



Water quality assessment using Sentinel-2 imagery with estimates of chlorophyll a, Secchi disk depth, and Cyanobacteria cell number: the Cantareira System reservoirs (São Paulo, Brazil)

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Abstract

Satellite images were used to assess surface water quality based on the concentration of chlorophyll a (chl_a), light penetration measured by the Secchi disk method (SD), and the Cyanobacteria cells number per mL (cyano). For this case study, six reservoirs interconnected were evaluated, comprising the Cantareira System (CS) in São Paulo State (Brazil). The work employed Sentinel-2 images from 2015 to 2018, SNAP image processing software, and the native products conc_chl and kd_z90max, treated using Case 2 Regional Coast Color (C2RCC) atmospheric correction. The database was obtained from CETESB, the agency legally responsible for operation of the Inland Water Quality Monitoring Network in São Paulo State. The results demonstrated robustness in the estimates of chl_a (RMSE = 3.73; NRMSE% = 19%) and SD (RMSE = 2,26; NRMSE% = 14%). Due to the strong relationship between cyano and chl_a ($r^2 = 0.84$, $p < 0.01$, $n = 90$), both obtained from field measurements, there was also robustness in cyano estimates based on the estimates of chl_a from the satellite images. The data revealed a clear pattern, with the upstream reservoirs being more eutrophic, compared to those downstream. There were evident concerns, about water quality, particularly due to the high numbers of Cyanobacteria cells, especially in the upstream reservoirs.

Keywords Remote sensing · Tropical reservoirs · C2RCC · Secchi disk · Chlorophyll · Cyanobacteria · Sentinel-2

Introduction

In studies of the water quality from lakes and reservoirs, satellite images based on different validated algorithms can be used to estimate chlorophyll a, suspended material, turbidity, and light penetration (Ritchie et al. 2003; Gholizadeh et al. 2016; Deutsch et al. 2018). The maps created with these algo-

gorithms enable observation of the horizontal spatial heterogeneity of various estimated environmental variables (Tyler et al. 2006; Zaraza-Aguilera and Manrique-Chacón 2019). The water quality of highly dendritic reservoirs can reflect the different contributions of the hydrographic basin for each arm. Spatial analysis employing satellite images enables understanding of the effects of land occupation and use, considering their relationship with water quality (Cavalcante et al. 2018; Chaves et al. 2019). In addition, the figures obtained are excellent tools for assessing areas at large scales. Complementing the information, it is possible to not only estimate concentrations but also infer differences in water quality, by transforming the estimated data into quality criteria, for example by using the trophic status index (Machado and Baptista 2016; Watanabe et al. 2017; Cairo et al. 2020; Martins et al. 2020). Hence, there are many possibilities for the use of satellite images to assess reservoir water quality, supporting decision-making by managers, so they should be considered a basic tool, particularly when supported by existing field monitoring infrastructure and

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established laboratories. This is the case in São Paulo State (Brazil), where there are many research groups working in this area, mainly linked to public universities and other research centers (Cardoso-Silva et al. 2013). This solid research infrastructure offers great potential for the implementation of a well-founded network for water quality monitoring, using field data and validated algorithms applied to satellite images.

CETESB (Environmental Company of São Paulo State) is the governmental agency responsible for the control, inspection, monitoring, and licensing of potentially pollution-generating activities, with the remit to preserve and restore the quality of water, air, and soil. Since 1974, CETESB has been responsible for operation of the Inland Water Quality Monitoring Network in São Paulo State (CETESB 2020b). This network has sampling points distributed throughout the State, with more than 300 monitoring stations (CETESB 2016). Since 1978, based on information collected in the field, CETESB has made publicly available an annual assessment report on water quality, representing a legal framework for monitoring purposes. Hence, there is already a large set of public information available, with environmental data for many inland water bodies in the State. For most reservoirs, the monitoring by CETESB involves sampling every 2 months, at a single collection point. However, for other reservoirs, mainly those employed for public supply and considered more eutrophic, there are databases with monthly collections and samplings performed at more than one collection point in each reservoir.

During the last decades, considerable progress has been made in water quality studies using remote sensing techniques. The Copernicus program of the European Union has put Earth observation satellites into orbit, which provide useful information that is accessible to all potential users. Among them, the Sentinel-2 mission incorporates a band configuration suitable for the study of water bodies (ESA 2020).

The main objective of this work was to use Sentinel-2 satellite images and test native products treated using SNAP (Sentinel Application Platform), a free image processing software package, as a viable and fast option for evaluation of the quality of inland waters. As a case study, six reservoirs of the Cantareira System (São Paulo State, Brazil) were evaluated, based on the Secchi disk depth, the concentration of chlorophyll a, and the Cyanobacteria cells number.

Materials and methods

Study area

Due to their importance for the supply of drinking water to the São Paulo metropolitan region, it was decided to study the Cantareira System (CS) reservoirs: Jaguari (JG), Jacarei (JC), Cachoeira (CA), Atibainha (AT), Paiva Castro (PC),

and Igaratá (IG). The reservoirs were observed using single scenes from Sentinel-2, at 23KLQ, within the following coordinates: 22° 49' 47" S, 46° 00' 30" W, 22° 49' 47" S, 46° 00' 30" W.

The JG, JC, CA, AT, and PC reservoirs comprise a basin transposition system and are interconnected by channels and tunnels (Fig. 1). The first stage of operation of the CS was completed in 1974 (Whately and Cunha 2007). In 2018, the IG reservoir was incorporated in the CS, transposing about 5 m³/s of water to the AT reservoir, through the Jaguari raw water pumping station located in the municipality of Santa Isabel (Fumes and Dardis 2020; SABESP 2020a). Table 1 shows some of the hydrological characteristics of the studied reservoirs.

The first CS reservoirs (JG and JC) are connected by a short open channel in the rock and usually have the same water levels. From JC, the water flows by gravity to CA and from there to AT and later to PC. The IG reservoir is connected by a channel to the AT reservoir. From PC, the water is pumped from the Santa Inês elevation to the small Águas Claras reservoir and from there to the Guarau water treatment station, where it is treated and sent to São Paulo city and the region (Whately and Cunha 2007).

According to Pompêo et al. (2017), with the exception of the IG reservoir (which was not studied at the time), for 2013, the observed dissolved inorganic nitrogen, total phosphorus, nitrite, nitrate, ammonium, chlorophyll a, suspended solids, and Secchi disk values for the CS were in agreement with the Cascading Reservoir Continuum Concept (CRCC) (Barbosa et al. 1999). Accordingly, the upstream reservoirs were more eutrophic and the downstream ones were more oligotrophic, suggesting low contributions from the basin areas of the intermediate reservoirs. Pompêo et al. (2017) also showed that the phytoplankton biomass in the reservoirs was regulated by the availability of nutrients, with the upstream reservoirs functioning as nutrient accumulators and the sediment as the main compartment for storage of P and N. The findings revealed an urgent need for restoration measures in the upstream reservoirs, especially JG and JC, which were more eutrophic than those located downstream.

By early 2014, the CS reservoir system regularly provided 33 m³/s of raw water, used to supply more than 9 million people. Between October 2013 and March 2014, the natural affluent flows were exceptionally low for that period, so the CS reservoirs did not receive the expected volumes of water (ANA 2020), with drastic reductions of the stored volumes, reflected in decreased water levels and areas. Figure 2a shows the variation of the water level (height above sea level) for the JG and JC set of reservoirs. For 2015, there were very low water levels and for the data presented in this figure, there was a difference of 30 m between the highest and the lowest water levels observed during the period. Figure 2b shows an overlap of the water surface areas obtained for the JG reservoir on two

Table 1 Characteristics and hydrological information of the Cantareira System reservoirs, according to ANA (2013)

	Unit	Jaguari/Jacarei	Cachoeira	Atibainha	Paiva Castro	Igaratá**
Average rainfall	mm	1592	1763	1642	1593	
Drainage area	km ²	1027 (JG) 203 (JC)	392	312	369	
Live/useful storage	hm ³	808.12	69.75	95.26	7.61	60.5
Dead storage	hm ³	239.43	46.81	194.93	25.33	793
Maximum flooded area	km ²	49.91	8.6	21.8	4.6	
Average flow	m ³ /s	25.2	8.5	6.0	4.6	28
Water level (height a.s.l.)	m	844.0	821.88	786.72	745.61	623
Residence time*	day	368.5	40.1	105.8	10.7	306

*Based on the average of the daily flows downstream of dams and through tunnels, using the input volume in the corresponding upstream reservoir and the daily volume of each reservoir. Data series for the period from 01/01/2004 to 31/12/2012, obtained from: http://arquivos.ana.gov.br/institucional/sof/Renovacao_Outorga/SeriedeHidrologicos-SistemaCantareira-2004-2012-SABESP.xlsx (29/09/2014), provided by ANA (National Water Agency)

**According to Prime Engenharia (2015), the dead storage corresponds to the portion of the total volume of the reservoir inactive or unavailable for the purpose of water catchment. The residence time that expresses the average time that water spends in a given reservoir

different occasions: in 2015, when the water surface area was estimated at 2.46 km², and in 2018, when it was 4.05 km², corresponding to an area reduction of about 1.5 km² in 2015, compared to 2018. Due to these exceptional events, new conditions of operation of the CS were established, authorizing the removal of raw water according to the percentage of storage in the system, with values ranging from 33 m³/s to a minimum of 15.5 m³/s, depending on the stored volume (ANA/DAEE 2017).

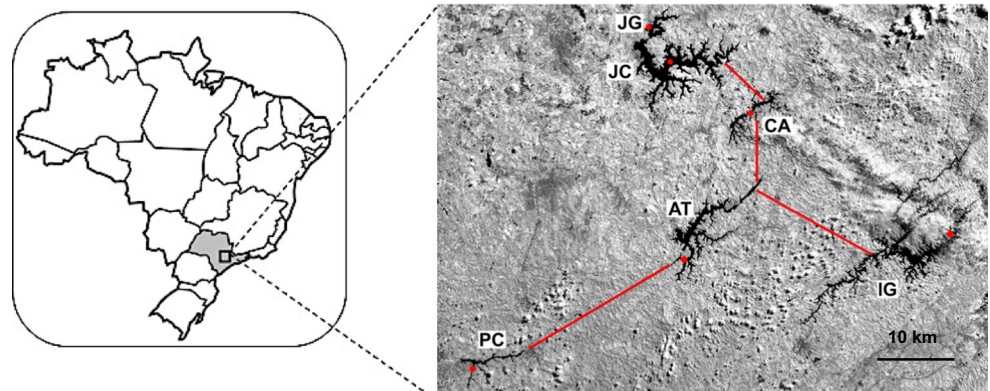
Data base and Sentinel 2 images

For this work, data were obtained from CETESB (2020a) water quality reports from 2015 to 2018. The data included chlorophyll a concentration (spectrophotometric method, 90% acetone), turbidity, Cyanobacteria cell number, and Secchi disk depth (SD) measured in situ (<https://cetesb.sp.gov.br/aguas-interiores/publicacoes-e-relatorios/>). For these

reservoirs, CETESB monitored surface water bimonthly, with sampling at a single collection station (Table 2, Fig. 1).

The two satellites of the European Space Agency (ESA) Sentinel-2 mission are in polar orbit, placed in the same sun-synchronous orbit in the sun, with 180° phases between them. Sentinel A has been operating since June 2015 and Sentinel B since March 2017. The purpose of these satellites is to monitor the variability in surface conditions. Their wide bandwidth (290 km) and fast revisit time, of 10 days at the equator with one satellite and 5 days with 2 satellites, in cloudless conditions, which results in 2–3 days at mid-latitudes, is intended to support monitoring of changes on the Earth's surface (ESA 2021). There are 13 spectral bands: four bands at 10 m, six bands at 20 m, and three bands at 60 m (ESA 2020). Sentinel-2 has been shown to be suitable for estimating chlorophyll a concentration and the Secchi disk depth, enabling tracking of the spatial and temporal dynamics in lakes (Ansper and Alikas 2019; Delegido et al. 2019; Pereira-Sandoval et al. 2019; Sòria-Perpinyà et al. 2020) and rivers (Pereira et al. 2020).

