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Modeling water quality in a tropical reservoir using CE-QUAL-W2: handling data scarcity, urban pollution and hydroclimatic seasonality

Modelagem da qualidade da água em um reservatório tropical usando CE-QUAL-W2: lidando com a escassez de dados, poluição urbana e sazonalidade hidroclimática

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ABSTRACT

This study applies a 2-D hydrodynamic model (CE-QUAL-W2) for simulating water quality dynamics in a tropical reservoir located in Fortaleza, Ceará, Brazil. While rainfall concentrates basically in the first semester, this reservoir receives untreated sewage from an urban catchment throughout the year. To deal with data scarcity, model simplifications are justified and several adjustments are carried out, so that only the parameters temperature (T), dissolved oxygen (DO), chlorophyll a (Chla) and phosphate (PO_4) are kept in the modeling process. Additionally, different assumptions are performed regarding the time-evolution of reservoir inlet concentrations: constant values, step and linear variations. The results indicate that the simplified model can predict well the seasonal variations of T, DO, Chla and PO_4. The best fitting between model results and measurements are obtained with the assumption of linear variation in inlet concentrations, followed by the assumptions of constant values and step variation. Moreover, the results reveal that while PO_4 presents a complete mixing behavior with a clear increase in concentration from the wet to the dry season, T, DO and Chla show an alternating stratification-destratification patter during the day-night but without relevant variations throughout the year. Model simulations of different scenarios also indicate a significant reduction in Chla concentration in the second semester, but external load reduction has a stronger impact on model outputs than hydroclimatic variability. The modeling approach developed in the present study is proposed as a simple way to cope with data scarcity, urban pollution and hydroclimatic seasonality in tropical reservoirs.

Keywords: Computational modeling; Eutrophication; Stratification.

RESUMO

Este estudo aplica um modelo hidrodinâmico 2-D (CE-QUAL-W2) para simular a dinâmica da qualidade da água em um reservatório tropical localizado em Fortaleza, Ceará, Brasil. Enquanto as chuvas se concentram basicamente no primeiro semestre, esse reservatório recebe esgoto bruto de uma bacia urbana ao longo do ano. Com o intuito de contornar o problema de escassez de dados, simplificações do modelo são justificadas e diversos ajustes são realizados, de forma que apenas os parâmetros temperatura (T), oxigênio dissolvido (DO), clorofila a (Cla) e fosfato (PO_4) sejam mantidos no processo de modelagem. Adicionalmente, diferentes suposições são realizadas em relação à evolução temporal das concentrações de entrada do reservatório: valores constantes, variações em degrau e variações lineares. Os resultados indicam que o modelo simplificado pode prever bem as variações sazonais de T, DO, Cla e PO_4. O melhor ajuste entre os resultados do modelo e as medições é obtido com a hipótese de variação linear nas concentrações de entrada, seguida pelas hipóteses de valores constantes e variação em degrau. Além disso, os resultados revelam que enquanto PO_4 apresenta um comportamento de mistura completa com um claro aumento na concentração da estação chuvosa para a seca, T, OD e Cla apresentam um padrão alternado de estratificação-desestratificação durante o dia-noite, mas sem variações relevantes ao longo do ano. As simulações do modelo para diferentes cenários também indicam uma redução significativa de Cla no segundo semestre, mas a redução da carga externa tem um maior impacto nos resultados do modelo do que a variabilidade hidroclimática. A abordagem de modelagem desenvolvida no presente estudo é proposta como uma maneira simples de lidar com a escassez de dados, poluição urbana e sazonalidade hidroclimática em reservatórios tropicais.

Palavras-chave: Modelagem computacional; Eutrofização; Estratificação.

INTRODUCTION

Lake and reservoir eutrophication is a critical problem, specially in developing countries. In order to improve water resources management, water quality modeling in such water bodies has long been used as an important tool (Chapra, 2008). In this sense, several modeling approaches can be applied, including zero-dimensional (Vollenweider, 1968; Mannich et al., 2015; Rocha & Lima Neto, 2021a, 2021b), one-dimensional (Araújo & Lima Neto, 2018; Araújo et al., 2019; Fraga et al., 2020; Carvalho & Bleninger, 2021), two-dimensional (Deus et al., 2013b; Lindenschmidt et al., 2019; Mesquita & Lima Neto, 2022; Rocha et al., 2022b) and tridimensional models (Deus et al., 2013a; Polli & Bleninger, 2019; Rocha et al., 2022a). A review of the effects of dimensionality on the performance of hydrodynamic models for lakes and reservoirs has been provided by Ishikawa et al. (2022). Multidimensional models including 2-D and 3-D approaches are generally used to simulate the hydrodynamics and thermal regime of the lakes and reservoirs, without necessarily modeling water quality parameters such dissolved oxygen, nutrients, algae, among others which are relevant to characterize the levels of eutrophication and compliance with respect to the required standards (Mesquita et al., 2020; Rocha et al., 2022a, 2022c). On the other hand, because of data scarcity and for the sake of simplicity, most recent water quality modeling studies still have focused on zero-dimensional models (Rocha & Lima Neto, 2021a, 2021b; Ferreira & Fernandes, 2022; Lima Neto et al., 2022).

CE-QUAL-W2 is a 2-D laterally-averaged hydrodynamic model that combines a relatively low computational cost, when compared to 3-D systems, and a wide range of water quality parameters, including more than 60 variables that interact at different compartments: air, water and sediments. This model has been in development for decades and its source code is freely available. Details of the model can be found in its comprehensive manual (see Cole & Wells, 2017). Since it is a laterally-averaged model, most of its applications focus on relatively narrow water bodies such as rivers and reservoirs. Examples of such applications are: simulating density currents and their effects on thermal stratification in lakes (Kim & Kim, 2006); evaluating the impact of pisciculture in the water quality of reservoirs (Deus et al., 2013b); investigating the biogeochemical responses to climatic and hydrologic forcing in river-reservoir systems (Zhang et al., 2018); modelling the impact of dam operations on nutrient dynamics (Lindenschmidt et al., 2019), assessing the effects of hydrodynamics on lake evaporation (Mesquita et al., 2020), and quantifying the impact of rainfall-inflow on the thermal stability of reservoirs (Rocha et al., 2022c).

