitoramento.

I. INTRODUCTION

Artificial eutrophication of rivers and reservoirs is a prevalent issue in urban centers, particularly those with high population density, inadequate sanitation infrastructure, and intense industrial activity (Jannuzzi; Travassos; Silva, 2024; Oliver; Corburn; Ribeiro, 2019). In addition to reducing water availability and degrading water quality, eutrophication poses significant public health risks, primarily due to the presence of cyanotoxins. These toxins are compounds produced by certain cyanobacteria species thriving in environments enriched by untreated effluents and nutrients transported from river basins (Jacinavicius et al., 2023; Lopes, 2023).

The impacts of cyanotoxins on organisms range from chronic effects, such as neurotoxicity, hepatotoxicity, dermatotoxicity, and carcinogenicity, to acute effects, which can lead to death (Rajput et al., 2024; Chen et al., 2021). Effective control of eutrophication and cyanotoxin contamination requires rigorous management of nutrient inputs - primarily phosphorus (P) and nitrogen (N) - and the strict regulation of effluent discharge, particularly in reservoirs designated for public water supply (Passos et al., 2022).

To guarantee the effectiveness of such controls, monitoring programs tailored to the environmental, social, and economic realities of river basins are crucial for identifying diffuse sources of pollution and assessing their impacts (Morais et al., 2020). In São Paulo State, the Environmental Company of São Paulo (CETESB) monitors water quality and publishes annual reports on major water bodies. Despite its relevance, the current monitoring program exhibits shortcomings, such as low sampling frequency and the absence of complementary parameters that could facilitate more comprehensive water quality management.

However, increasing sampling frequency and incorporating additional parameters can be economically and logistically impractical. To overcome these limitations, studies have focused on developing mathematical models that simulate environmental phenomena and enable the prediction of future scenarios, thereby supporting more rapid and informed decision-making (Tan; Özesmi; Kurtt, 2006).

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Accordingly, this study aimed to develop models for estimating cyanobacteria cell density in São Paulo reservoirs based on field-measured chlorophyll-a concentration data, employing statistical methods centered on linear regression. Furthermore, the study sought to integrate these models with complementary monitoring approaches using remote sensing technologies. Thus, estimates can be produced by analyzing orbital images even during periods without field data collection.

II. Materials and Methods

Study Area

The study area comprised municipalities within the state of São Paulo whose reservoirs are monitored by the São Paulo State Environmental Company (CETESB). Reservoirs selected for analysis met the following criteria: (1) inclusion in CETESB's Basic Monitoring Network; (2) availability of sampling points located either near the central body of the reservoir or at least 50 meters away from shores, bridges, piers, or other public facilities; and (3) the presence of chlorophyll-a concentration and cyanobacteria cell density data spanning from 2015 to 2022, with a minimum sampling frequency of three measurements per year.

Data collection and analysis

Field data were extracted from CETESB's Inland Water Quality Reports, publicly accessible for the period from 2015 to 2022 (available at: https://cetesb.sp.gov.br/aguas-interiores/publicacoes-e-relatorios/). These data were organized in Excel spreadsheets, which included reservoir identification details (water system name, municipality, UGRHI, geographical coordinates, and CETESB monitoring code), chlorophyll-a concentrations, cyanobacteria cell densities, and respective sampling dates.

Orbital images used to estimate chlorophyll-a concentrations in the reservoirs were acquired from the Sentinel-2A and Sentinel-2B satellites operated by the European Space Agency (ESA). These satellites provide a temporal resolution of five days, spatial resolutions of 10, 20, and 60 meters, and spectral resolution spanning 13 bands (Sentiwiki). The images were downloaded from the Copernicus Browser platform (https://browser.dataspace.copernicus.eu/) and processed using ESA's Sentinel Application Platform (SNAP). Image selection criteria included scenes free of clouds and cloud shadows. Initially, the images were searched to coincide precisely with the dates of field sampling. Due to the unavailability of images on certain sampling dates, a five-day temporal window before or after each sampling date was adopted, consistent with methods described by Schröde et al. (2024).

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Images downloaded at the L1C processing level (top-of-atmosphere reflectance, without atmospheric correction) (Silva; Lacerda, 2020) underwent a resampling procedure to standardize pixel size to 20 meters. Atmospheric correction was then performed using SNAP's C2RCC-Nets processor (Pompêo; Moschini, 2022), which automatically provides the chlorophyll-a concentration estimation product, designated as conc_chl. This product derives chlorophyll-a estimates from satellite-measured reflectance and absorption characteristics of chlorophyll-a pigment wavelengths, utilizing neural-network-trained algorithms that have demonstrated high efficiency and accuracy in estimating field chlorophyll-a concentrations (Camargo et al., 2024).