Fig. 1 a Location of the Cantareira System reservoirs, in the State of São Paulo (Brazil), sampling stations (red bullets) and interconnection through channels and tunnels (line red) of the Jaguari (JG), Jacarei (JC), Cachoeira (CA), Atibainha (AT), Igaratá (IG), and Paiva Castro (PC) reservoirs



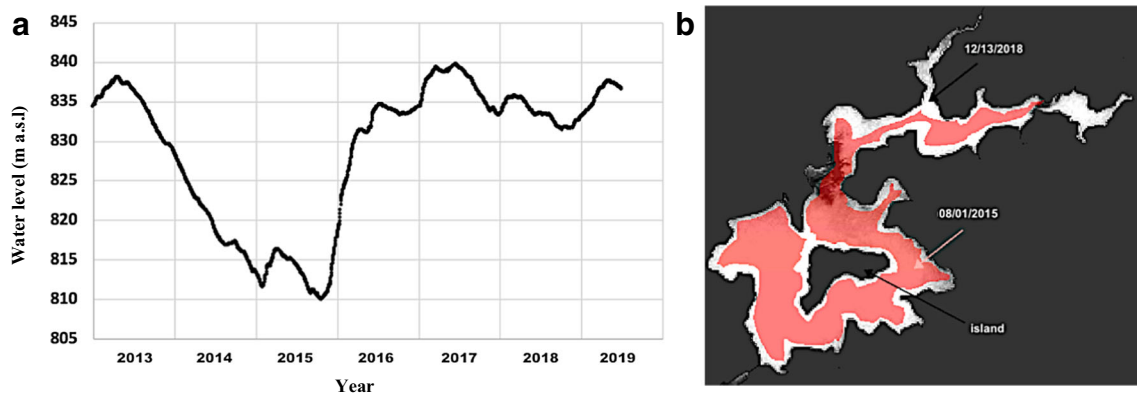


Fig. 2 a Daily variation of the water levels of the JG and JC reservoirs from January 2013 to June 2019, and b overlap of the water mirror areas for the JG reservoir, from Sentinel-2 images acquired on 01/08/2015 (in red) and on 12/13/2018 (in white)

Due to the low reflectivity of water, atmospheric correction is essential in studies of water quality employing remote sensing (Brockmann et al. 2016). Among the different methods developed, the Case 2 Regional Coast Color (C2RCC) technique was adapted to Sentinel-2 and is used for waters with low turbidity, such as marine waters (C2RCC-Nets networks), while the C2X processor (Case-2 Extreme) is used for darker waters. These methods of atmospheric correction are based on neural networks trained with a database of reflectance and radiation, obtained using simulations performed with radiative transfer models, and are included in the free SNAP software developed by ESA. The SNAP products include the absorption coefficients for different constituents, the reflectivity of each band, and the uncertainties, with the results of special interest for this study being the absolute concentrations of chlorophyll a (conc_chl, in µg/L) and the product kd_z90max.

Based on the dates of water quality evaluations performed by CETESB, Sentinel-2 images for level 1C were searched at Earthexplorer of the United States Geological Survey (USGS) (<https://earthexplorer.usgs.gov/>). Table 3 lists all the Sentinel-2 scenes downloaded from July 2015 to December 2018. After unpacking, the images were processed using SNAP 7.0.0 software (<http://step.esa.int/main/>). Firstly, a 10-m resampling was applied to all the images and a subset was cut out, retaining only the reservoirs of interest. The atmospheric

corrections C2RCC-Nets and C2RCC-C2X (Thematic Water Processing, C2RCC Processors, S2-MSI) (Delegido et al. 2019; Pereira-Sandoval et al. 2019) were then applied. After the atmospheric correction processes, it was possible to obtain, as SNAP native products, estimates of the chlorophyll a concentration (conc_chl, in µg/L) and kd_z90max (in m). The data were extracted from the images based on the coordinates (Table 1), with an average of 9 pixels and the coordinates of the sampling station as the central point (Delegido et al. 2019; Pereira-Sandoval et al. 2019).

Due to the presence of clouds, the image did not always provide data for all collection stations in the same scene. On the other hand, in the case of a good scene, field data were not always available, since for some dates, CETESB did not provide complete information in the spreadsheets. For a given collection station, there might be data for chlorophyll a, but not SD, or sometimes the reverse. Therefore, also due to the reduced number of images available for the period, reflecting the reduced number of points used for the calibration curves, it was decided to use Sentinel-2 images with a maximum of 9-day difference between the passage of the satellite and the collection date. For most dates, scenes were obtained with up to 6 days between the passage of the satellite and the corresponding collection.

Table 2 Coordinates of the CETESB monitoring stations in the Jaguari, Jacarei, Cachoeira, Atibainha, Paiva Castro, and Igaratá reservoirs (CETESB 2016)

Reservoir	Legend	Coordinates		Sampling station description
Jaguari	JG	22° 55' 40" S	46° 25' 27" W	In the central body, in front of the island
Jacarei	JC	22° 58' 16" S	46° 24' 03" W	In the central body
Cachoeira	CA	23° 02' 01" S	46° 17' 24" W	In the middle of the central body, about 3.5 km from the dam
Atibainha	AT	23° 12' 35" S	46° 23' 10" W	At intake pumps, near the road that connects the cities Nazaré and Guarulhos
Paiva Castro	PC	23° 20' 25" S	46° 39' 45" W	Santa Inês Bridge, on the highway that connects the cities Mairiporã and Franco da Rocha
Igaratá	IG	23° 11' 37" S	46° 01' 39" W	In the water intake of the reservoir, in the city of São José dos Campos

Table 3 Sentinel-2 (A and B) image references and sampling dates

Year	Sampling date	Image date	Sentinel-2 image reference (A and B)
2015	08/05/15	08/01/15	S2A_MSIL1C_20150801T131806_N0204_R138_T23KLQ_20150801T131809
	08/06/15		
	08/12/15	08/11/15	S2A_MSIL1C_20150811T131816_N0204_R138_T23KLQ_20150811T131811
2016	01/06/16	01/08/16	S2A_MSIL1C_20160108T131142_N0201_R138_T23KLQ_20160108T131626
	01/12/16		
	07/13/16 07/05/16	07/06/16	S2A_MSIL1C_20160706T131242_N0204_R138_T23KLQ_20160706T131549
2017	07/07/17	07/01/17	S2A_MSIL1C_20170701T131241_N0205_R138_T23KLQ_20170701T131632
	07/12/17	07/21/17	S2A_MSIL1C_20170721T131241_N0205_R138_T23KLQ_20170721T131244
	09/21/17	09/19/17	S2A_MSIL1C_20170919T131241_N0205_R138_T23KLQ_20170919T131238
2018	11/07/17	11/13/17	S2B_MSIL1C_20171113T131229_N0206_R138_T23KLQ_20171113T193925
	03/22/18	03/23/18	S2B_MSIL1C_20180323T131239_N0206_R138_T23KLQ_20180323T135825
	04/18/18	04/22/18	S2B_MSIL1C_20180422T131239_N0206_R138_T23KLQ_20180422T135336
	05/09/18	05/07/18	S2A_MSIL1C_20180507T131251_N0206_R138_T23KLQ_20180507T145606
	05/24/18	05/22/18	S2B_MSIL1C_20180522T131239_N0206_R138_T23KLQ_20180522T144941
	12/07/18	07/21/18	S2B_MSIL1C_20180721T131239_N0206_R138_T23KLQ_20180721T181454
	07/11/18		
	09/11/18	09/09/18	S2B_MSIL1C_20180909T131239_N0206_R138_T23KLQ_20180909T182556
	09/13/18	09/19/18	S2B_MSIL1C_20180919T131239_N0206_R138_T23KLQ_20180919T182219
	09/20/18		
	09/22/18	09/24/18	S2A_MSIL1C_20180924T131241_N0206_R138_T23KLQ_20180924T171325
11/07/18	11/03/18	S2A_MSIL1C_20181103T131241_N0206_R138_T23KLQ_20181103T145623	
11/03/18			
11/27/18	11/28/18	S2B_MSIL1C_20181128T131239_N0207_R138_T23KLQ_20181128T144314	
12/10/18	12/13/18	S2A_MSIL1C_20181213T131231_N0207_R138_T23KLQ_20181213T144242	

In order to validate the estimates obtained by the SNAP algorithms, the values were linearly correlated to the SD depths and chlorophyll a concentration obtained from the CETESB reports. Calculations were made of R^2 , RMSE (root mean square error), and NRMSE (normalized root mean square error) (Delegido et al. 2019; Pereira-Sandoval et al. 2019). A data analysis also was performed with the raw information retrieved from the CETESB reports.

The SNAP product kd_{z90max} represents the depth at which there is 90% extinction of surface light. In order to relate the SD values to kd_{z90max} , a correction algorithm was developed, using SD field measurements and light profiles ($\mu\text{mol of photons m}^{-2} \text{ s}^{-1}$) obtained at the same point using a Licor radiometer fitted with a photosynthetically active radiation cell. Based on these underwater radiation profiles, the depths corresponding to 90% light extinction (here denoted kd_{z90max_field}) were calculated for each sampling station. The estimated kd_{z90max_field} values were then related to the measured SD

depth data for the same seasons and days. In turn, the linear equation generated was used to estimate the SD depths, but now using the SNAP product kd_{z90max} . For validation, the SD depths estimated with the SNAP product were related to the SD depths measured in the field at the same collection stations in the reservoirs used for the study of chlorophyll a (JG, JC, CA, AT, IG, and PC). The data used to generate the conversion algorithm, both direct measurements of SD and light profiles, were obtained from numerous Spanish reservoirs, for the years 2017 to 2019, obtained from the Confederación Hidrográfica del Ebro (<http://www.chebro.es/contenido.visualizar.do?idContenido=7299&idMenu=3400>). For 2017, data were collected from 32 reservoirs, for 2018 from 15 reservoirs, and for 2019 from 11 reservoirs, all located in the Ebro river basin (Spain), and the collections in these reservoirs spanned the period from June 6 to August 9.

The Trophic State Index (TSI) aims to classify water bodies in different degrees of trophic, that is, it evaluates the water

Table 4 Ranges, averages, standard deviations (σ), and coefficients of variation (CV) for reservoir field data published in CETESB reports for the period from July 2015 to December 2018. The maximum values are shown in bold font; the minimum values are shown in bold italics. For the italicized values, see the text. *ND*, not determined

		Secchi disk (m)	Turbidity (NTU)	Chlorophyll a ($\mu\text{g/L}$)	Cyanobacteria (cells/mL)
Jaguari	Average	1.23	<i>15.21</i>	13.25	61.698
	Minimum	0.40	<i>0.50</i>	1.07	230
	Maximum	2.20	66.90	33.95	251.850
	σ	0.55	17.80	9.45	78.155
	CV	44.36	117.04	71.32	126.67
Jacarei	Average	1.33	5.39	10.63	53.651
	Minimum	0.60	<i>0.50</i>	1.97	795
	Maximum	2.10	15.80	29.40	221.435
	σ	0.40	3.28	6.04	56.682
	CV	29.92	60.78	56.80	105.65
Cachoeira	Average	1.26	6.53	<i>13.63</i>	<i>93.186</i>
	Minimum	0.50	1.30	6.24	10.620
	Maximum	2.00	24.50	41.88	354.205
	σ	0.36	4.85	9.43	98.974
	CV	28.88	74.31	69.22	106.21
Atibainha	Average	<i>2.07</i>	3.26	4.90	29.478
	Minimum	1.10	1.14	<i>0.75</i>	3.300
	Maximum	2.90	6.80	12.60	194.255
	σ	0.64	1.70	3.50	44.627
	CV	31.05	52.16	71.43	151.40
Igaratá	Average	ND	2.86	0.70	ND
	Minimum	ND	1.80	<i>0.50</i>	ND
	Maximum	ND	6.19	1.30	ND
	σ	ND	1.20	0.21	ND
	CV	ND	41.81	30.17	ND
Paiva Castro	Average	1.73	3.55	4.57	31.344
	Minimum	0.90	1.10	0.89	1.670
	Maximum	3.10	10.90	12.70	126.190
	σ	0.52	2.21	3.47	35.557
	CV	30.10	62.43	75.89	113.44

quality in terms of enrichment by nutrients and its effect related to the excessive growth of algae or to the increase in infestation of aquatic macrophytes (CETESB - Companhia Ambiental do Estado de São Paulo 2020a, 2020b). In this work, the TSI calculations and their respective trophic categories for chlorophyll a and SD, followed CETESB - Companhia Ambiental do Estado de São Paulo (2020a, 2020b), according to the equations developed by Lamparelli (2004).