Although the CE-QUAL-W2 model has been used worldwide for water quality modeling studies, in tropical regions, such applications have usually been limited to simulations of the hydrodynamics and thermal regime of lakes and reservoirs (Barros, 2019; Golyjeswki, 2020; Mesquita et al., 2020; Rocha et al., 2022c). It is important to mention that recent studies have also coupled the CE-QUAL-W2 hydrodynamic model outputs to zero-dimensional water quality models to predict total phosphorus concentrations in tropical reservoirs (Mesquita & Lima Neto, 2022; Rocha et al., 2022b). However, direct applications of the CE-QUAL-W2 model to predict water quality patterns in tropical reservoirs, also including the dynamics of other parameters such as dissolved oxygen, algae, soluble reactive phosphate, and so on, are still scarce in the literature.

In the present study, the CE-QUAL-W2 model was employed to simulate water quality dynamics in a tropical reservoir subject to significant urban pollution and hydroclimatic seasonality. The objectives were: (1) to discuss and perform adaptations in the water quality modeling procedures of CE-QUAL-W2 to manage data scarcity; (2) to evaluate the impact of different time-evolution patterns of reservoir inlet concentrations in the water quality modeling outputs; (3) to calibrate/validate the model with field data and investigate the spatio-temporal variations of water quality parameters in the reservoir; and (4) to simulate different scenarios of input load reduction and hydroclimatic variability with respect to the compliance with the mandatory water quality standards and the trophic state categories of the reservoir.

METHODOLOGY

Study area

The study site is the Santo Anastácio Reservoir (SAR), an eutrophic urban lake located in a low-income area of Fortaleza, capital of the State of Ceará, which is the city with the highest population density in Brazil (~8,700 hab/km^2). Figure 1 shows the catchment area of SAR and the reservoir discretization in the CE-QUAL-W2 model. The location where the measurements were taken at the inlet and outlet of SAR is also indicated both in the plan and side views. The fitting of the elevation-volume curve generated in CE-QUAL-W2 to the measured one is depicted in Figure 2, which was considered sufficient for the purposes of the present study. The annual precipitation measured in a meteorological station located at 500 m from the reservoir outlet ranges from about 1,000 to 2,500 mm, with two well-defined seasons: the wet period, concentrated basically in the first semester, and the dry period, concentrated in the second semester. Figures 3 and 4 show the daily variations of hydroclimatic conditions for a typical year (2018) with annual precipitation of 1,770 mm. On the other hand, water temperature variation in the reservoir is relatively small (27-31 °C). SAR is supplied from a catchment area of about 4 km^2 drained by a 2.5 km long and 5.0 m wide channel. This catchment area is covered by a sewage network, but most residences surrounding the drainage channel (about 1/5 of the watershed area) are not connected to the system, resulting in an almost constant inflow of untreated sewage to the reservoir throughout the year. The water is discharged from SAR through a 2.0 m wide Creager spillway. More details of the study area can be found in previous studies (Pacheco & Lima Neto, 2017; Araújo & Lima Neto, 2018; Araújo et al., 2019; Fraga et al., 2020; Mesquita et al., 2020; Mesquita & Lima Neto, 2022).

Hydrodynamic modeling

The CE-QUAL-W2 model solves the Reynolds Averaged Navier-Stokes (RANS) equations in the longitudinal and vertical directions. The equations are written in the conservative form using the Boussinesq and hydrostatic approximations. The model

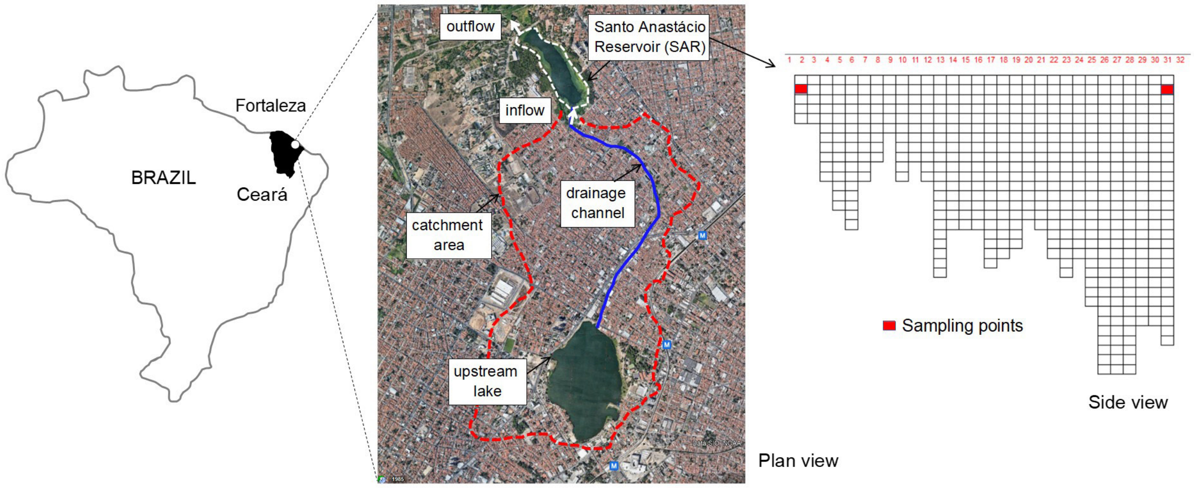

Figure 1. Catchment area and discretization of Santo Anastácio Reservoir (SAR) in the CE-QUAL-W2 model. Measurements taken at the inflow and outflow sections (plan view), which correspond to the second cell of segments 2 and 31 (side view), respectively.

uses input data of bathymetry and hydroclimatic conditions to solve the water balance, the laterally-averaged velocity field and the thermal regime of the reservoir. Temperature is included in the hydrodynamics to account for the water density effect on stratification. Different turbulence-closure models can be used. In the present study, the simple turbulence-closure model named W2 was considered, as it presents a lower computational effort than more complex closure schemes such as the k-ε turbulence model. The W2 model assumes the maximum vertical-grid spacing as the mixing length and uses the turbulence-viscosity formulation derived by Cole & Buchak (1995). Calibration and validation of this model to SAR have been performed by Mesquita et al. (2020), Mesquita & Lima Neto (2022) and Rocha et al. (2022b). Therefore, the same hydrodynamic modeling approach and input files, which include data of bathymetry (see Figure 2) and hydroclimatic conditions from January 1st to December 31st of 2009-2019, covering both daily and sub-daily data (see Figures 3 and 4), will be used in this study. The discretization of SAR in the CE-QUAL-W2 model (side view) is depicted in Figure 1. Comparisons between the model outputs by using the W2 and k-ε approaches are also carried out in this study.