The chlorophyll-a concentration for each sampling location was obtained by calculating the mean value from the nine pixels adjacent to the sampling coordinates. Statistical validation of satellite-estimated conc_chl values was conducted by performing a one-way ANOVA using the software Past (version 4.16; Hammer; Harper; Ryan, 2001) to identify significant differences between satellite-derived and field-measured values. Subsequently, the satellite-derived concentrations were validated through scatter plot comparisons with CETESB field data using Excel software.

Relationship between chlorophyll-a and cyanobacteria cell density

Field data for chlorophyll-a concentration and cyanobacteria cell density from CETESB's Inland Water Quality Reports (2015–2022) were compiled into a spreadsheet containing reservoir identification details (water system name, municipality, UGRHI, geographical coordinates, and CETESB monitoring code), along with the respective sampling dates.

Satellite images from Sentinel-2A and 2B (ESA), which possess a temporal resolution of five days, spatial resolutions of 10, 20, and 60 meters, and 13 spectral bands (Sentiwiki), were downloaded through the Copernicus Browser platform and processed with SNAP. Images selected were cloud-free and temporally proximate to the field sampling dates, adopting a five-day window (Schröde et al., 2024).

Images at the L1C processing level (without atmospheric correction; Silva; Lacerda, 2020) were standardized to a 20-meter pixel resolution via resampling. Subsequently, atmospheric correction was implemented using the C2RCC-Nets processor within SNAP (Pompêo; Moschini, 2022), generating the conc_chl product. The conc_chl estimates the concentration of chlorophyll-a based on reflectance captured by satellite sensors, employing neural network algorithms previously validated against field data (Camargo et al., 2024).

For each sampling location, the chlorophyll-a concentration was computed as the mean value of the nine pixels surrounding the geographical coordinates. Satellite-derived conc_chl values underwent one-way ANOVA analysis using Past software (version 4.16; Hammer; Harper; Ryan, 2001) to assess potential statistical

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differences compared to field observations. The concentrations obtained via satellite imagery were further validated against CETESB field data through scatter plots created using Excel.

Table 1 – Classification of trophic states in lentic ecosystems.

Categoria	Clorofila *a*(mg.m³)
Ultraoligotrófico	CL ≤ 1,17
Oligotrófico	1,17 CL ≤ 3,24
Mesotrófico	3,24 CL ≤ 11,03
Eutrófico	11,03 CL ≤ 30,55
Supereutrófico	30,55 CL ≤ 69,05
Hipereutrófico	CL > 69,05

Source: São Paulo State Environmental Company (https://www.cetesb.sp.gov.br/aguas-interiores/wp-content/uploads/sites/12/2013/11/04).

To construct the statistical models relating chlorophyll-a concentrations to cyanobacteria cell density, data sets demonstrating strong correlations (R^2 > 0.60) were identified. These data were randomly partitioned into two subsets: 70% for model calibration (equation development) and 30% for validation, following methods established by Camargo et al. (2024). Model robustness was evaluated by employing standard statistical metrics: Root Mean Square Error (RMSE), Relative Root Mean Square Error (RRMSE), Normalized Root Mean Square Error (NRMSE), and Bias.

III. Results and discussion

Based on the selection criteria established in this study, twelve reservoirs from CETESB's Basic Monitoring Network were included in the analysis (Box 1). The Billings, Guarapiranga, Itupararanga, and Rio Grande reservoirs each contained multiple CETESB-defined monitoring points, all of which were incorporated into the final dataset. Figure 1 illustrates the spatial distribution of the selected reservoirs across São Paulo State.