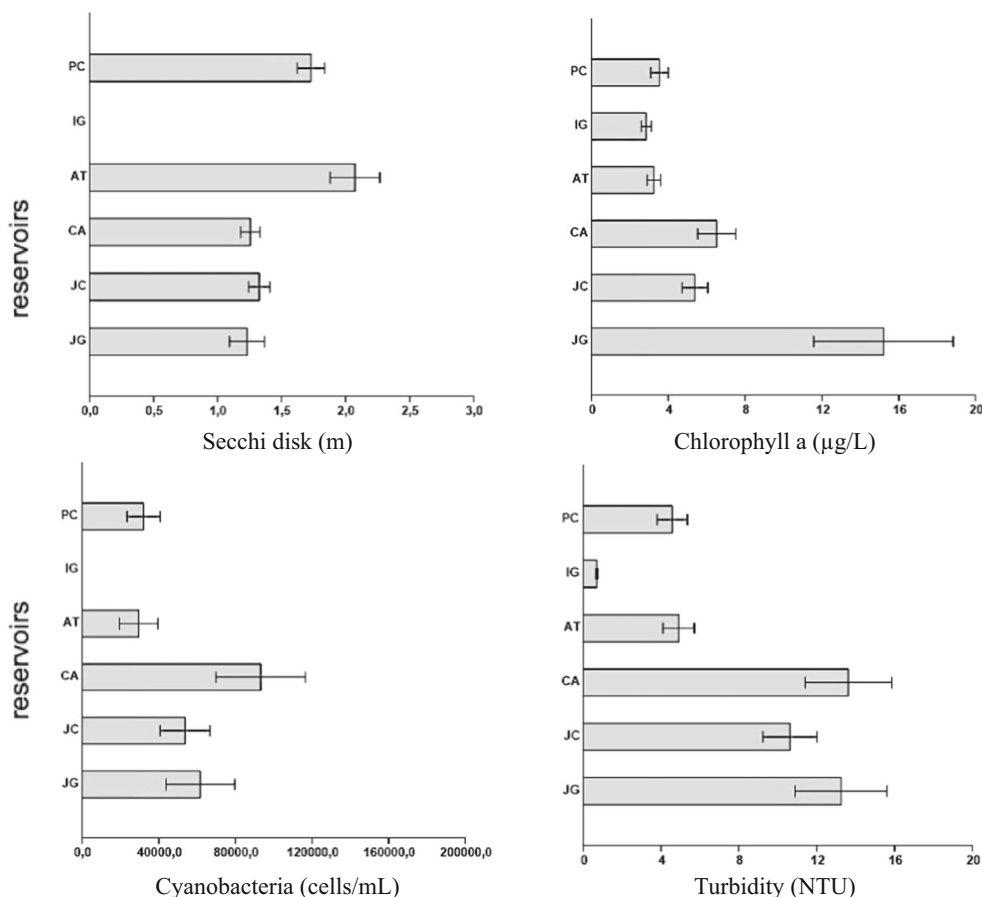
Results and discussion

CETESB data analysis

Table 4 shows the amplitudes of variations of the data obtained from the CETESB reports, together with the means,

standard deviations (σ), and coefficients of variation (CV) for the raw water samples collected in the field during the period from July 2015 to December 2018, according to reservoir. For some dates, the CETESB reports only provided minimum limit values for turbidity and chlorophyll a. When this occurred, half of this value was used in the table. The method of using half the detection limit has been reported to be sufficiently accurate to obtain descriptive statistics, such as the mean and standard deviation (Dodds et al. 2006), as shown italicized in Table 4. High values for turbidity and chlorophyll a, but low values for SD were found in JG reservoir. In general, the PC and IG reservoirs presented lower values for turbidity and chlorophyll a, with high values for SD (Table 4). However, the CA reservoir presented high values for chlorophyll a, as well as the highest value for the Cyanobacteria cell number. The JG and JC reservoirs also showed high concentrations of Cyanobacteria cells.

Fig. 3 Averages and standard errors for the Secchi disk, chlorophyll a, turbidity, and Cyanobacteria cell number values for the reservoirs studied, considering the period from July 2015 to December 2018: Jaguari (JG), Jacarei (JC), Cachoeira (CA), Atibainha (AT), Igaratá (IG), and Paiva Castro (PC)

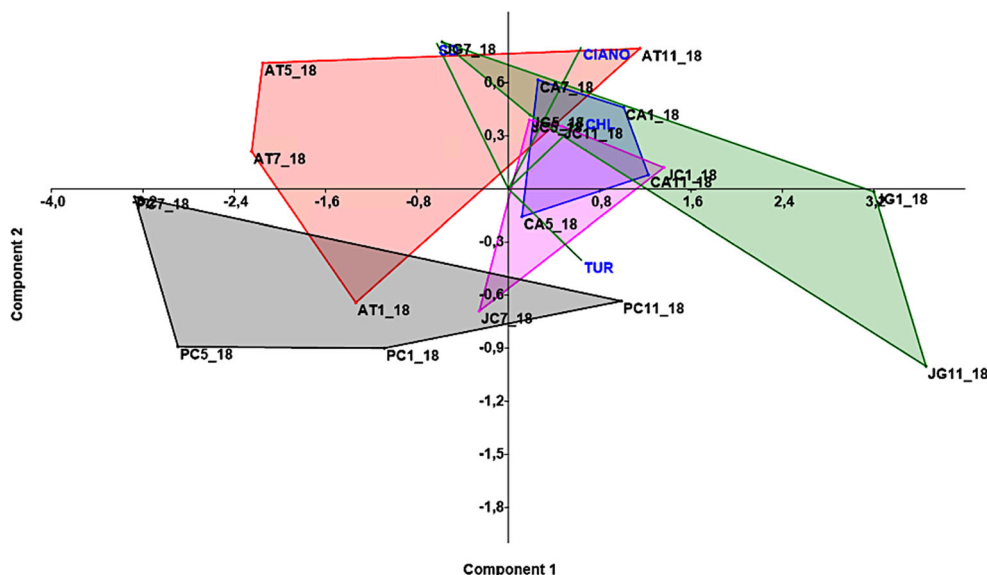


This manner, the more turbid reservoirs presented higher concentrations of chlorophyll a and lower values for SD (Fig. 3), suggesting that the organic fraction was mainly responsible for the total material in suspension. Pompêo et al. (2017) also observed that the organic fraction accounted

for the highest percentage of the suspended material in the CS reservoirs, in 2013.

Principal component analysis (PCA) (Fig. 4), using the data retrieved from the CETESB reports, showed that the JG, JC, and CA reservoirs were more associated with

Fig. 4 Principal component analysis, with log transformed data for turbidity (TUR), chlorophyll a concentration (CHL), Secchi disk depth (SD), and Cyanobacteria cell number (CIANO). The legends indicate the reservoir and the month and year of sampling (e.g., JG11_18: Jaguari, November 2018)



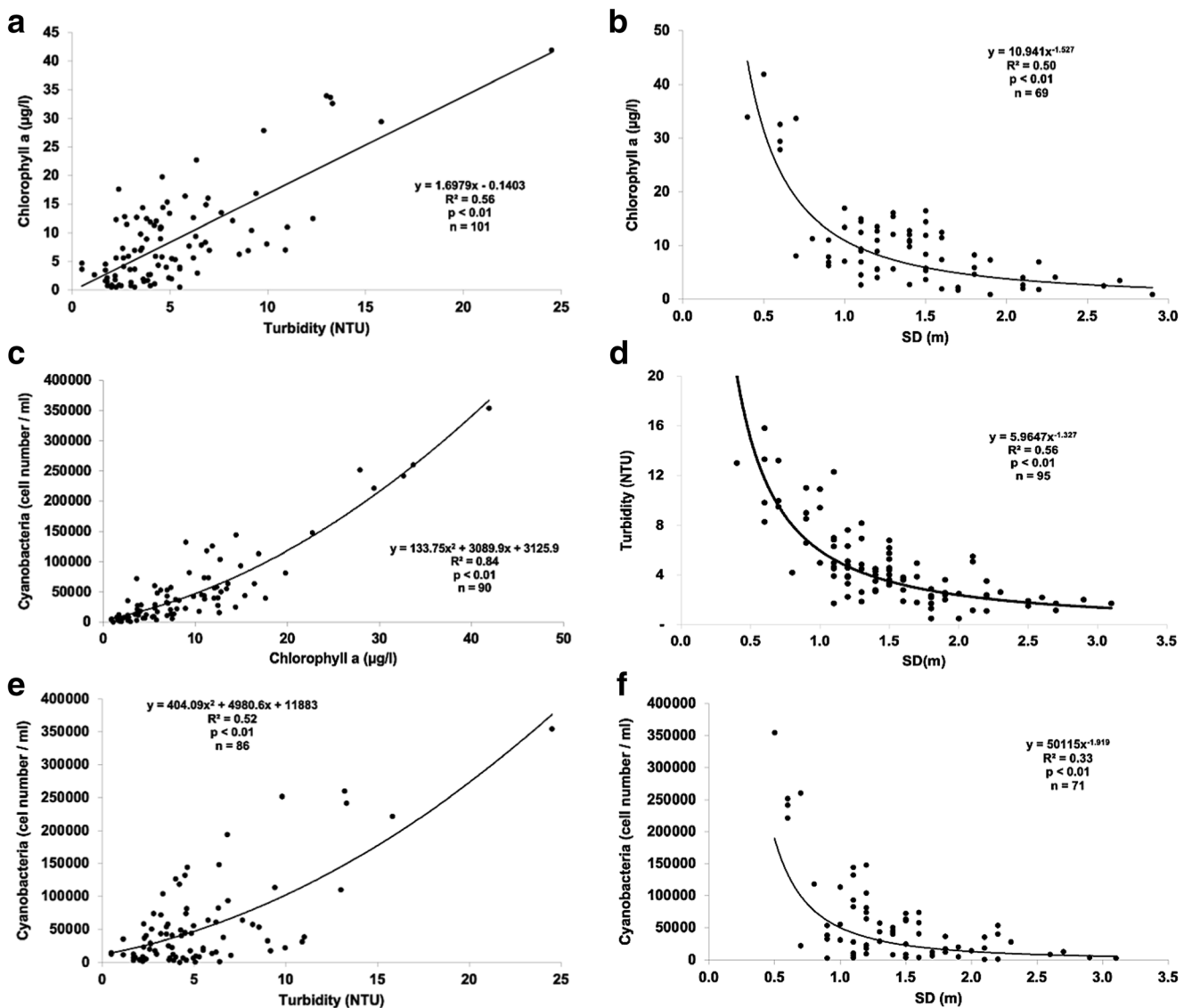


Fig. 5 Relationships between the environmental variables determined in the field by CETESB, for the period from July 2015 to December 2018. Best fit curves: a, c, and e 2nd-order polynomial; b, d, and f log

chlorophyll a, turbidity, and Cyanobacteria cell number. The PC and AT reservoirs were associated with SD. In this analysis, axis 1 explained 82.6% of the variance, while axis 2 explained 9.03%. For PCA were used only sampling dates and stations with complete information for chlorophyll a, SD, turbidity, and Cyanobacteria cell number.

The results obtained using the field data collected by CETESB revealed clear relationships among chlorophyll a, turbidity, SD, and Cyanobacteria cell number (Fig. 5). These classical relationships showed that increase of the chlorophyll a concentration was associated with increases of the Cyanobacteria cell number and turbidity, and decrease of the SD depth. Despite this, according to Søndergaard et al. (2011), when the goal is to estimate Chla, but predictability is not always high. As the authors report, Chla was

significantly related to TP, but the variability was high, with R^2 reaching 0.47, 0.59, and 0.61 in shallow, stratified, and siliceous lakes, respectively, based on summer averages. According to those authors, the Chla is also related to TN, but the correlation coefficients were low throughout the year and, in a multiple regression with TP included, TN only added little to the total variability. Likewise, the proportion of Cyanobacteria increased significantly with TP, but the correlation was also low. This suggests that other factors, such as availability of light, temperature, or competition, may interfere with the growth of Cyanobacteria's.

The clear relationships observed among chlorophyll a, SD, turbidity, and Cyanobacteria cell number (Fig. 5) indicated that the chlorophyll a concentration could in large part be explained by the presence of Cyanobacteria. They also

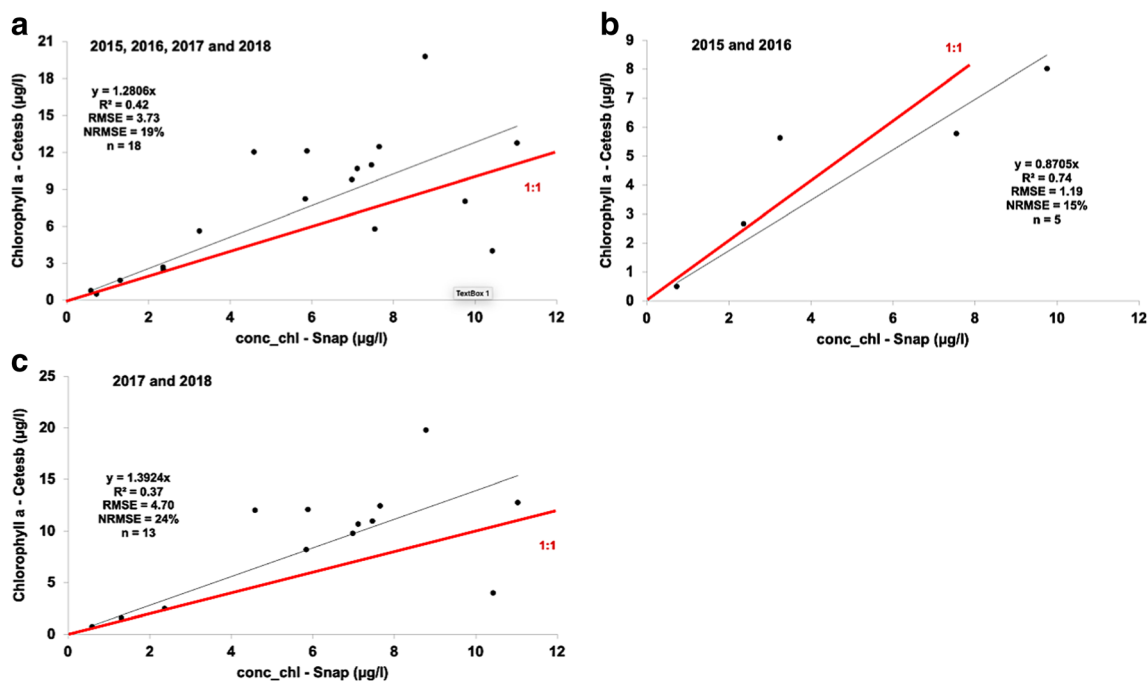


Fig. 6 Linear relationships between chlorophyll concentrations measured in the field by CETESB and the values estimated using the C2RCC-Nets model (conc_chl)

suggested that although the Chlorophyceae were important algal components of phytoplankton, during the study period, the main component of the phytoplankton population in the CS was Cyanobacteria. This is a worrying observation, since Cyanobacteria are potentially toxic (Codd 1995; Bláha et al.