Water quality modeling

The CE-QUAL-W2 model solves the 2-D advection-diffusion-reaction equation (Equation 1) for water temperature and other water quality parameters such as suspended solids, nutrients, dissolved oxygen, organic matter and algal dynamics. In total, the model version 4.1, used in the present study, computes over 60 water quality parameters (Cole & Wells, 2017).

$$\frac{\partial B\phi}{\partial t}+\frac{\partial UB\phi}{\partial x}+\frac{\partial WB\phi}{\partial z}=\frac{\partial\left(BD_x\frac{\partial\phi}{\partial x}\right)}{\partial x}+\frac{\partial\left(BD_z\frac{\partial\phi}{\partial z}\right)}{\partial z}+S\phi B \qquad (1)$$

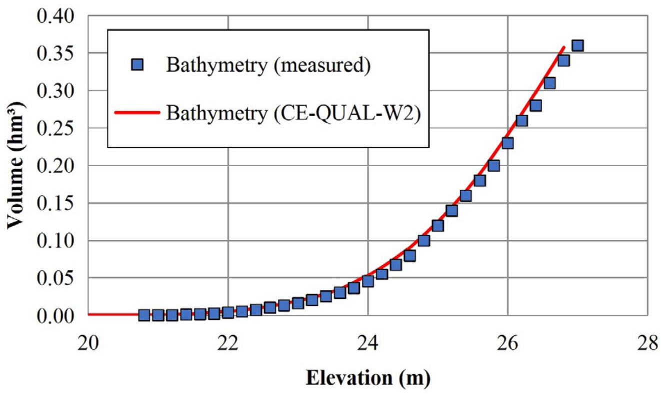

Figure 2. Fitting of the elevation-volume curve generated in CE-QUAL-W2 to the measured one in SAR.

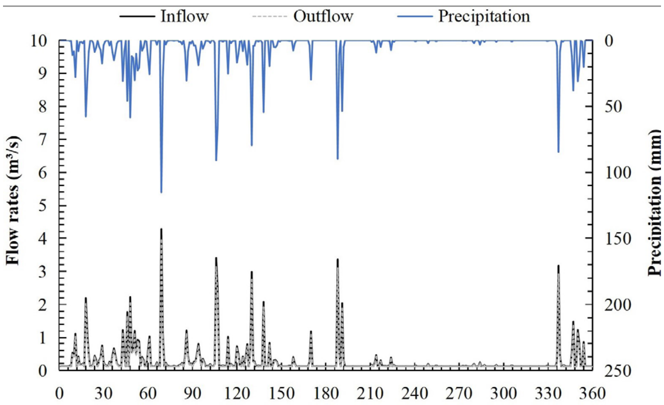

Figure 3. Daily precipitations, inflows and outflows measured at SAR in a typical year (2018).

in which B is the cell width (m), U and W are the longitudinal and vertical velocity components (m/s), respectively, t is time (s), x and z are the longitudinal and vertical coordinates (m), respectively, ϕ is the laterally-averaged constituent concentration (mg/L), D_x and D_z are the longitudinal and vertical dispersion coefficients (m^2/s),

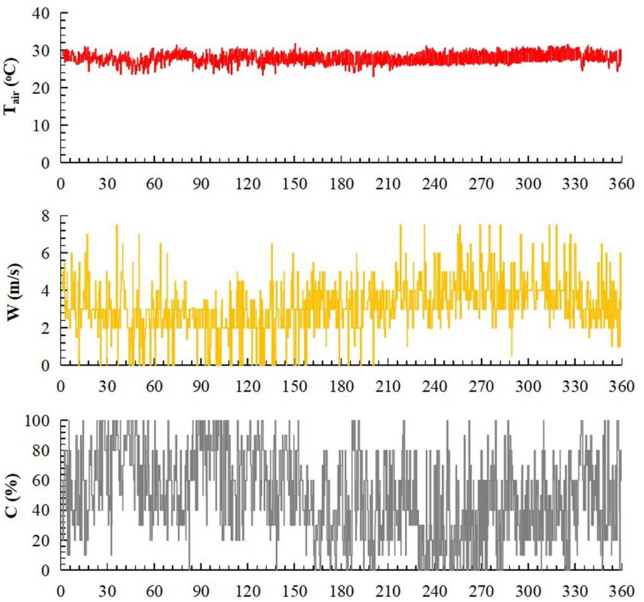

Figure 4. Sub-daily variations of air temperature (T_{air}), 10m wind speed (W) and cloud cover (C) measured at SAR in a typical year (2018).

respectively, and S_ϕ is the laterally-averaged source/sink term for each constituent [mg/(L.s)]. Note that here the lateral inflow or outflow of constituents is neglected and the concentration of heat is determined to be $\varrho c_p T$, where ϱ is the fluid density, c_p is the specific heat of water and T is water temperature.

The water quality data used in the present study was obtained from Pacheco & Lima Neto (2017) and Rocha et al. (2022b). The measurements were taken in 2013 and 2019 at the reservoir inlet and outlet, which correspond to the second cell of segments 2 and 31 (see Figure 1), and were limited to the following parameters: temperature (T), dissolved oxygen (DO), chlorophyll a (Chla) and phosphate (PO_4). Therefore, although the CE-QUAL-W2 model can handle several water quality parameters, these four were the only ones kept in the modeling process. Hence, to deal with data scarcity, it was assumed that the interactions among T, DO, Chla and PO_4 could be described by the following equations for the laterally-averaged source/sink terms in Equation 1:

$$S_a = K_{ag}\phi_a - K_{ar}\phi_a - K_{ae}\phi_a - K_{am}\phi_a - \omega_a \frac{\partial \phi_a}{\partial z} \quad (2)$$

$$S_p = \left(K_{ar} - K_{ag}\right)\delta_{pa}\phi_a + PO4R.SOD\frac{A_{sed}}{V} \quad (3)$$

$$S_{DO} = \left(K_{ag} - K_{ar}\right)\phi_a + \frac{A_{sur}}{V_{sur}}K_L\left(\phi_{SDO} - \phi_{DO}\right) - SOD\frac{A_{sed}}{V} \quad (4)$$

In which S_a, S_p and S_{DO} are the source/sink terms of Chla, PO_4 and DO [mg/(L.day)], respectively, K_{ag}, K_{ar}, K_{ae} and K_{am} are the algal growth, respiration, excretion and mortality rates (1/day), respectively, ϕ_a is the concentration of Chla (mg/L), ω_a is the algal settling rate (m/day), δ_{pa} is the algal stoichiometric coefficient for phosphorus, PO4R is the sediment release rate of PO_4 under anaerobic conditions specified as a fraction of the sediment oxygen demand, SOD [g/(m^{2}day)], A_{sed} is the sediment surface area (m^2), V is the cell volume (m^3), K_L is the interfacial exchange rate for oxygen (m/s), ϕ_{SDO} and ϕ_{DO} are the saturation and actual DO concentration (mg/L), respectively, and A_{sur} and V_{sur} are the surface area (m^2) and volume (m^3), respectively. Observe that the effect of T on the source/sink terms is described by Arrhenius temperature dependence functions (see Cole & Wells, 2017).