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ISSN eletrônico 2177-2738
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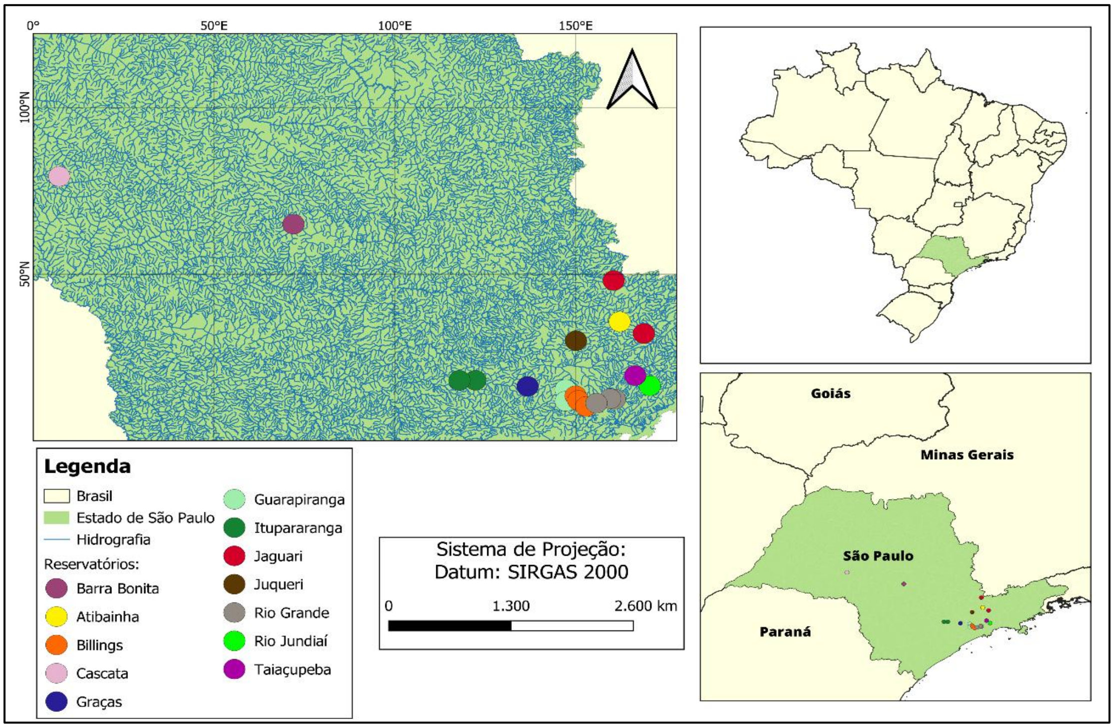

Figure 1 – Spatial distribution of the reservoirs analyzed within the state of São Paulo. (Author).

A total of 681 raw data points for chlorophyll-a concentrations and cyanobacteria cell densities were obtained from CETESB's Inland Water Quality Reports. Applying the established threshold, 149 data pairs with cyanobacteria densities lower than 10,000 cells/mL were identified and subsequently excluded from the database. Additionally, visual analysis identified and excluded 36 pairs that lacked valid results, exhibited outliers far from the overall data distribution, or had values significantly divergent from those previously reported in literature and prior studies conducted by researchers and CETESB itself for the same reservoirs. Descriptive statistical analysis was conducted to verify the data range and distribution characteristics (Box 2).

Box 1 – Reservoirs evaluated in the study, including their municipality, CETESB monitoring codes, water use classification (CONAMA Resolution 357/05), and the number of available data points used.

Water System	Municipality	Code CETESB	Use Class	No. of data
Jaguari Reservoir	Bragança Paulista	JARI00800	1	41
	Santa Isabel	JAGJ00200	1	31
Atibainha River Dam	Nazaré Paulista	RAIN00880	1	38
Billings Reservoir	São Paulo	BILL 02030	1	27
	São Paulo	BILL 02100	1	29
	São Bernardo do Campo	BILL 02500	1	26
Cascata Reservoir	Marília	CASC 02050	1	31
Graças Reservoir	Cotia	COGR 00900	1	29
Barra Bonita Reservoir	São Manuel	TIBB02700	1	31

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Guarapiranga Reservoir	São Paulo	GUAR 00100	1	33
	São Paulo	GUAR 00900	1	33
Juqueri or Paiva Castro Reservoir	Mairiporã	JQJU00900	1	39
Rio Grande Reservoir	Ribeirão Pires	RGDE02030	1	51
	Ribeirão Pires	RGDE02200	1	32
	São Bernardo do Campo	RGDE02900	1	59
Jundiaí River Reservoir	Mogi das Cruzes	JNDI 00500	1	32
Itupararanga Reservoir	Ibiúna	SOIT02100	1	29
	Votorantim	SOIT02900	1	33
Taiaçupeba Reservoir	Suzano	PEBA00900	1	57
Total of points				681

Source: Prepared by the author.