2009), which might compromise the water quality in this important water source for the São Paulo city and the region.

Since 1995, applications of algacide (copper sulfate pentahydrate) have been used in the CS to control the growth of algae, particularly in the entry channel of the PC reservoir.

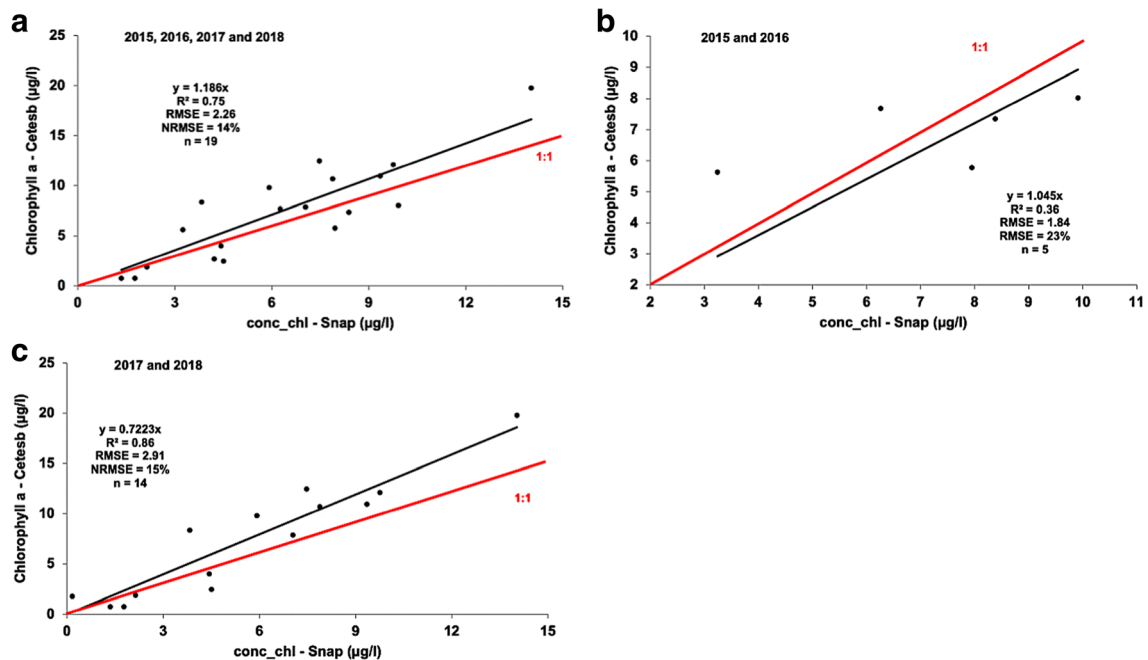


Fig. 7 Linear relationships between chlorophyll a concentration measured in the field by CETESB and the values estimated using the C2RCC-C2X model (conc_chl)

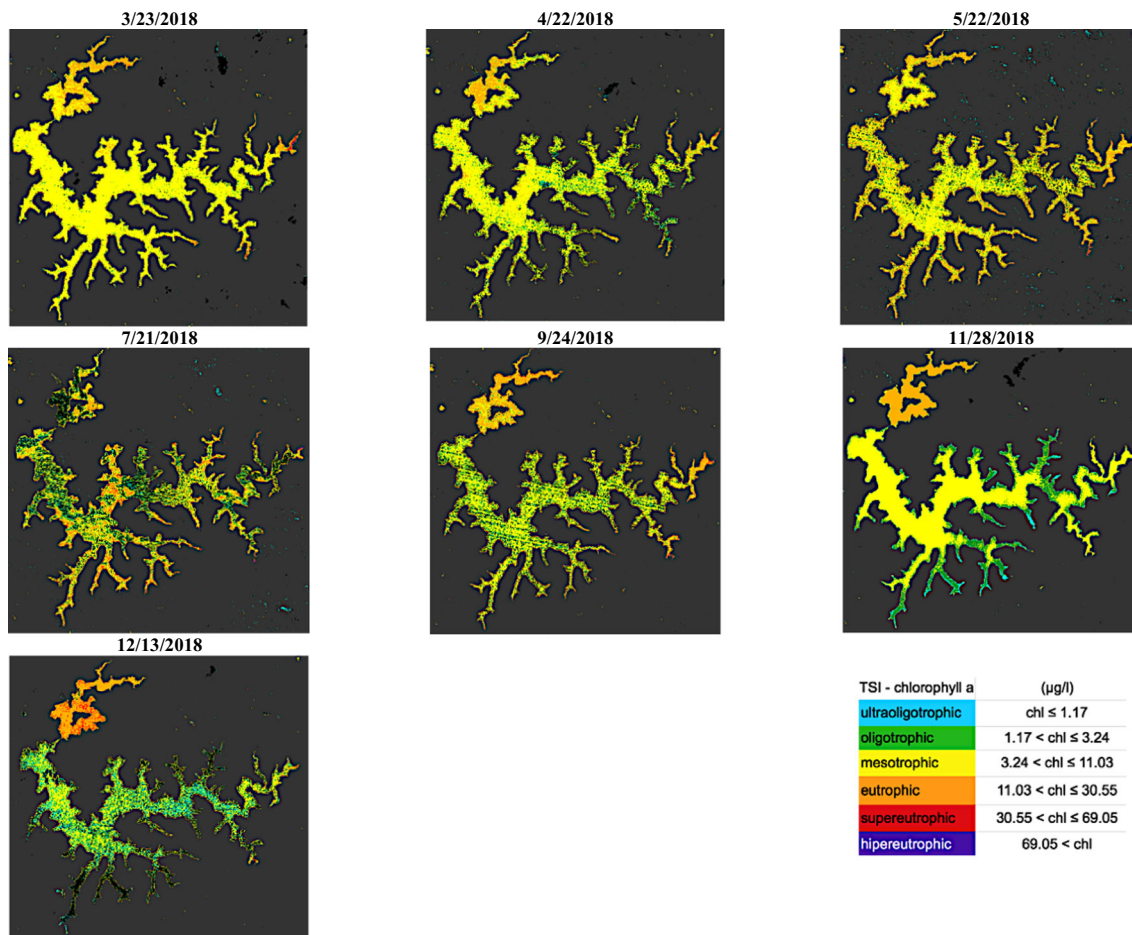


Fig. 8 Maps of chlorophyll a concentration ($\mu\text{g/L}$) in the JG and JC reservoirs for 2018, estimated from the C2RCC-C2X product conc_chl. The colors represent different trophic levels. TSI, trophic state index; chl, chlorophyll a

This strategy is already reflected in the copper concentrations measured in the sediment of this reservoir (Cardoso-Silva et al. 2016). The Cyanobacteria predominance and algaecide applications are facets of the same problem and indicate the need to rethink the monitoring program for these reservoirs, as well as the wider management strategies affecting water quality in the CS. The CS needs to be sustainable in the long term, in order to continue to ensure the provision of water with satisfactory quality for public supply. Hence, the predominance of Cyanobacteria and the control of these microorganisms using copper sulfate applications must be avoided (Pompêo 2020). The strong relationships obtained here among chlorophyll a, SD, turbidity, and Cyanobacteria cell number were in agreement with the observed by Pompêo et al. (2017).

The SD values for the period from 2015 to 2018 were close to those observed for the JG reservoir in May 2013 (Hackbart et al. 2015), but lower than those observed by the same authors for the JC reservoir (around 3 m). Hackbart et al. (2015) reported lower values of chlorophyll a for JC, compared to JG, as observed in the present work. Pompêo et al. (2017) observed SD values above 3 m for JG in 2013. For chlorophyll a, the concentrations observed by Pompêo et al. (2017) were

close to those found in this study, but (depending on the time of year) with higher values for JG, compared to JC. Based on field data published by CETESB, Pompêo et al. (2017) reported a gradient between the reservoirs studied, going from JG towards PC. In general, JG has been the reservoir with the highest chlorophyll a concentration and turbidity, while the AT and PC reservoirs have shown the highest SD values. It should be noted that unlike the observations of Pompêo et al. (2017), in this study, the CA reservoir presented worrying chlorophyll a concentrations and significant Cyanobacteria cell numbers. Pompêo et al. (2017) reported chlorophyll a concentration in the CA reservoir below $4 \mu\text{g/L}$, in 2013, for samples collected at five points in this reservoir, at two times during the year, with the values being much lower than those reported by CETESB (Fig. 6). Similarly, for SD, the authors observed much higher values for the PC reservoir, ranging from 1.6 to 3.7 m.

Chlorophyll a estimate

In validation of the C2RCC-Nets model (conc_chl), a clear correlation was observed between the chlorophyll a field data

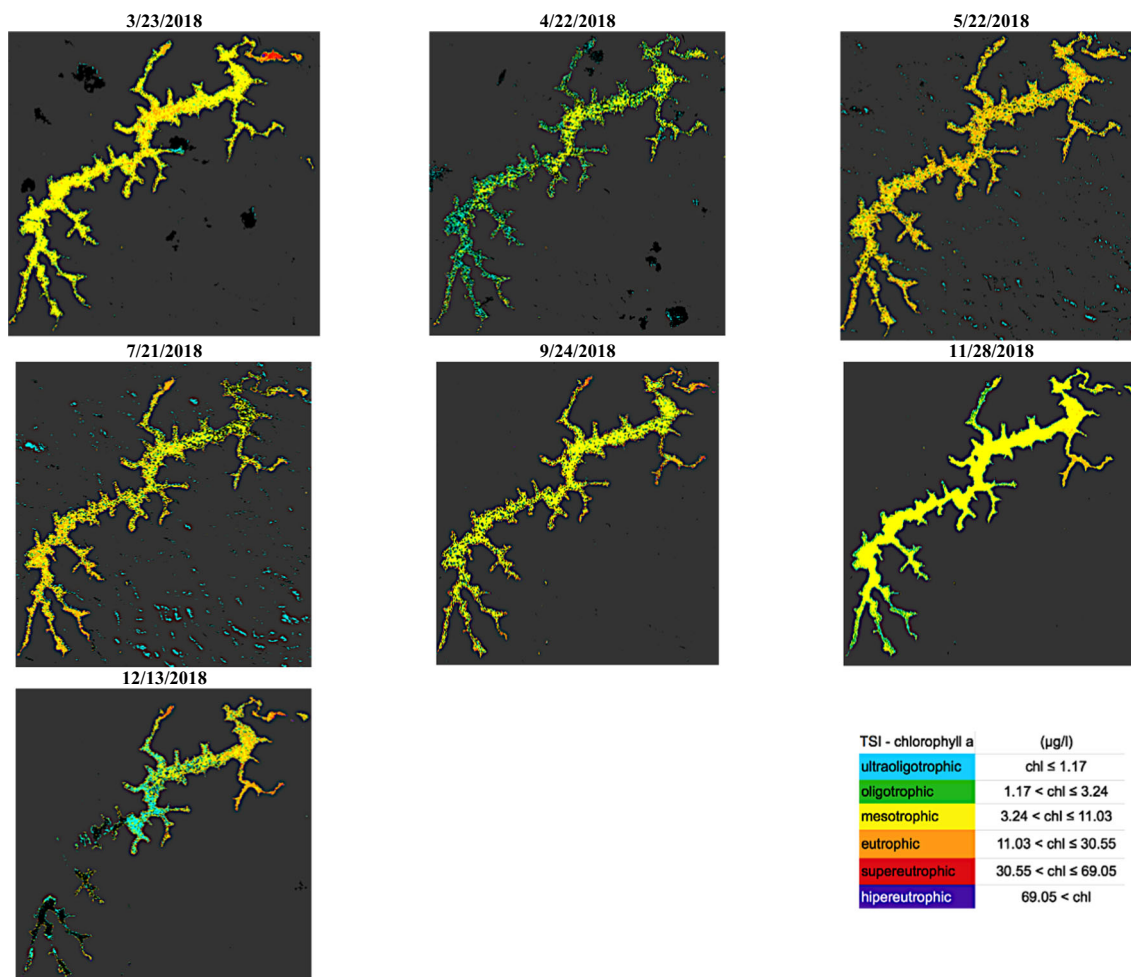


Fig. 9 Maps of chlorophyll a concentration ($\mu\text{g/L}$) in the CA reservoir for 2018, estimated from the C2RCC-C2X product conc_chl. The colors represent different trophic levels. TSI, trophic state index; chl, chlorophyll a