Equations 2 to 4 are simplifications of the complete equations presented by Cole & Wells (2017) for algae, phosphorus and dissolved oxygen, which include several additional terms to account for the interactions among different inorganic solids, organic matter and nitrogen fractions, phytoplankton, zooplankton and macrophyte species, methane, hydrogen sulfide, iron and manganese. The selection of the parameters K_{ag}, K_{ar}, K_{ae}, K_{am}, ω_a and SOD was also supported by a sensitivity analysis.

The calibration of K_{ag}, K_{ar}, K_{ae}, K_{am}, ω_a and SOD was performed by statistical analysis, comparing the model results and measurements of Chla, PO_4 and DO taken near the reservoir outlet (second cell of segment 31 in Figure 1) through minimization of the average relative deviation (RD) among these three parameters. Note that other dimensionless metrics, namely the percent bias (PBIAS) and determination coefficient (R^2), were also calculated for comparison purposes. A similar calibration procedure was conducted by Deus et al. (2013b). Since both K_{ag} and K_{ar} are included in the three equations for the source/sink terms (Equations 2 to 4), these were assumed to be the main fitting parameters controlling the dynamics of water quality. Then, K_{ae}, K_{am} and ω_a were adjusted for refinement of Chla prediction, while a fixed value of SOD was considered, assuming that all the sinks of DO (except for $K_{ar}\phi_a$) can be included in this factor, in absence of data of organic matter and other intervenient parameters. On the other hand, the interfacial exchange rate for oxygen (K_L) was calculated by the formula of Cole and Buchak (1995): $K_L = 0.5 + 0.05W^2$, in which W is the 10m wind speed. This is considered an update of the classical equation of Wanninkhof et al. (1991). The model was tested for both equations, and the deviations in the simulated DO concentrations were lower than 1%. In fact, for the typical range of wind speeds (2-6 m/s) considered in the present study (see Figure 4), the results from these equations tend to overlap. Therefore, the formula of Cole & Buchak (1995) was used in the simulations. Additionally, to cope with data scarcity, average values of Chla, PO_4 and DO were assumed as initial inlet and reservoir conditions. However, different assumptions were made regarding the evolution of inlet concentrations: constant averaged-values, step variation from wet to dry periods, and linear variation throughout the year. Finally, default values and empirical formulae from Cole & Wells (2017) were used for the other parameters in Equations 1 to 4.

The CE-QUAL-W2 model solved the hydrodynamics and water quality (Equations 1 to 4) considering the three time-evolution patterns of inlet concentrations (constant averaged-values, step and linear variations) and the best fit of K_{ag}, K_{ar}, K_{ae}, K_{am}, ω_a and SOD was obtained by minimizing the deviations between model results and the data of Chla, PO_4 and DO obtained in 2013 (calibration process). Then, the model was validated by comparing the deviations between simulations and measurements of PO_4 obtained in 2019 (validation process). Lastly, the validated model was used to investigate the impacts of PO_4 reduction and hydroclimatic variability on Chla outpus, which were also compared with the national water quality standards (Brasil, 2005) and the trophic state categories of Cunha et al. (2013).

A step-by-step summary of the methodology is presented as follows:

1. Preparation of input files: bathymetry, sub-daily time series of meteorological parameters, and daily time series of inflow;
2. Calibration of the model using 2013 data of T, Chla, PO_4 and DO measured at the reservoir outlet, assuming different time-evolution patterns of inflow temperature and concentration: constant averaged-values, step and linear variations. The objective-function was the minimization of RD, but PBIAS and R^2 were also used for comparison;
3. Sensitivity analysis on the average variation of model outputs for PO_4, Chla and DO;
4. Analysis of the spatio-temporal variations of T, Chla, PO_4 and DO in the reservoir;
5. Validation of the model using the 2019 data of PO_4 measured at the reservoir outlet, assuming the above-mentioned time-evolution patterns of inflow temperature and concentration. The metrics RD, PBIAS and R^2 were also used for comparison;
6. Simulations of Chla with the validated model considering two scenarios: a wet (2009) and a dry (2013) year; and input load reduction;
7. Analysis of the results with respect to the changes in the water quality class and trophic status of the reservoir.

RESULTS AND DISCUSSION

The CE-QUAL-W2 model results confirm a relatively weak stratification pattern in SAR with water temperature contrasts between top and bottom water layers of up to about 3°C throughout the year, as already pointed out by Mesquita et al. (2020), Mesquita & Lima Neto (2022) and Rocha et al. (2022b) by using the same turbulence-closure model (W2). Figure 5 shows a typical output of the CE-QUAL-W2 model. Because of the simple geometry of SAR and weak stratification patterns, additional simulations with the k-ε turbulence model resulted in similar outputs as those obtained with the W2 scheme, with RD and PBIAS lower than 1% and R^2 higher than 0.99. Therefore, all the water quality modeling processes carried out in this study (calibration, validation and simulations) considered the simpler W2 turbulence-closure model.

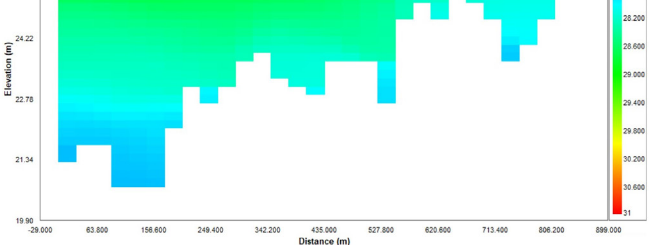

Figure 5. Typical output of the CE-QUAL-W2 model simulation of water temperature distribution in SAR, indicating a relatively weak stratification pattern with temperature contrasts between top and bottom water layers of about 2 °C (10:00h, January 30, 2013).