Box 2 – Range of variation in the dataset used in this study. N – number of data points; SD – standard deviation; CV% – coefficient of variation.

Data range						
Parameter:	**N**	**Minimum**	**Maximum**	**Average**	**SD**	**CV (%)**
Chlorophyll-a concentration (µg/L)	495	1.67	510.54	39.76	58.847231	1.4801743
Cyanobacteria density (cells/mL)		10,035	1,478,460	111,883	189,392.58	1.6927682

Source: Prepared by the author.

According to São Paulo State Decree No. 8,468 (1976), all reservoirs evaluated in this study are classified as class 1 waters. The classification of water bodies into usage classes is a mechanism prescribed within the National Policy on Water Resources, aimed at preserving water quality and preventing further environmental degradation (Silva; Mariani, Pompêo, 2015). The responsibility for assigning classes to water bodies resides with state authorities in collaboration with basin committees, based on the basin's priority uses. According to CONAMA Resolution No. 357 (2005), freshwater bodies are classified into five categories: Special Class, Class 1, Class 2, Class 3, and Class 4, in descending order of water quality and increasingly less demanding applications. Class 1 waters are the focus of this study and are suitable for human consumption following simple treatment, protection of aquatic ecosystems, primary contact recreation activities such as swimming, water skiing, and diving (as regulated by CONAMA Resolution No. 274/2000), irrigation of vegetables consumed raw and fruits consumed with the peel, and the preservation of aquatic communities in Indigenous Territories. Notably, classification as class 1 alone does not guarantee adherence to all water quality parameters or the effectiveness of pollution control actions implemented in respective river basins. Specifically, the maximum permitted limits defined by CONAMA Resolution No. 357 (2005) for chlorophyll-a concentration and cyanobacteria cell density are 10 µg/L and 20,000 cells/mL, respectively, values significantly below the average levels identified in this

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O ESPAÇO GEOGRÁFICO EM ANÁLISE
https://revistas.ufpr.br/raega
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study (Box 2). These findings highlight the disparity between actual water quality and intended standards, reflecting insufficient pollution control efforts. Studies by Buzelli and Cunha-Santino (2013) on the Barra Bonita reservoir, Frascarelli et al. (2015) on the Itupararanga reservoir, and Sonobe, Lamperelli, and Cunha (2019) on the Cascata, Guarapiranga, Jundiaí, and Itupararanga reservoirs similarly reported that chlorophyll-a and cyanobacteria cell density parameters consistently exceeded the maximum permissible limits established by CONAMA Resolution No. 357 (2005).

Elevated cyanobacteria densities and high chlorophyll-a concentrations typically indicate eutrophication, reflecting ongoing nutrient enrichment. Persistent eutrophic conditions highlight continuous discharge of nitrogen- and phosphorus-rich effluents and diffuse pollution sources (Barboza; Teixeira Filho, 2013a, 2013b). De Carli et al. (2018) have emphasized that eutrophication in public supply reservoirs within the metropolitan region of São Paulo is directly linked to untreated pollutant discharge and inadequate sewage management practices.

After refining the dataset, trophic states were categorized as previously described, and chlorophyll-a concentrations and cyanobacteria cell densities were correlated across nine proposed data subsets using scatter plots and determination coefficients (R^2). Only two subsets exhibited strong correlations ($R^2 > 0.60$): the "General" dataset, incorporating all trophic levels, and the combined dataset comprising Eutrophic, Supereutrophic, and Hypereutrophic trophic states ("Hyper ESH"). The remaining subsets showed weak correlations ($R^2 < 0.60$) and were thus excluded from further model development. Consequently, only the "General" and "Hyper ESH" datasets were used to construct predictive models, termed the General Model and the Hyper ESH Model, respectively (Figures 2 and 3).