and the values reported by CETESB (Fig. 7a), with high R^2 and low NRMSE. Due to the extreme variation in the water levels and areas of the reservoirs during the study period, it was decided to check whether validation was maintained for specific periods. For other periods in 2015 and 2016 (Fig. 5b), when the water levels were very low, and between 2017 and 2018 (Fig. 5c), after reaching water levels close to those observed before the stress period started in mid-2013 (SABESP 2020b), the C2RCC-Nets model also provided satisfactory estimation of the chlorophyll a concentration in the CS reservoirs. However, the C2RCC-C2X algorithm proved to be more robust for the estimation of chlorophyll a concentration. For the same periods analyzed, there was a close relationship between the chlorophyll a concentration (Fig. 7) estimated by this model and those determined in the field, with lower NRMSE values, compared to use of the C2RCC-Nets model, with the exception of the scenario shown in Fig. 7b.

Figures 8, 9, 10, 11, and 12 show the estimated chlorophyll a concentration maps obtained with the C2RCC-C2X SNAP

product for all the CS reservoirs in 2018. No image for the PC reservoir was available for 4/22/2018. For all the dates considered, the JG and JC reservoirs (Fig. 9) showed trophic levels ranging from oligotrophic to hypertrophic, with the JG reservoir showing a tendency for higher trophic levels, compared to the JC reservoir, as also observed by Pompéo et al. (2017).

The color scale employed in these figures was as described by Lamparelli (2004) and used by CETESB in the annual water quality monitoring reports. The amplitudes of the classes used followed the modified Carson's trophic state index (TSI), developed based on a series of historical data for reservoirs in São Paulo State (ultraoligotrophic: $\text{chl} \leq 1.17$; oligotrophic: $1.17 < \text{chl} \leq 3.24$; mesotrophic: $3.24 < \text{chl} \leq 11.03$; eutrophic: $11.03 < \text{chl} \leq 30.55$; supereutrophic: $30.55 < \text{chl} \leq 69.05$; and hypereutrophic: $\text{chl} > 69.05$). Therefore, the images also represented the degrees of reservoir impairment for water quality, based on the TSI.

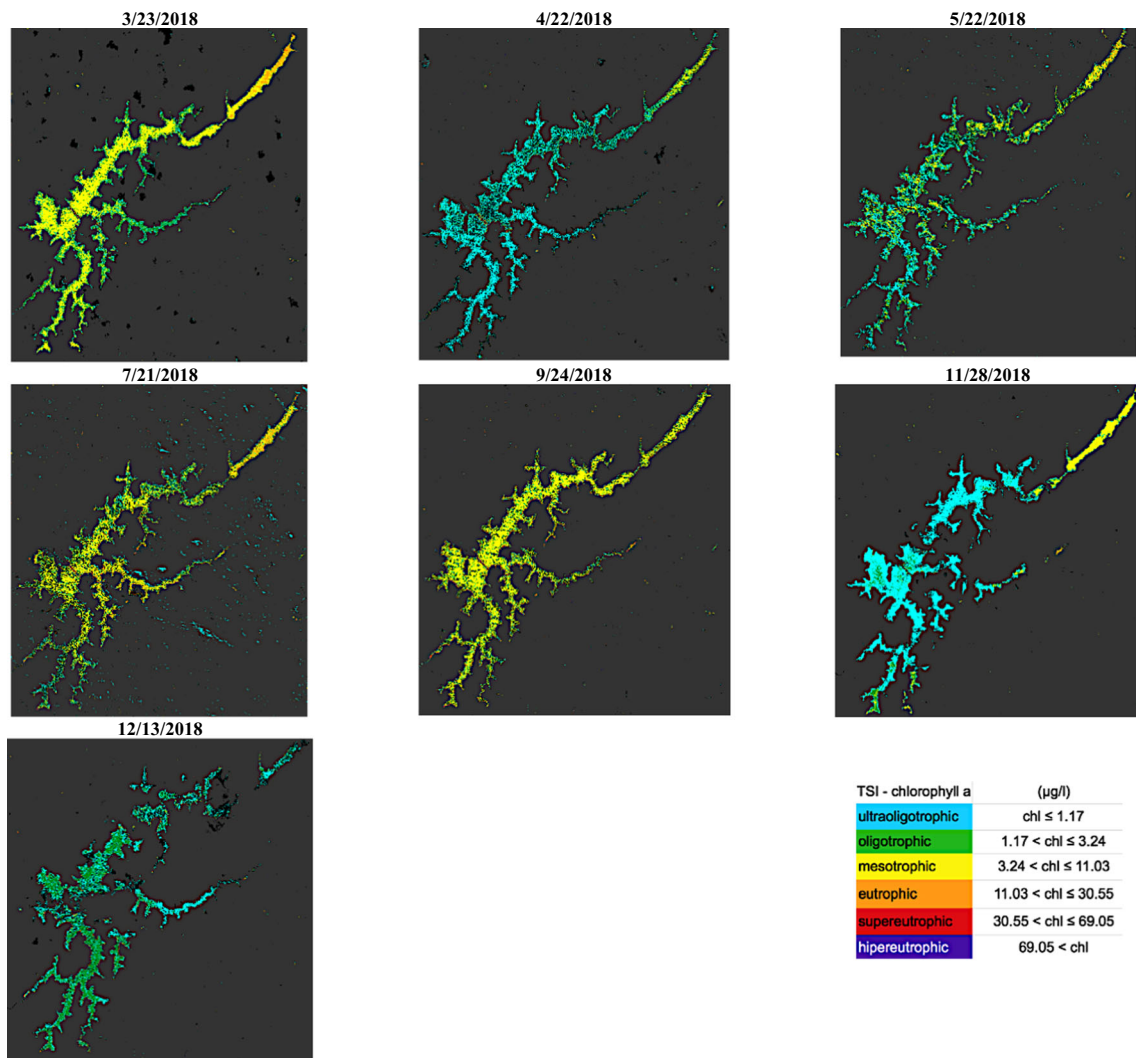


Fig. 10 Maps of chlorophyll a concentration (µg/L) in the AT reservoir for 2018, estimated from the C2RCC-C2X product conc_chl. The colors represent different trophic levels. TSI, trophic state index; chl, chlorophyll a

For the CA reservoir, the data suggested oligotrophic to eutrophic conditions, which was not observed in 2013 by Pompêo et al. (2017). This apparent change in the trophic state may have been due to the drastic reductions in flow and water depth (water level) observed in the CS reservoirs from 2013 to 2015. With the return to water level levels close to normal, there may have been greater entry of nutrients from adjacent areas, due to surface runoff. There may also have been changes in land use and occupation in the watershed, which was also reflected in greater inputs of nutrients to the CA reservoir. The observed trend indicated deterioration of water quality, compared to the earlier period (Pompêo et al. 2017). The observations suggest the need for a higher sampling frequency, as well as the use of a larger number of sampling stations to monitor the water quality in this reservoir.

For the AT and IG reservoirs (Figs. 10 and 11), that they presented satisfactory trophic levels during most of 2018, but higher levels between July and September, the drier months of

the year with lower rainfall. This was especially evident for July, the driest month, as observed from the Bragança Paulista weather station database (climate-data.org).

The PC reservoir (Fig. 12) presented ultraoligotrophic to eutrophic conditions, but with a predominance of oligo-mesotrophy. Oligotrophic conditions were observed near the dam area, while eutrophic conditions occurred in the upper part of the reservoir. Of the CS reservoirs, the PC reservoir has the shortest residence time, which affects the plankton (Matta 2016), as well as compartmentalization of the quality of the surface water (Macedo 2011) and sediment (Cardoso-Silva et al. 2016), with the superficial sediment having low potential toxicity (Silva et al. 2018). Martins et al. (2020), working on the PC reservoir in 2008 and 2009, calculated the TSI as described by Lamparelli (2004), but using the average chlorophyll a and total phosphorus concentrations obtained for surface water

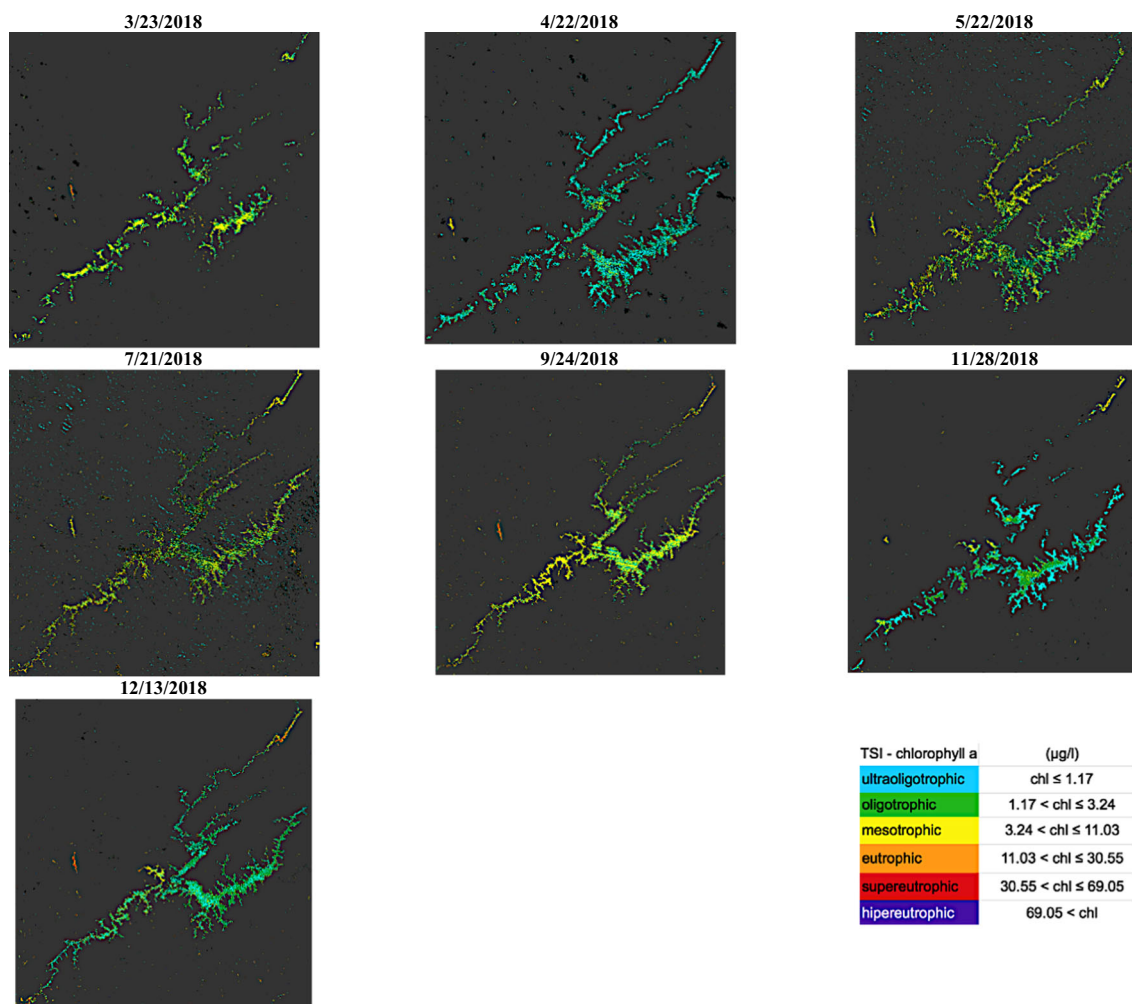


Fig. 11 Maps of chlorophyll a concentration ($\mu\text{g/L}$) in the IG reservoir for 2018, estimated from the C2RCC-C2X product conc_chl. The colors represent different trophic levels. TSI, trophic state index; chl, chlorophyll a

samples. The water samples were geocoded and the TSI values were submitted to TIN (Triangulated Irregular Network) interpolation, converting them into polygons and resulting in a surface image. Based on the empirical images from the TSI, it was concluded that the maps generated using remote sensing were highly significant, with the trophic level of this reservoir estimated as mesotrophic for November 2008 and June 2009, corroborating the findings of Pompêo et al. (2017) and the present work. It should be noted that the city of Mairiporã is located near the upper part of the PC reservoir, close to its entrance. Furthermore, a sewage treatment station adjacent to the city discharges partially treated waters into the access channel to the PC. Hence, these possible sources of N and P could also contribute to the higher trophic levels in the upper part of this reservoir, suggested by the images. Since the CS is a cascade reservoir system, there is a tendency for nutrients to be accumulated in the upstream reservoirs, as suggested by Pompêo et al. (2017).