Average values of T = 28.2 °C, Chla = 72.0 mg/L, PO_4 = 0.6 mg/L and DO = 5.5 mg/L were adopted as initial reservoir conditions, as indicated in Table 1. On the other hand, the inlet conditions for the different time-evolution patterns were: constant averaged-values (T = 29.0 °C, Chla = 18.1 mg/L, PO_4 = 0.8 mg/L and DO = 0.9 mg/L); step variation (wet period: T = 29.2 °C, Chla = 27.5 mg/L, PO_4 = 0.2 mg/L and DO = 0.9 mg/L; dry period: T = 28.8 °C, Chla = 8.6 mg/L, PO_4 = 1.6 mg/L and DO = 0.8 mg/L); and linear variation throughout the year (T = 29.2-28.8 °C, Chla = 27.5-8.6 mg/L, PO_4 = 0.2-1.6 mg/L and DO = 0.9-0.8 mg/L). The above-mentioned data were obtained from Pacheco & Lima Neto (2017) and Rocha et al. (2022b) and were used for model calibration considering the year of 2013. Note that the total annual heat/mass influx for each parameter (T, Chla, PO_4 and DO) was approximately the same (< 5% difference due to the use of one decimal place in the CE-QUAL-W2 input files) for the three time-evolution patterns of inlet concentrations. Figure 6 shows the measured inlet conditions of T, DO, PO_4 and Chla and their corresponding time-evolution patterns considering the constant averaged-values, step and linear variations.

Figure 7 shows that the best fitting between model results and measurements of DO, Chla and PO_4 were obtained with the assumption of linear variation in inlet concentrations (RD = 28%, PBIAS = -19% and R^2 = 0.32), followed by the assumptions of constant values (RD = 60%, PBIAS = -58% and R^2 = 0.08) and step variation (RD = 76%, PBIAS = -63% and R^2 = 0.20). This is consistent with the results of Fraga et al. (2020), Mesquita & Lima Neto (2022), Rocha & Lima Neto (2021a), and Rocha et al. (2022b), in which the inlet concentrations of total and thermotolerant coliforms and total phosphorus could be described as functions of inflows, which presented an overall trend of decrease from January to December. The optimum values for the fitted coefficients were: K_{ag} = 2.0/day, K_{ar} = 1.2/day, K_{ae} = 0.1/day, K_{am} = 0.1/day, ω_a = 1.0 m/s, and SOD = 1.0 g/m²/day (see Table 2). Note that while the fitted values for K_{ag}, K_{ar}, K_{ae}, K_{am} and ω_a were close to the typical ones recommended by Cole & Wells (2017), the fitted value for SOD is the upper limit of their suggested range, which implies that the assumption that all sinks of DO (except for $K_{ar}\phi_a$) can be included in this factor is reasonable, as SAR is an eutrophic reservoir that receives large input loads of organic matter and nutrients (Araújo & Lima Neto, 2018; Araújo et al.,

Table 1. Summary of initial reservoir conditions of T, Chla, PO_4 and DO.

Parameters	Initial values
Temperature, T (°C)	28.2
Chlorophyll a, Chla (μg/L)	72.0
Phosphate, PO_4 (mg/L)	0.6
Dissolved oxygen, DO (mg/L)	5.5

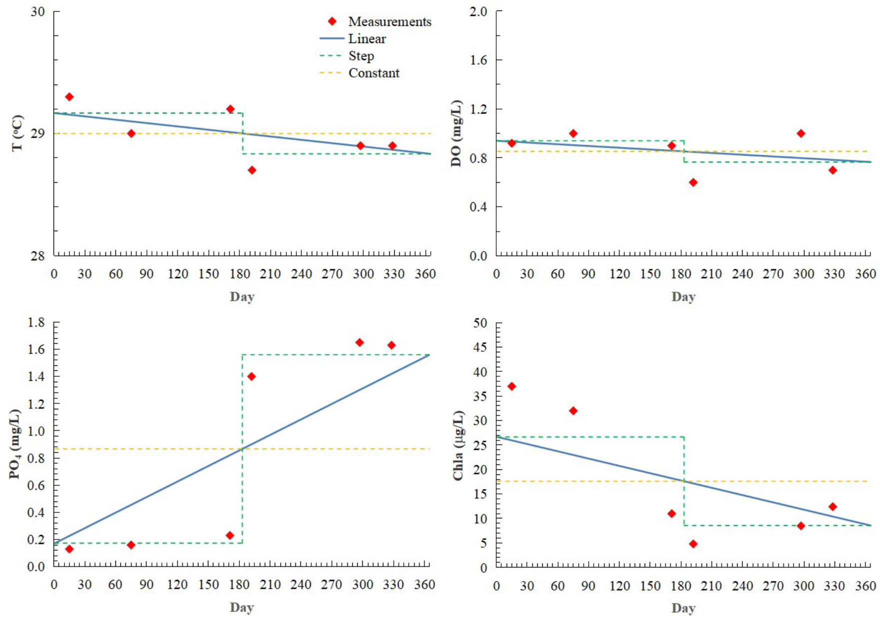

Figure 6. Measured inlet conditions of T, DO, PO_4 and Chla and their corresponding time-evolution patterns considering the constant averaged-values, step and linear variations.