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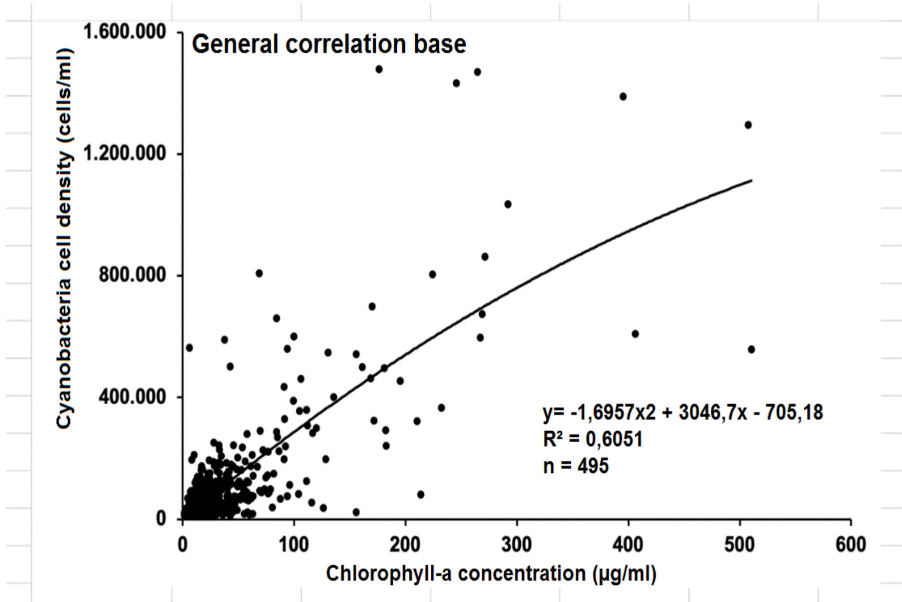

Figure 2 – General base correlation. (Author).

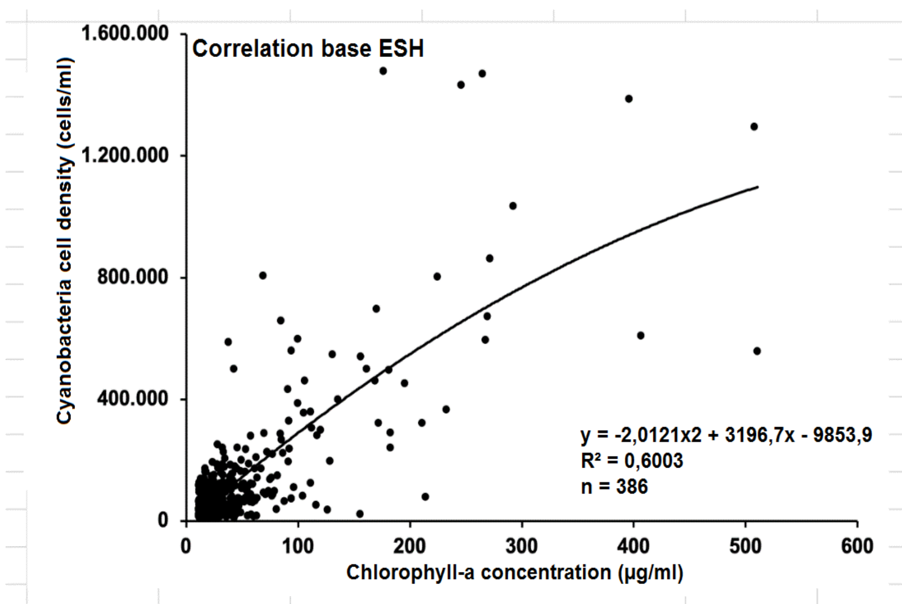

Figure 3 – Base ESH correlation. (Author).

In developing these predictive models, datasets were randomly divided into calibration (70% of data) and validation (30% of data) subsets. For the General Model, 346 data points were employed for calibration (Figure 4), while the remaining 149 points served as validation. The Hyper ESH Model utilized 270 points for model construction (Figure 5) and 116 points for validation purposes. To improve model accuracy, certain outliers were removed; however, these exclusions did not exceed 10% of the total dataset, thus ensuring the robustness and unbiased nature of the generated models.