Secchi disk estimates

The field data for light profiles and SD measurements obtained at Spanish reservoirs in the years 2017, 2018, and 2019 showed a strong relationship between kd_{z90max_field} and SD depth, measured at the same sampling points of these reservoirs (Fig. 13). For practical purposes, the relationship could be described by the following equation:

$$SD = 0.7 * kd_{z90max}, \quad (1)$$

where SD and kd_{z90max} are in m. Based on this fitted equation, strong relationships were also observed between the SD values observed in the field by CETESB and those estimated by Eq. 1 (Fig. 14), using both C2RCC-Nets and C2RCC-C2X. However, the C2RCC-Nets algorithm (Fig. 14b) generated a slightly more robust model, compared to C2RCC-C2X. In the same way as observed for the chlorophyll a concentration estimated with C2RCC-C2X, the maps of the SD values (Figs. 15, 16, 17, 18, and 19) corroborated the findings of

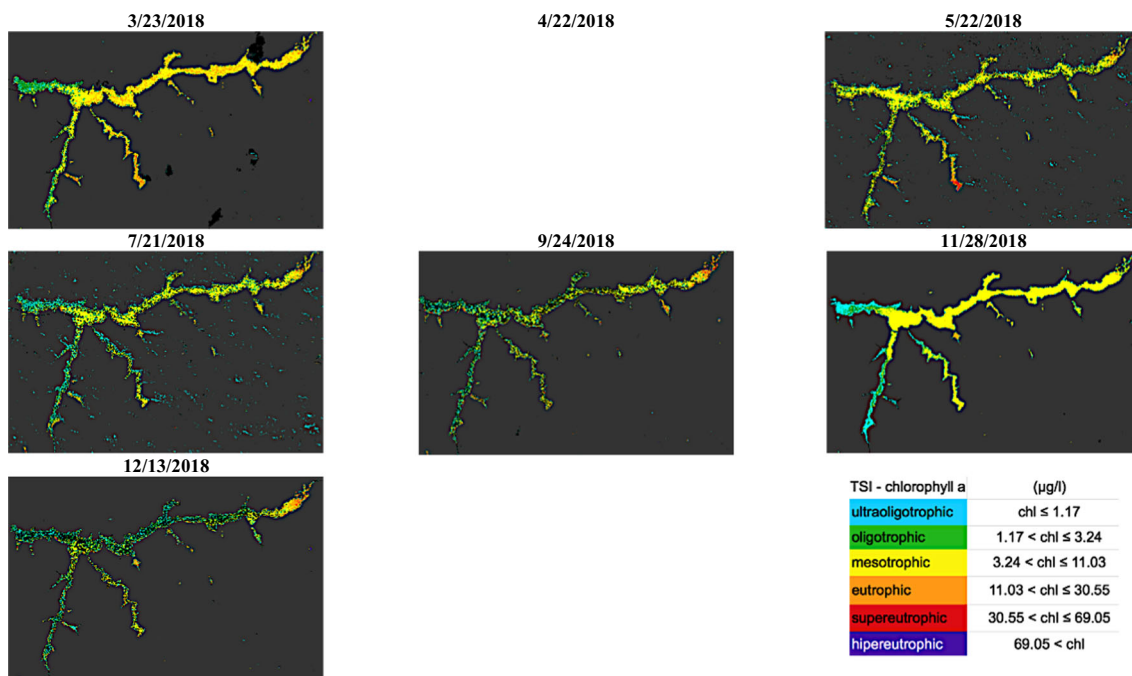


Fig. 12 Map of chlorophyll a concentration (µg/L) in the PC reservoir for 2018, estimated from the C2RCC-C2X product conc_chl. The colors represent different trophic levels. TSI, trophic state index; chl, chlorophyll a

Pompêo et al. (2017), with higher chlorophyll a values and lower SD values for the JG reservoir and the upper section of the PC reservoir.

In previous work, Sòria-Perpinyà et al. (2020) used the Sen2cor atmospheric correction with Sentinel 2 images of the Valencia Lagoon (Spain), obtaining a robust fitted model for SD depth estimates ($R^2 = 0.673$, RMSE = 0.06 m). The model enabled observation of an annual bimodal pattern, with increase of SD explained by a significant increase in water renewal. It was concluded that the algorithm developed to estimate SD values from Sentinel 2 images was accurate and

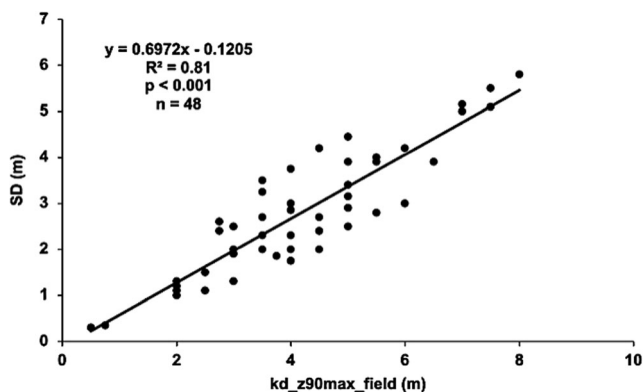


Fig. 13 Relationship between SD depths measured in the field and the depth for 90% extinction of light intensity (kd_{z90max_field}) in Spanish reservoirs

appropriate for use in protocols for monitoring the ecological status of lakes.

As for chlorophyll a, the scales used in Figs. 15, 16, 17, 18, and 19 were as described by Lamparelli (2004), with the range of classes for SD depth also defined using the modified Carlson trophic state index, but for SD (in m), based on a historical series of data for reservoirs in São Paulo State. Therefore, Figs. 16, 17, 18, 19, and 20 also represent the levels of impairment of the surface water quality, based on the TSI for SD. As shown in Fig. 16, the JG reservoir presented higher trophic levels from September to December, for both chlorophyll a and SD. For the CA reservoir (Supplementary Material), the trophic levels varied throughout the year, ranging from ultraoligotrophic (using SD) and from mesotrophic (using chlorophyll a). For the AT and IG reservoirs (Supplementary Material), the conditions were more ultraoligotrophic, using SD, and mesotrophic, using chlorophyll a (especially for the AT reservoir). For the PC reservoir (Supplementary Material), the region closest to the dam was more ultraoligotrophic, using SD and chlorophyll a.

Cyanobacteria cell number estimates

A strong relationship (Fig. 5c) was obtained between chlorophyll a concentration measured in the field by CETESB and the corresponding Cyanobacteria cell numbers determined under a microscope, for the same

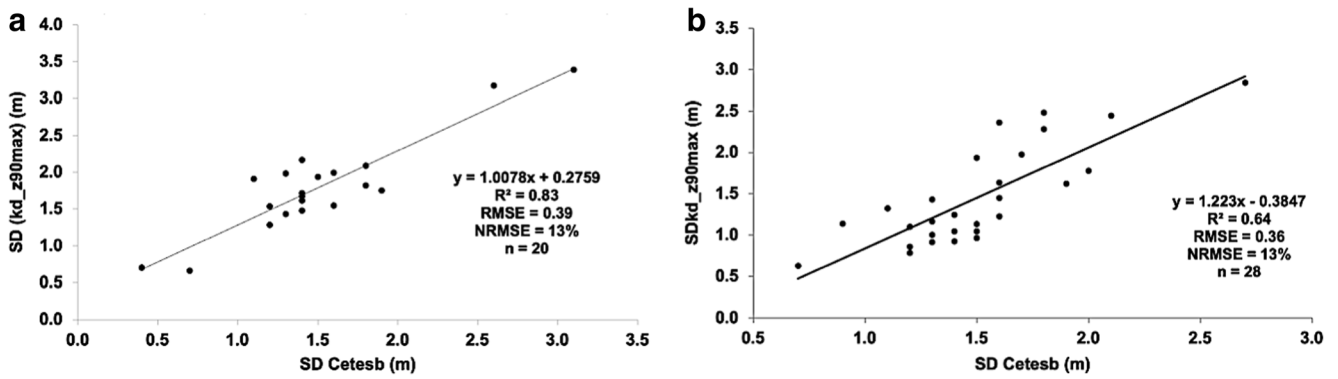


Fig. 14 **a** Relationship between SD depth measured by CETESB in the CS reservoirs and the depth for 90% extinction of light intensity (SDkd_z90max, C2RCC-Nets). **b** Relationship between SD depth measured by CETESB in the CS reservoirs and the depth for 90% extinction of light intensity (SDkd_z90max, C2RCC-C2X)

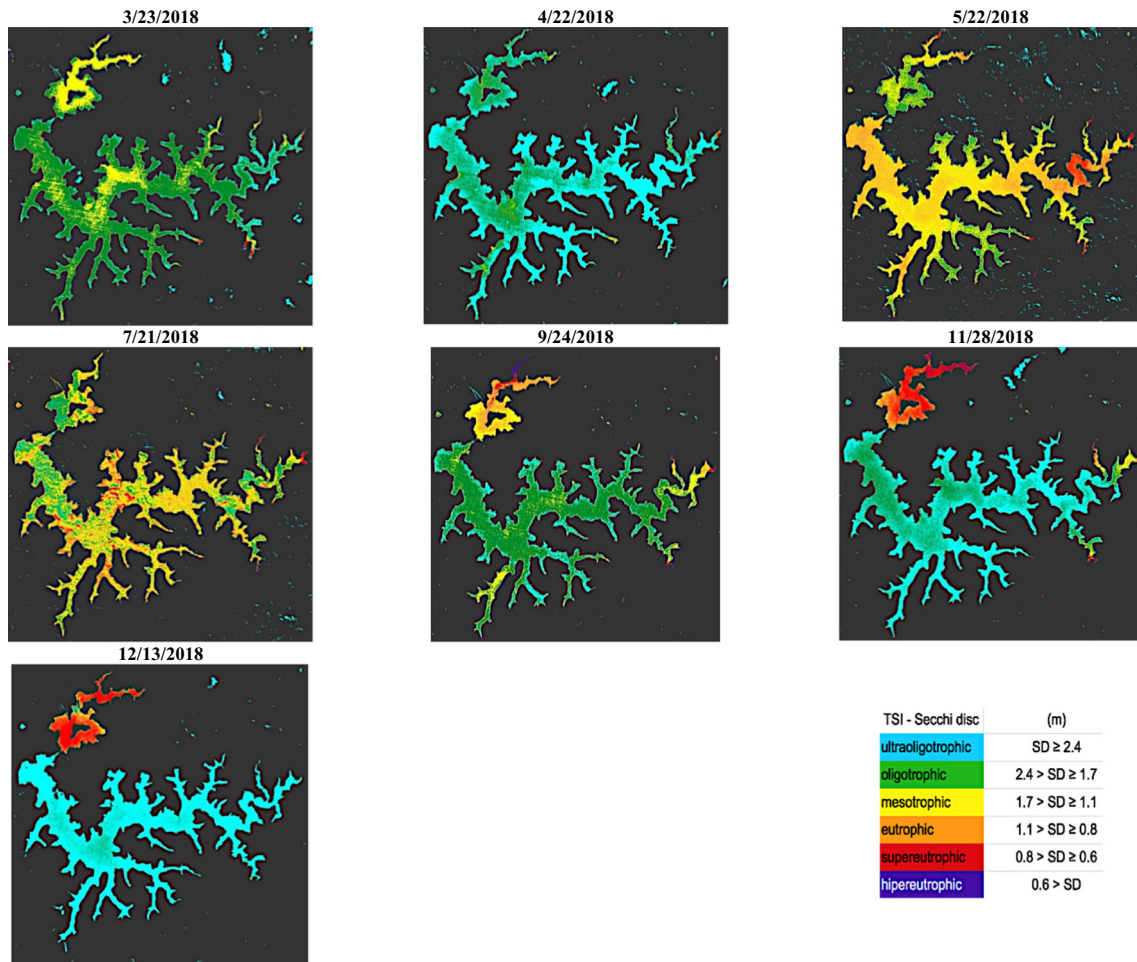


Fig. 15 Maps of the SD depths (m) of the JG and JC reservoirs for 2018, estimated from the fitted equation for the C2RCC-Nets product (kd_z90max). The colors represent different trophic levels. TSI, trophic state index