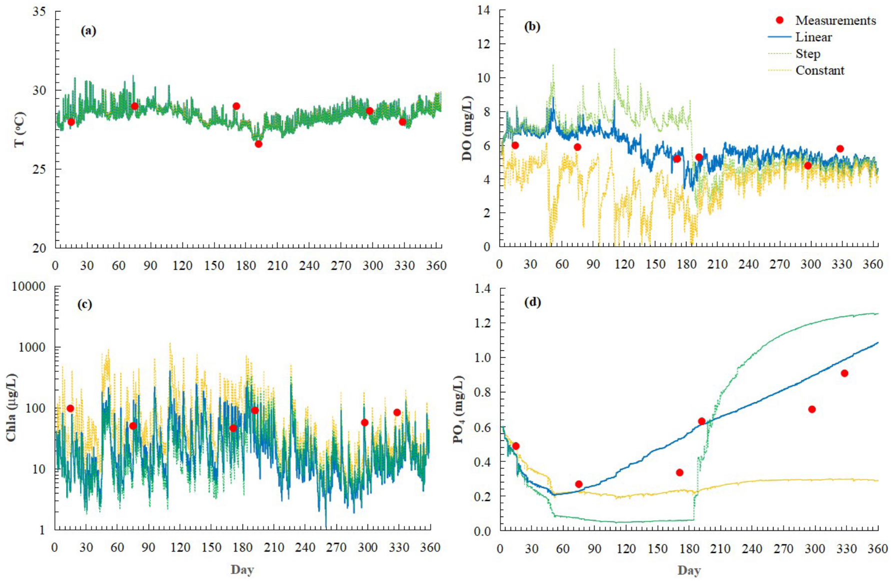

Figure 7. Model calibration using the data of 2013 and comparison among the different time-evolution patterns of inlet concentrations (constant averaged-values, step variation from wet to dry periods, and linear variation throughout the year): (a) temperature, (b) dissolved oxygen, (c) chlorophyll a, and (d) phosphate.

Table 2. Kinetic coefficients, fitted values and their sensitivity analysis (±50%) on the average variation of model outputs for PO_4, Chla and DO.

Kinetic coefficients	Fitted values	Average variation
Algal growth, K_{ag} (1/day)	2.0	25%
Algal respiration, K_{ar} (1/day)	1.2	39%
Algal excretion, K_{ae} (1/day)	0.1	17%
Algal mortality, K_{am} (1/day)	0.1	18%
Algal settling, ω_a (m/day)	1.0	19%
Sediment oxygen demand, SOD [g/(m^2 day)]	1.0	17%
Algal half-saturation for phosphorus limited growth (mg/L)	0.003	15%
Algal light saturation intensity at maximum photosynthetic rate (W/m^2)	100	17%

2019). It is also interesting to mention that the fitted values for K_{ag}, K_{ar}, K_{ae}, K_{am} and ω_a were all higher than the ones adjusted by Deus et al. (2013b) for a large reservoir located in the north region of Brazil, while the value of SOD was lower. Even though the results of the present study cannot be directly compared with those of Deus et al. (2013b), as they also included other water quality parameters such as suspended solids, nitrate and ammonia in their modeling process, the fitted values suggest that algal activity was more intense in SAR, as this urban reservoir had much higher concentrations of PO_4. On the other hand, SOD in SAR was lower possible due to wind-induced sediment resuspension and outflow transport in this shallow reservoir (see Araújo et al., 2019; Mesquita et al., 2020). Figure 7 also shows that while the impact of the different time-evolution patterns of inlet concentrations of Chla, PO_4 and DO on water quality dynamics is relevant, the impact of T variation is negligible as the results for the different approaches are overlapped. This occurred because the temperature variability from the wet to the dry periods was very small (< 2%), which may not necessarily be the case in other reservoirs.

Table 2 also shows the results of a sensitivity analysis (±50%) on the average variation of model outputs for PO_4, Chla and DO. As expected, K_{ag} and K_{ar} are the most sensitive coefficients as they are included in the three equations for the source/sink terms (Equations 2 to 4). Therefore, K_{ag} and K_{ar} can be seen as the main fitting parameters controlling the dynamics of Chla, PO_4 and DO. Observe that the algal half-saturation for phosphorus limited growth and the light saturation intensity at maximum photosynthetic rate were also included in the sensitivity analysis, as these coefficients have also been calibrated in previous studies (see Deus et al., 2013b). However, the results indicate their lower impact on model outputs and that the use of default values from Cole & Wells (2017), as in the present study, is reasonable.

It is interesting to stress that the only parameter the exhibited a clear seasonal behavior was PO_4 (see Figure 7). Additionally, as depicted in Figure 8, PO_4 was the only parameter that presented a near complete mixing pattern, which supports previous applications considering this simplified modeling approach for phosphorus dynamics in SAR and other tropical reservoirs located in the Brazilian Northeast (Rocha & Lima Neto, 2021a, 2021b; Lima Neto et al., 2022; Mesquita & Lima Neto, 2022; Rocha et al., 2022b). On the other hand, all the other parameters (T, Chla and DO) presented an alternating stratification-destratification patter during the day-night but without significant variations throughout the year, as indicated in Figure 9. Similar trends for T, PO_4, Chla and DO were observed by Deus et al. (2013b) in a large reservoir located in the North region of Brazil.

Figure 10 shows the validation of the model using the data of phosphate of 2019 as well as a comparison among the different time-evolution patterns of inlet concentrations (constant averaged-values, step variation from wet to dry periods, and linear variation throughout the year). Because of data scarcity, the initial reservoir and inlet conditions of T, Chla, PO_4 and DO were the same shown in Table 1 and Figure 6. On the other hand, the kinetic coefficients were the same obtained in the calibration process (see Table 2). The results confirm that the best fitting between model results and measurements was obtained assuming a linear variation in inlet concentrations (RD = 29%, PBIAS = -10% and R^2 = 0.41), followed by the assumptions of constant values (RD = 136%, PBIAS = -136% and R^2 = 0.01) and step variation (RD = 205%, PBIAS = -192% and R^2 = 0.52). The quality of this fitting (linear assumption) was similar to that reported by Deus et al. (2013b), Sadeghian et al. (2018) and Terry et al. (2018) considering a more complete set of water quality parameters in the CE-QUAL-W2 modeling, which gives credence to the assumptions adopted in the present study.