O ESPAÇO GEOGRÁFICO EM ANÁLISE
https://revistas.ufpr.br/raega
ISSN eletrônico 2177-2738
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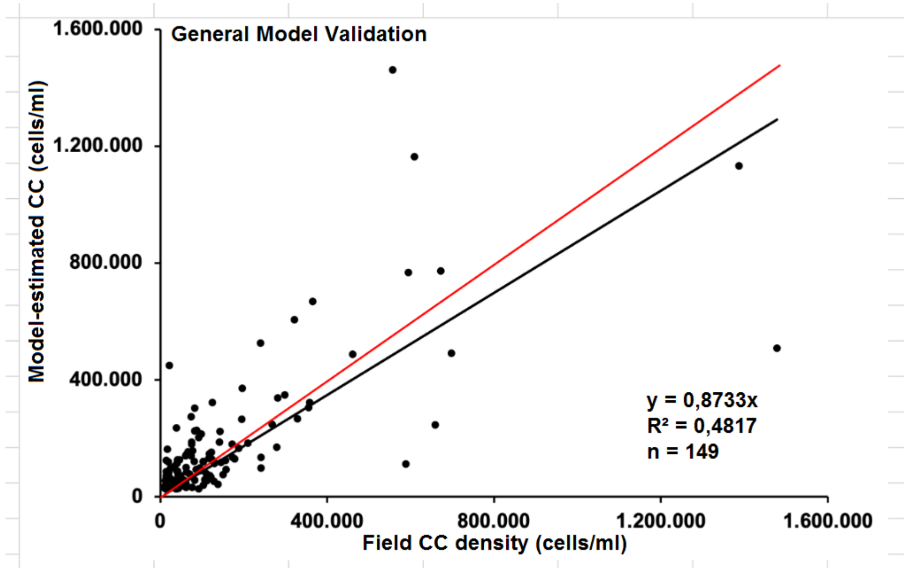

Figure 4 – General Model. (Author).

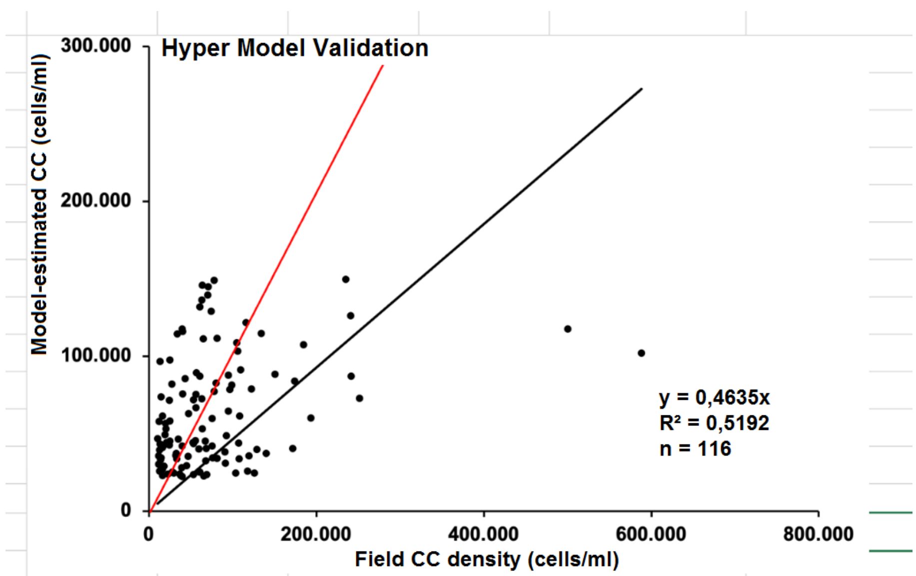

Figure 5 – Hyper Model. (Author).

Upon evaluating the distribution of data points relative to the regression trend lines and the associated determination coefficients (R^2), the developed models demonstrated satisfactory fits to the data. Similar outcomes were reported by Caballero et al. (2022) in Mirim Lake, where cyanobacteria cell density estimates were derived from chlorophyll-a concentrations measured both in the field and through remote sensing. According to those authors, the strong correlation between chlorophyll-a concentration and cyanobacteria density is influenced by environmental conditions that facilitate cyanobacteria proliferation and dominance within phytoplankton communities, including factors such as pH, temperature, nutrient availability, and solar

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RA'EGA, Curitiba, PR, V.63, n.1, p. 152 – 170, 8/2025
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radiation. Likewise; Pompêo et al. (2021) observed a significant relationship between chlorophyll-a concentrations and cyanobacteria cell densities in Brazilian reservoirs. Utilizing CETESB's dataset for the Cantareira System reservoirs from July 2015 to December 2018, these authors developed a second-order exponential model from a set of 90 data points, obtaining an R^2 value of 0.84.