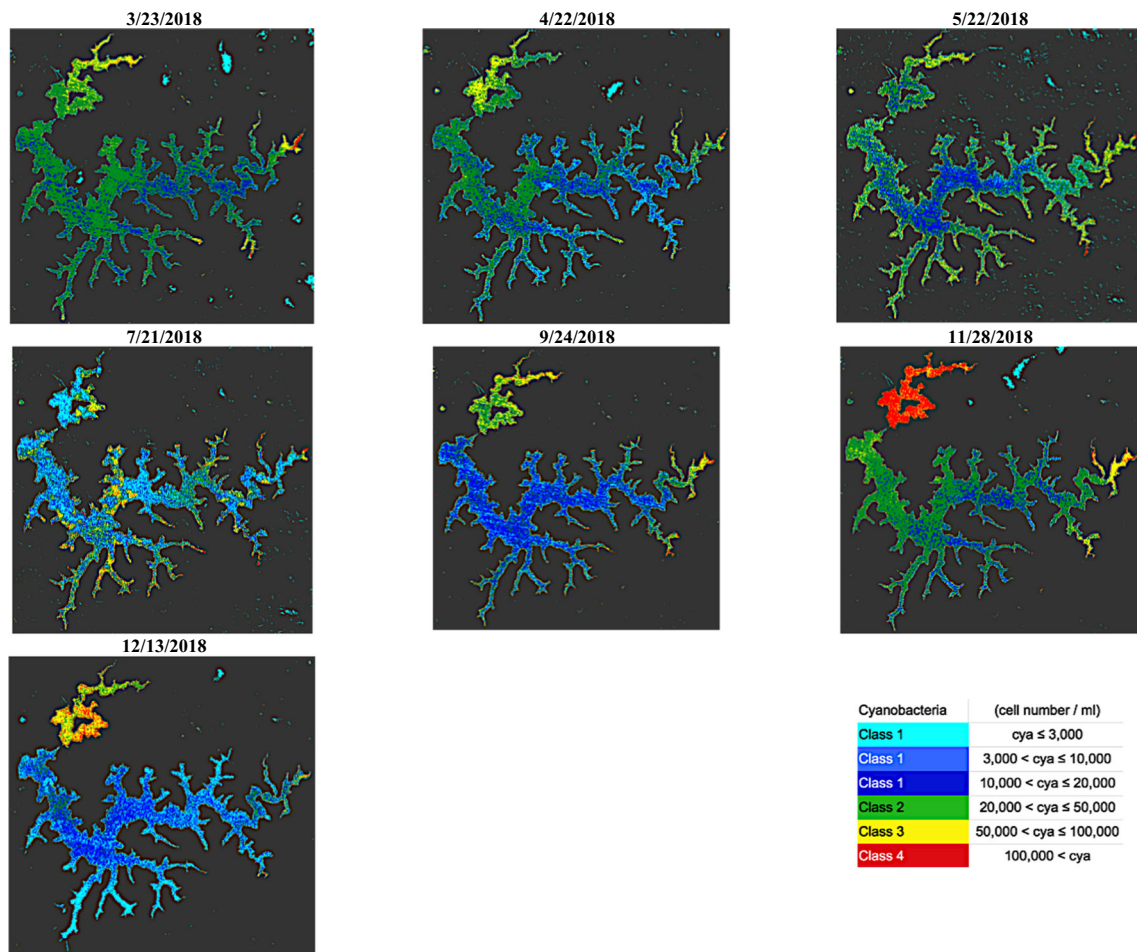


Fig. 16 Maps of estimated Cyanobacteria (cya) cell numbers (cells/mL) in the JG and JC reservoirs, obtained from Sentinel-2 images for the year 2018. The colors also represent different classes of uses (adapted from Brazil, 2005)

sampling stations and data sampling, described by the following equation:

$$cyano = 133.75 \cdot chla^2 + 3089.9 \cdot chla + 3125.9, \quad (2)$$

where cyano is the Cyanobacteria cell number (per mL) and chla is the chlorophyll a concentration (in $\mu\text{g/L}$).

Use of the polynomial model presented in Eq. 2 enabled estimation of the Cyanobacteria cell numbers for the CS reservoirs (Figs. 16, 17, 18, 19, and 20). The chlorophyll a concentration obtained using C2RCC-C2X was used for these estimates. In the same way as for chlorophyll a and SD, the JG reservoir was distinguished from the other reservoirs, since it presented higher numbers of Cyanobacteria cells, with values above 100,000 cells/mL in November 2018 for almost the entire water body. The maps for the other reservoirs showed values below 50,000 cells/mL throughout the year, with the exception of the PC reservoir in November 2018, where the values were between 50,000 and 100,000 cells/

mL. The maps indicated annual patterns with values lower than 20,000 cells/mL only for the AT and IG reservoirs.

The Brazilian law CONAMA Resolution 357 (Brazil 2005) classifies water bodies according to the type of use and provides environmental guidelines for their classification. It also establishes the conditions and standards for the discharge of effluents. The CS reservoirs are classified as class 1, corresponding to water intended for human consumption, after simplified treatment. For class 1, the upper limit for the presence of Cyanobacteria is 20,000 cells/mL. Hence, for much of the year, the estimates obtained using the maps indicated that the JG, JC, and CA reservoirs did not comply with the designated class. In some periods of the year, these reservoirs could be considered class 2, 3, or even 4, the worst of the classes. For class 2, the maximum permitted concentration of Cyanobacteria is 50,000 cells/mL, while for class 3, it is 100,000 cells/mL. For class 4, there is no upper limit for Cyanobacteria cell number. Class 2 reservoirs can supply

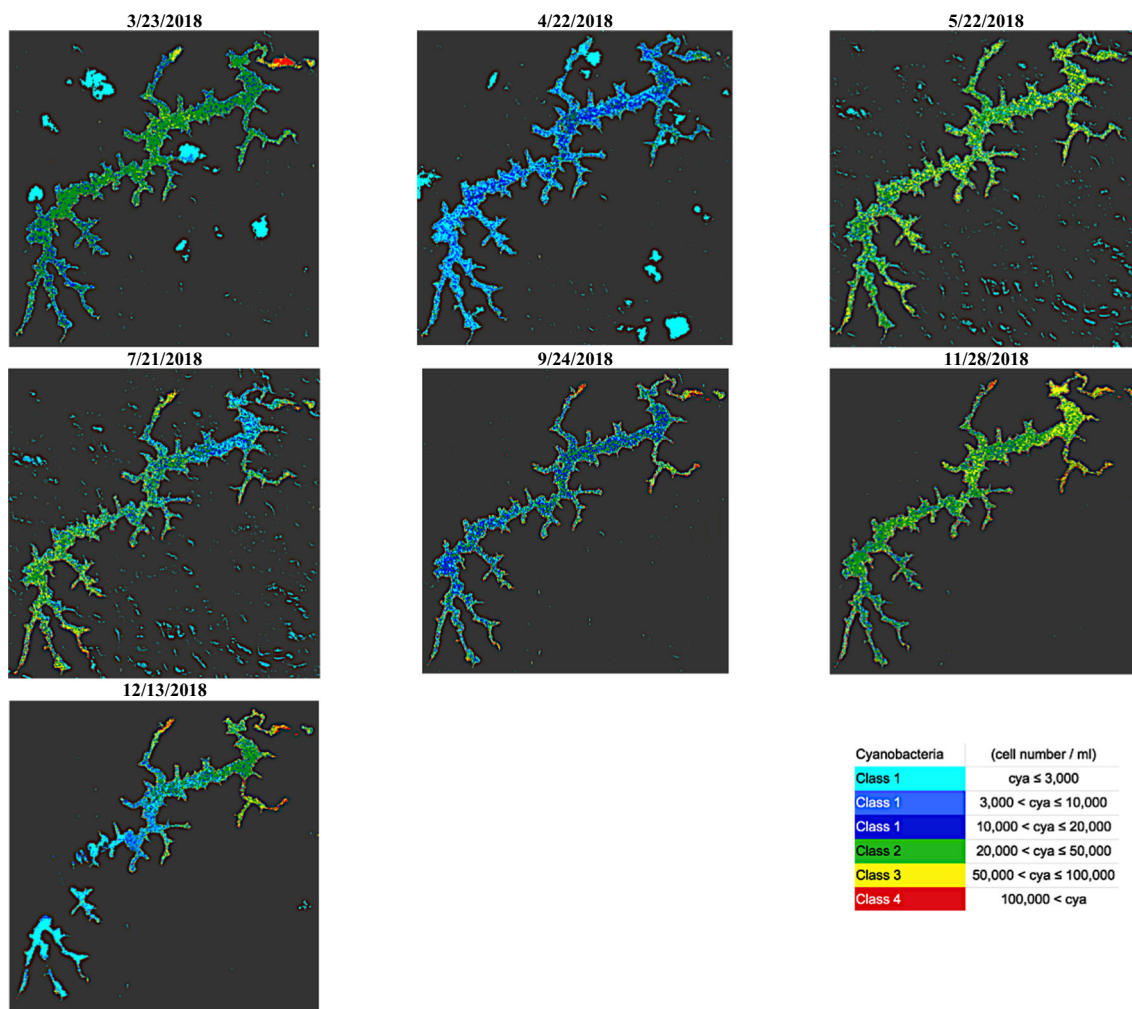


Fig. 17 Maps of estimated Cyanobacteria cell numbers (cells/mL) in the CA reservoir, obtained from Sentinel-2 images for the year 2018. The colors also represent different classes of uses (adapted from Brazil, 2005)

water for human consumption after conventional treatment. Water from class 3 reservoirs can be used for human consumption after conventional or advanced treatment, while class 4 reservoirs are only considered suitable for navigation and landscape purposes. Adopting the principle of “one out all out” (Borja 2010; Hering et al. 2010), if applied to the CS based on the framework classes (Brazil 2005), it could be concluded from the map estimates of Cyanobacteria cell numbers that in 2018, the reservoirs remained in non-compliance with the class 1 classification almost all year round.

Another Brazilian law, Consolidation Ordinance no. 5, of 11/16/2017 (Brazil 2017), states that when the Cyanobacteria number is below 10,000 cells/mL, monitoring of water quality should occur on a monthly basis. For values above 10,000 cells/mL, the monitoring must be weekly. The standard states that for values above 20,000 cells/mL, due to the significance

of Cyanobacteria as potentially toxin-producing organisms, with corresponding negative socioeconomic effects (Steffen et al. 2014), there must be weekly monitoring together with complementary analysis of cyanotoxins, at least at the raw water collection point. Consequently, based on the Cyanobacteria cell numbers and the existing legislation, the JG, JC, CA, and PC reservoirs require complementary monitoring, with quantitative assessments of the cyanotoxin concentrations, especially in the JG, JC, and CA reservoirs.