Figure 11 shows simulations of Chla with the validated model considering two scenarios: (a) a wet (2009) and a dry (2013) year, and (b) an external load reduction by maintaining throughout the year the inlet concentration of PO_4 at 0.1 mg/L, which corresponds to a 50% reduction in the wet period

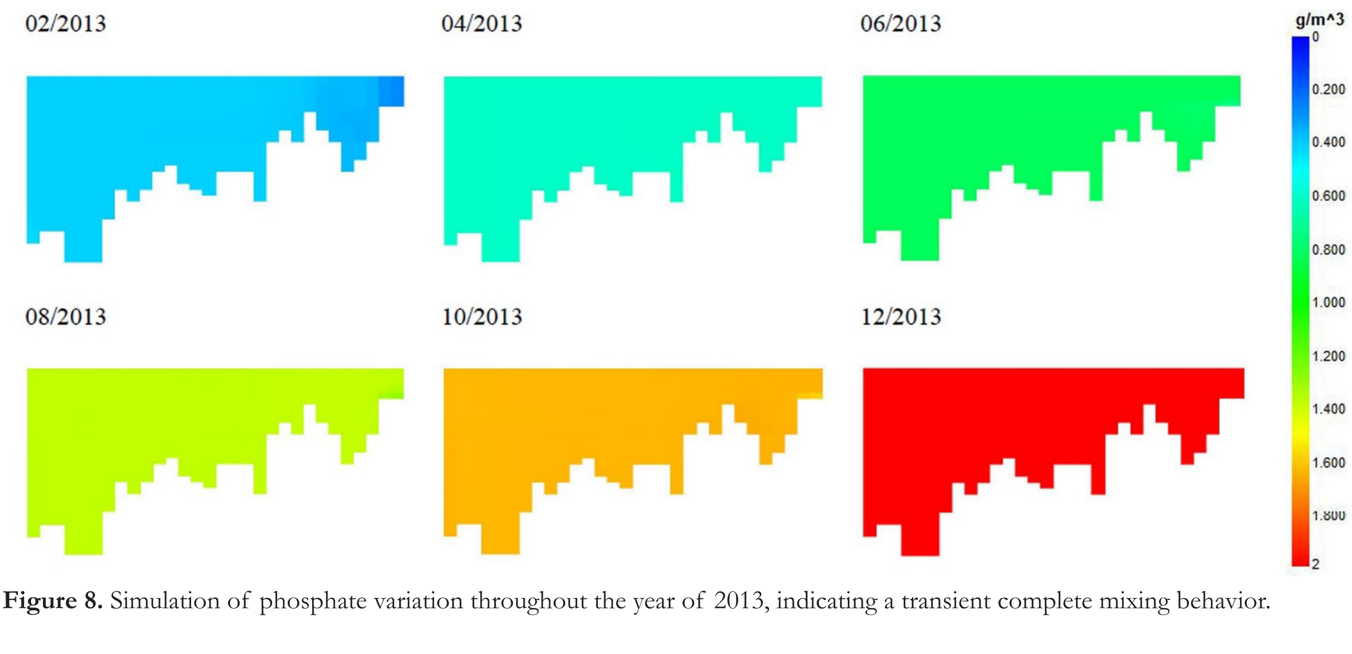

Figure 8. Simulation of phosphate variation throughout the year of 2013, indicating a transient complete mixing behavior.

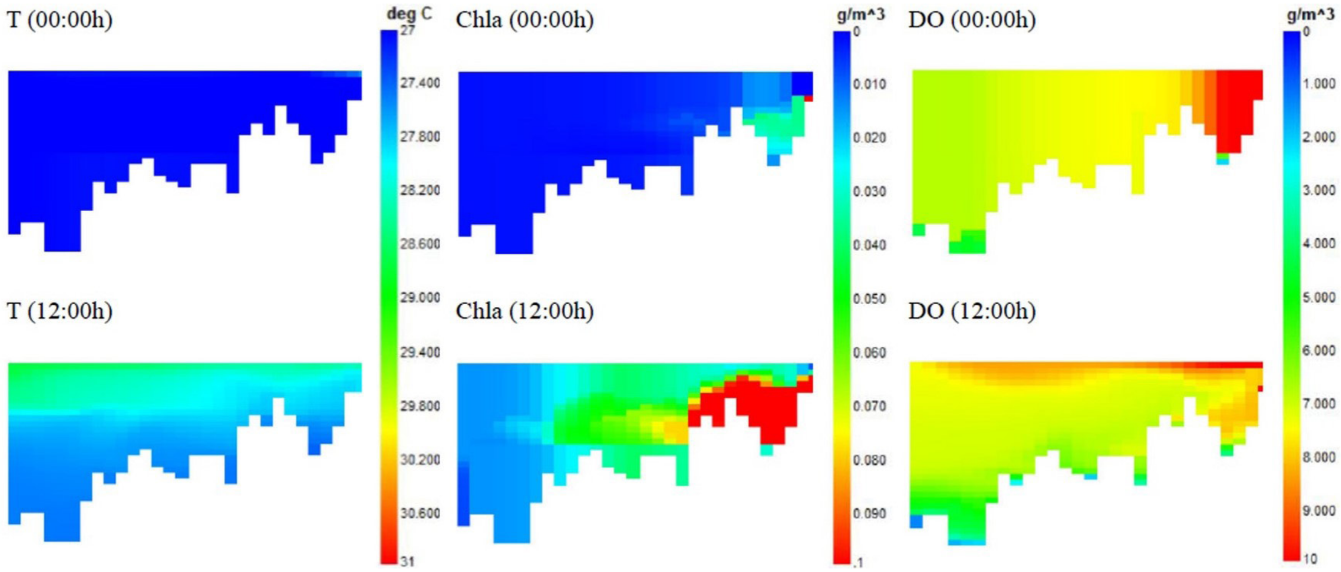

Figure 9. Simulation of the daily variation of temperature, chlorophyll a and dissolved oxygen in June 30, 2013.

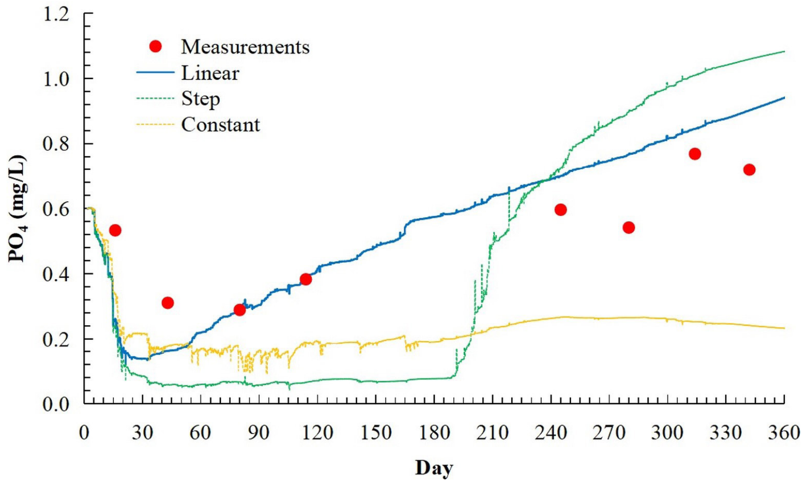

Figure 10. Model validation using the data of phosphate of 2019 and comparison among the different time-evolution patterns of inlet concentrations (constant averaged-values, step variation from wet to dry periods, and linear variation throughout the year).