Datasets demonstrating weak correlations between chlorophyll-a and cyanobacteria cell density could result from the presence of phytoplankton groups other than cyanobacteria. In reservoirs dominated by Chlorophyceae, chlorophyll-a concentrations typically correlate more closely with this algal group than with cyanobacteria. Conversely, in cyanobacteria-dominated systems, chlorophyll-a concentrations strongly correlate with cyanobacteria presence. Silva, Albuquerque, and Becker (2022), studying four reservoirs in the metropolitan area of Fortaleza (CE), demonstrated that phycocyanin is a more suitable pigment for estimating cyanobacteria cell densities, as this pigment exclusively occurs in cyanobacteria. They also highlighted difficulties in using chlorophyll-a to estimate cyanobacteria densities, primarily because chlorophyll-a is a pigment common to various algal groups and aquatic macrophytes. Accurate phytoplankton identification and quantification are thus crucial for establishing precise relationships between chlorophyll-a concentrations and cyanobacteria densities or for determining the dominant algal group influencing the chlorophyll-a signal. Unfortunately, CETESB's Water Quality Reports do not include data on phycocyanin or total phytoplankton cell densities. Moreover, phytoplankton identification and counting involve substantial costs, requiring regular field sampling, laboratory infrastructure, and trained technical personnel (Hanish; Freire-Nordi, 2015). Consequently, routine phycocyanin monitoring could significantly enhance the accuracy of cyanobacteria estimation models, as previously demonstrated by Simis et al. (2007), Kudela et al. (2015), Yan, Bao, and Shao (2018), and Silva, Albuquerque and Becker (2022).

It is important to emphasize that this study does not advocate the replacement of traditional, in-situ water quality monitoring. Field monitoring remains indispensable, as it provides actual data essential for validating remote sensing-based approaches. However, remote sensing represents a highly viable and cost-effective complementary solution, enabling the expansion of water quality monitoring coverage for all Brazilian reservoirs and thereby positively influencing overall water management. Additionally, Sentinel-2 satellite images, and the SNAP processing software are freely accessible, providing nationwide image coverage across Brazil (Pompêo et al., 2022).

RA'EGA O ESPAÇO GEOGRÁFICO EM ANÁLISE
https://revistas.ufpr.br/raega
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Figures 6 and 7 illustrate validation plots comparing cyanobacteria cell densities measured in field samples against densities estimated by each developed model. These graphs also include a 1:1 reference line and a linear trend line through the origin, facilitating assessment of estimation robustness.

To quantitatively assess model performance, the coefficient of determination (R^2) and error metrics, including Root Mean Square Error (RMSE), Relative Root Mean Square Error (RRMSE), Normalized Root Mean Square Error (NRMSE), and Bias, were evaluated (Box 3).

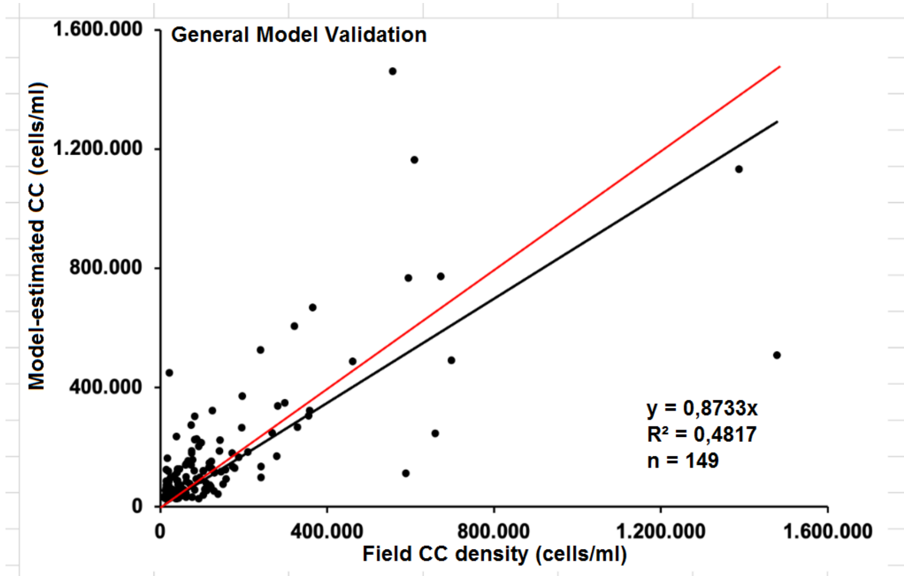

Figure 6 – General Model Validation. (Author).