Conclusions

The joint analysis of chlorophyll a, SD, Cyanobacteria cell number, and turbidity data for the CS reservoirs, obtained from surveys carried out by CETESB for the years 2015 to

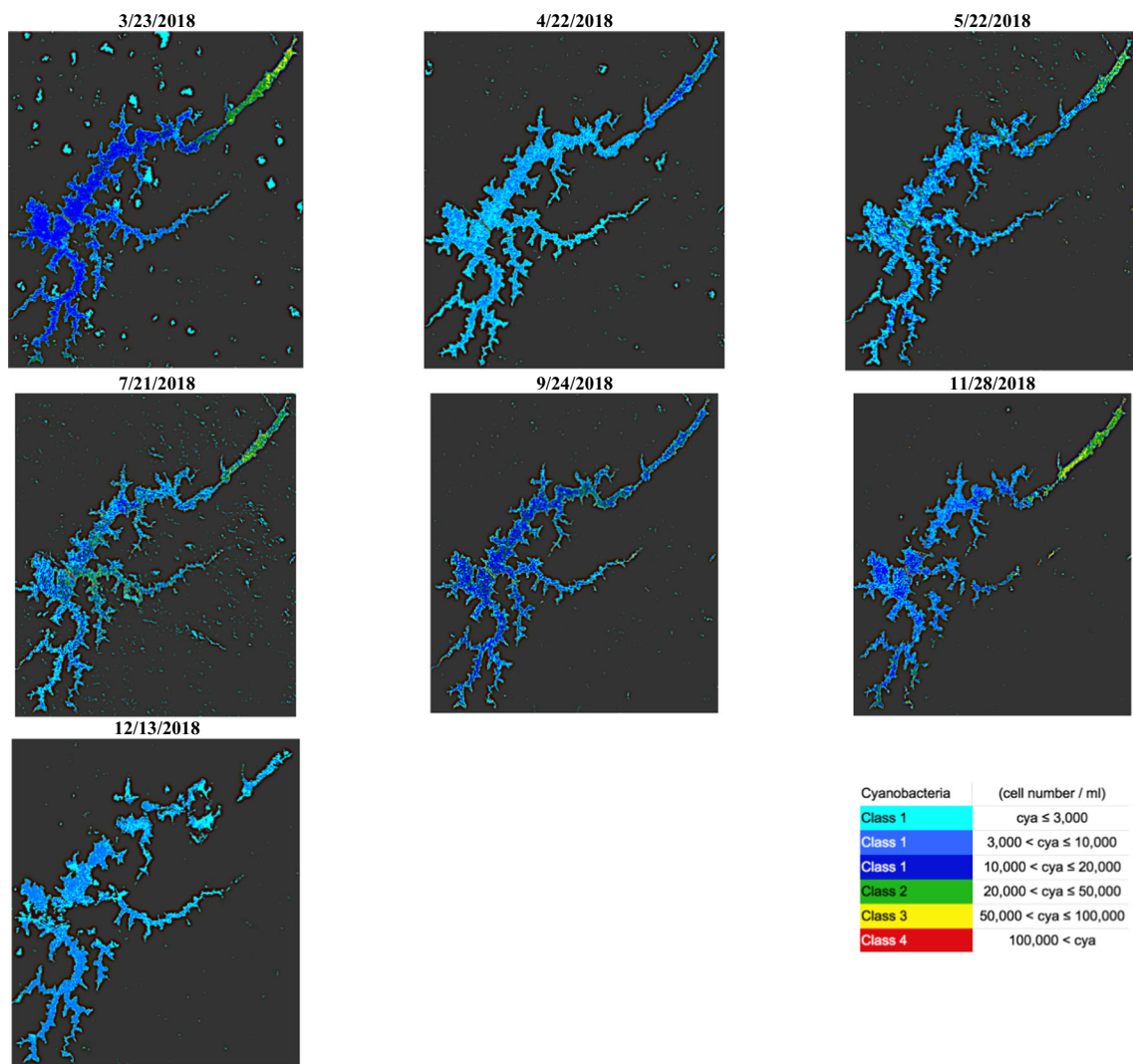


Fig. 18 Maps of estimated Cyanobacteria cell numbers (cells/mL) in the AT reservoir, obtained from Sentinel-2 images for the year 2018. The colors also represent different classes of uses (adapted from Brazil, 2005)

2018, revealed strong relationships among these parameters and also showed that there was a great predominance of Cyanobacteria during the study period. Due to their potential to cause toxicity, these microorganisms can compromise the quality of raw water used in the public supply of 9 million people. The worrying conditions observed in this study indicate the need for changes in the water quality monitoring program of these reservoirs. Therefore, it is necessary to evaluate the feasibility of increasing the sampling frequency, in order to improve monitoring of the evolution of algal growth, especially considering Cyanobacteria. The findings also suggested that the hydrographic basin itself should be monitored (Pompêo 2017), in order to assist in elucidating the influence of greater nutrient inputs caused by changes in the uses of the basin, particularly for the JG, JC, and CA reservoirs, which

were the most eutrophic and presented the highest Cyanobacteria cell numbers.

This study also demonstrated that two native SNAP products, *conc_chl* and *kd_z90max*, obtained using C2RCC (Nets and C2X) atmospheric corrections, were sufficiently robust to allow estimates of chlorophyll a concentrations and SD depths for the waters of the CS reservoirs. This robustness demonstrated the excellent potential of these tools to assist in the development of alternative ways of assessing the water quality in the CS and probably other reservoirs in the region, which could complement existing environmental management programs, as suggested by Machado and Baptista (2016), Pompêo (2017), Pompêo and Moschini-Carlos (2020), and Sòria-Perpinyà et al. (2020).

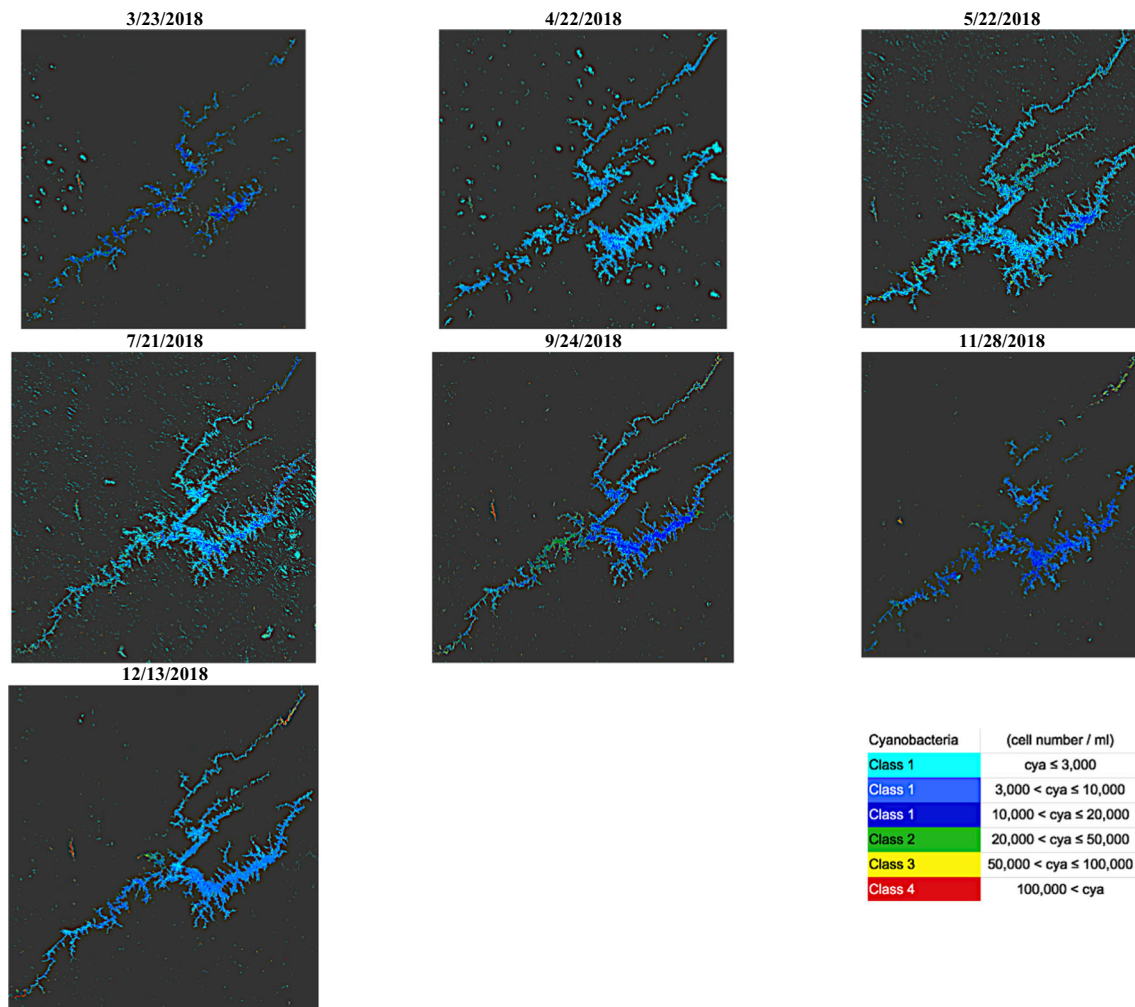


Fig. 19 Maps of estimated Cyanobacteria cell numbers (cells/mL) in the IG reservoir, obtained from Sentinel-2 images for the year 2018. The colors also represent different classes of uses (adapted from Brazil, 2005)

In addition, the values generated may be converted into water quality criteria, using either the TSI or the quality classes based on use, as defined by Brazilian regulations (Brazil 2005; 2017). These products, with calculations performed automatically and the information provided in the form of maps, can speed up the monitoring of water quality, since there is no need to previously generate and validate new models. In addition, the SNAP and Sentinel-2 images are both free, the images have good resolution, and the satellites with a five-day revisit period greatly expand the possibilities for obtaining images. These features, added to release of the images by ESA on an almost daily basis, provide the system with excellent potential for use in the management of South American inland water quality. It is known that Brazilian States are very heterogeneous from the point of view of water quality management and monitoring systems (Cardoso-Silva et al. 2013; Pompêo et al. 2015), with many differences in the parameters

monitored and the frequency of sampling. This same situation may be extended to all of South America. The standardized use of Sentinel-2 products and images would allow the creation of a solid comparative database, which is not possible at present. Hence, free products, robust native algorithms, and good quality estimates, such as those offered by ESA in the forms of Sentinel-2 images and SNAP software, should be considered for use, not least because they require little financial investment and offer an excellent return. In order to maximize the benefits of using this system, it would be valuable to obtain complementary reservoir monitoring information, including quantitative data for total and dissolved solids, as well as the total number of cells making up the phytoplankton population, rather than only the Cyanobacteria number, with this strategy extended to all monitoring stations.

The maps generated in this work, together with the analysis using field data, indicated that there are already problems

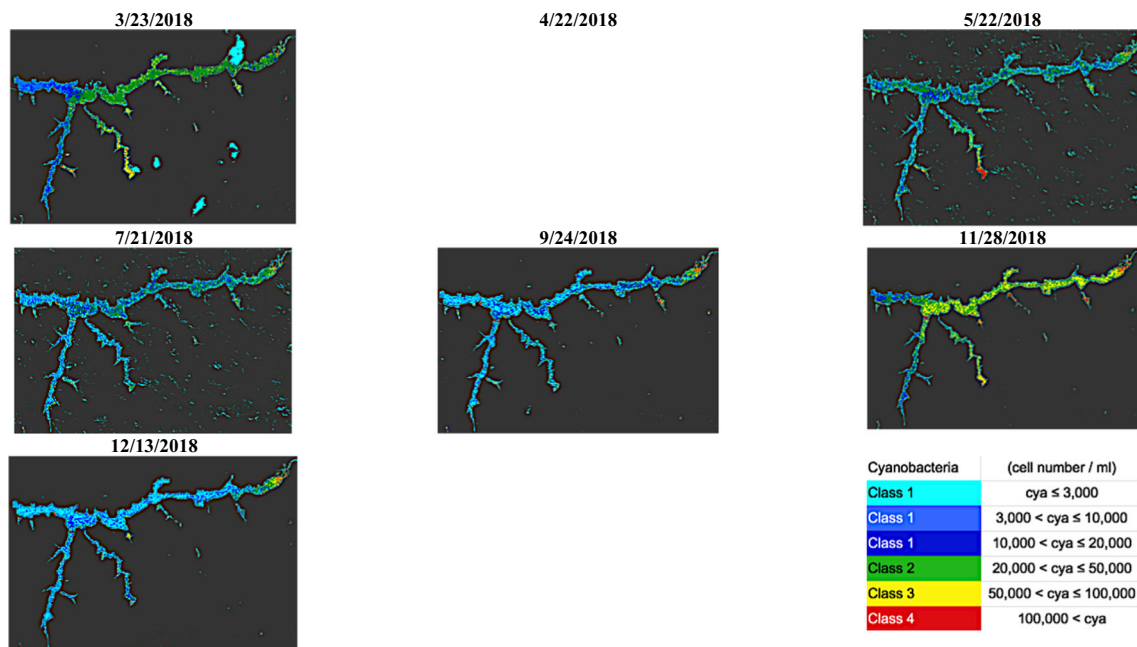


Fig. 20 Maps of estimated Cyanobacteria cell numbers (cells/mL) in the PC reservoir, obtained from Sentinel-2 images for the year 2018. The colors also represent different classes of uses (adapted from Brazil, 2005)

regarding the quality of the water in the CS reservoirs. This is highly concerning, considering that the CS supplies water to around 9 million inhabitants. The findings revealed that at some times of the year, the reservoirs present large regions of the water column with significant chlorophyll a concentration and, more worryingly, high Cyanobacteria numbers. The data also suggested that these features are not occasional, but persist over time, making some of these reservoirs non-conforming to their classification class for most of the year.

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Author contribution All authors contributed to the design of this study, as follows: Marcelo Pompêo: writing original draft, formal analysis, funding acquisition; Viviane Moschini-Carlos: formal analysis, writing review; Marisa Dantas Bitencourt: formal analysis; Xavier Sòria-Perpinyà: formal analysis, writing review; Eduardo Vicente: formal analysis, writing review; Jesus Delegido: formal analysis, writing review. All authors commented on previous versions of the manuscript and read and approved the final manuscript.

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Data Availability The datasets analyzed during the current study are available in the São Paulo environmental agency website, CETESB repository: <https://cetesb.sp.gov.br/aguas-390interiores/publicacoes-e-relatorios/>

Declarations

Ethical approval and consent to participate “Not applicable”

Consent to publish “Not applicable”

Competing interests The authors declare no competing interests.

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