concentration. The national water quality standards for classes 1, 2, 3 and 4 according to CONAMA 357/05 are also indicated respectively by layers with different colors: blue, yellow, orange and red. Overall, the simulations showed that the optimistic scenarios promoted a clear shift in water quality to class 1 in the second semester. However, during the first semester of the dry year, the compliance with the mandatory water quality standard of Chla (30 mg/L) for class 2 increased in comparison with the same period of the wet year, which can be attributed to the lower input loads due to lower inflows, as the same inlet concentration patterns of 2013 were considered for 2009. Contrastingly, during the second semester, the compliance in the dry year dropped from 78.2 to 73.3%, possibly due to lower volumes stored as compared to the wet year. On the other hand, the external load reduction had a stronger impact on model outputs, as the compliance increased from 73.3 to 94.1%. This suggests that load reduction is still a necessary measure to improve water quality of tropical reservoirs, as pointed out by Rocha & Lima Neto (2021a), Ferreira & Fernandes (2022), Lima Neto et al. (2022). Finally, it is also interesting to evaluate the impact of the above-mentioned mitigation measures on the trophic status of the reservoir. The analysis was based on the methodology of Cunha et al. (2013), in which the trophic state category is given by the geometric mean of Chla. The results shown in Figure 12 confirmed that load reduction had a stronger positive impact on the cumulative frequency of the trophic state than the hydroclimatic variability, as Chla was about 77% (against 59%) of the time under the mesotrophic category. Observe that the percentage dropped to 33% considering the standard condition of 2013 (dry year).

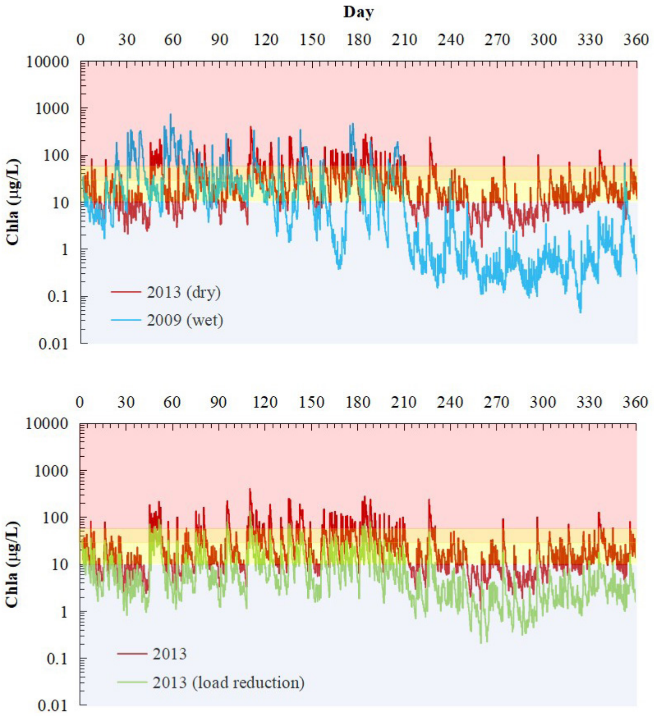

Figure 11. Simulations of Chla with the validated model considering two scenarios: (a) a wet (2009) and a dry (2013) year; and (b) a load reduction by maintaining the inlet concentration of PO_4 at 0.1 mg/L. The national water quality standards for classes 1, 2, 3 and 4 (CONAMA 357/05) are also indicated respectively by layers with different colors: blue, yellow, orange and red.

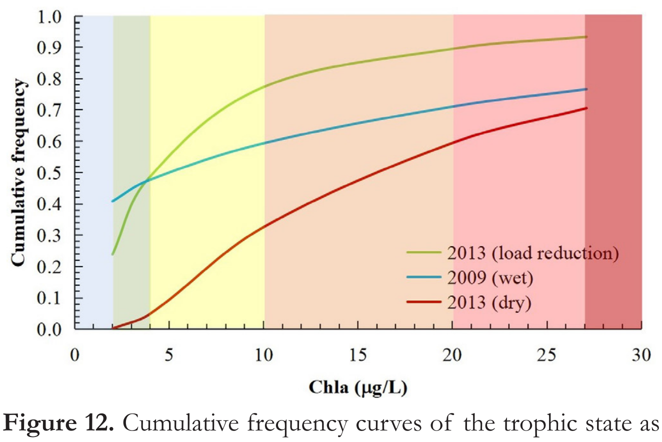

Figure 12. Cumulative frequency curves of the trophic state as a function of Chla for the scenarios of hydroclimatic variability and input load reduction. The different categories according to Cunha et al. (2013) are indicated by layers with different colors: blue (ultraoligotrophic), green (oligotrophic), yellow (mesotrophic), orange (eutrophic), light red (supereutrophic) and dark red (hypereutrophic).

CONCLUSIONS

The present study applied the two-dimensional CE-QUAL-W2 model for simulating water quality dynamics in a tropical reservoir in Brazil, subject to strong hydroclimatic variability and urban pollution. In order to manage data scarcity, model simplifications were justified based on the relevance of each process and several adjustments were performed to reduce the dynamic modeling to four water quality parameters: temperature (T), dissolved oxygen (DO), chlorophyll a (Chla) and phosphate (PO_4). Moreover, different patterns for the time-evolution of reservoir inlet concentrations were tested: constant averaged-values, step variation from the wet to the dry periods, and linear variation throughout the year. The results showed that the simplified model can predict well the seasonal variations of T, DO, Chla and PO_4. The best fitting between model simulations and measured data were found by considering the linear variation in inlet concentrations, followed by the assumptions of constant values and step variation. PO_4 presented a transient complete mixing behavior with a significant increase in concentration from the wet to the dry season, while T, DO and Chla displayed an alternating stratification-destratification patter during the day-night but with small variations along the year. Model predictions of different scenarios also revealed a clear improvement in both the water quality class and the trophic status of the reservoir, especially in the second semester. However, PO_4 load reduction had a more significant impact than hydroclimatic variability. Finally, the present study proposed a relatively simple and efficient tool to improve water quality management in tropical reservoirs by dealing with data scarcity, urban pollution and hydroclimatic seasonality.

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