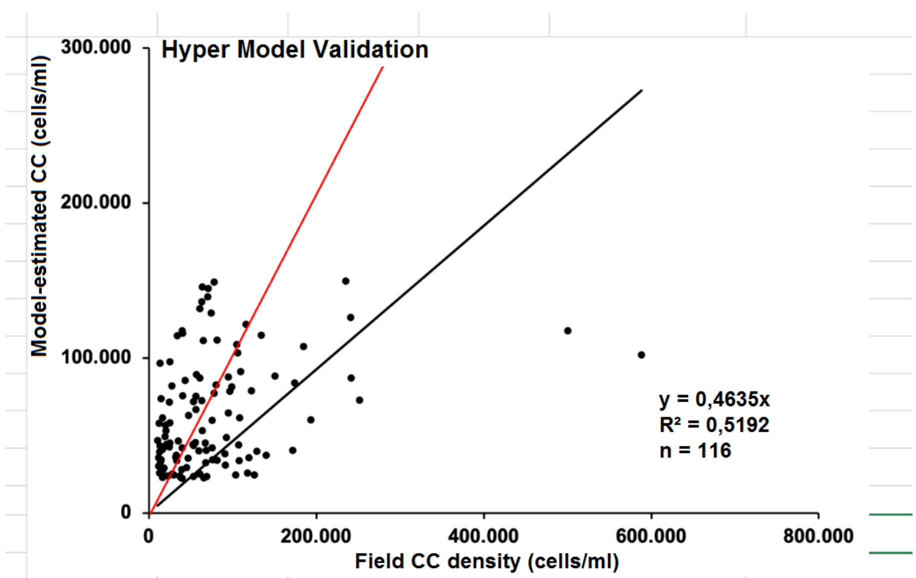

Figure 7 – Hyper ESH Model Validation. (Author).

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Box 3 – Summary of the models developed based on trophic states, including respective equations, regression models employed, the number of points used for model development and validation, and robustness indicators (R^2, RMSE, RRMSE, NRMSE, and Bias).

Model	Equation	Regression model	No. of data model	No. of data validation	R^2	RMSE	RRMSE (%)	NRMSE	BIAS
General	y = 2851.3x + 5088.4	Linear	324	149	0.8	155,851	99.3518	1.18	25049
Hyper (ESH)	y = 3009x - 11154	Linear	235	116	0.9	77,956	124.647	1.01	-13,988

Source: Prepared by the author.

The coefficient of determination (R^2) measures how well model predictions fit observed data, specifically indicating how much variability in cyanobacteria cell density is explained by chlorophyll-a concentration (Camargo; Ferrari, 2016). The models developed herein exhibited high degrees of fit, yielding R^2 values of 0.82 for the General model and 0.85 for the Hyper ESH model. Thus, chlorophyll-a concentrations explained 82% and 85% of the variability in cyanobacteria cell densities in the respective models.

The Root Mean Square Error (RMSE), representing the average prediction error of each model, showed that the General model produced an average error of approximately 155,851 cyanobacteria cells. The Relative Root Mean Square Error (RRMSE) translates RMSE values into percentage terms, offering a clearer understanding of estimation accuracy (Castro; Ferrari, 2016). According to this metric, the General model presented errors nearing 100%, whereas the Hyper ESH model surpassed this, reaching an error magnitude of approximately 124%.

The Normalized Root Mean Square Error (NRMSE), unlike the RMSE, normalizes both observed and predicted data to facilitate better comparability across datasets (Castro; Ferrari, 2016). NRMSE values close to zero indicate optimal model performance, while values approaching or exceeding one suggest poor predictive capability. Both developed models exhibited NRMSE values greater than one, indicating insufficient accuracy for reliable estimates.

Bias calculations were employed to assess systematic tendencies in model predictions, identifying either overestimation or underestimation trends. The General model tended to overestimate cyanobacteria densities by an average of 25,049 cells, whereas the Hyper ESH model underestimated densities by approximately 13,988 cells.

Given these results, neither model demonstrated sufficient robustness for confidently estimating cyanobacteria densities, suggesting that, in their current state, these models should not be utilized as reliable tools for cyanobacteria monitoring in São Paulo reservoirs.

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IV. Concluding Remarks and Recommendations

The findings of this study indicate that robust estimation models based solely on the direct relationship between chlorophyll-a concentrations and cyanobacteria cell densities could not be reliably developed for the reservoirs analyzed. This limitation likely results from the difficulty of isolating cyanobacteria-specific data from other phytoplankton groups, information currently absent in CETESB's Water Quality Reports. Consequently, future research should prioritize expanding the database, clearly differentiating cyanobacteria from total phytoplankton, and assessing the inclusion of phycocyanin pigment monitoring in standard water quality assessments.

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