Modeling the Responses of Dissolved Oxygen and Nitrate Concentrations due to Land Use and Land Cover Change Scenarios in a Large Subtropical Reservoir

Carolina Cerqueira Barbosa[a*], Maria do Carmo Calijuri[a], Phelipe da Silva Anjinho[b], André Cordeiro Alves dos Santos[c]

[a]*Hydraulics and Sanitation Department, University of São Paulo at São Carlos School of Engineering, São Carlos, SP, Brazil*

[b]University of São Paulo, Center of Water Resources and Environmental Studies, São Carlos, SP, Brazil

[c]*Biology Department, University of São Carlos-Sorocaba, Sorocaba, SP, Brazil*

***Corresponding author**

E-mail address: carolina.cbarbosa@usp.br

ABSTRACT

Itupararanga reservoir is a large reservoir built in the Southeast of Brazil to support multiple uses, mainly hydropower generation and drinking water supply for almost 1 million people. We applied a process-based biogeochemical model and a distributed basin load model to assess the responses of dissolved oxygen and nitrate concentrations in the Itupararanga reservoir based on three land use and land cover (LULC) scenarios. The proposed LULC management actions resulted in a set of diverse ecosystem responses of the Itupararanga reservoir and the biogeochemical model highlighted the impact of allochthonous nutrient loads on reservoir water quality conditions, as well as the overall low biogeochemical turnover in the Itupararanga reservoir. The proposed modeling framework is a coupling of open science tools, which can be used to estimate future changes in the water quality of standing freshwater bodies due to likely changes in the land use and land cover in watersheds.

Keywords: land use and land cover changes, GLM-AED2, Lake Ecosystem modeling.

1. INTRODUCTION

The deterioration of freshwater quality worldwide has resulted in various factors, mainly due to water level changes and inflow nutrient loadings (Gilboa et al., 2014). It is important to identify and quantify the drivers and pressures related to water pollution, especially in urban water bodies (Tuerlinckx et al., 2019). The main ongoing challenges facing inland waters (Downing, 2014) are eutrophication (Liu et al., 2021), agriculture impacts (Lopes et al., 2020), super exploration of the water resource (Simonovic and Arunkumar, 2016), water withdrawal (Feldbauer et al., 2020) and climate change (O'Reilly et al., 2015; Woolway et al., 2020).

According to Gregorio and Jansen (1998), land cover is the observed (bio) physical cover on the earth's surface and land use is explained by human activities, arrangements and inputs to produce, change or maintain some types of land cover. The literature has been investigated internal and external factors associated with consequences on water quality (Laura et al., 2021; Lopes et al., 2020). The main driver associated with the alterations in water quality that causes direct consequences on ecosystem services (e.g., water provisioning for drinking and water purification) is catchments' land use change (Grizzetti et al., 2016). A recent study has proved that total phosphorus release and climate change have equal importance as drivers of water quality deterioration in lakes (Shuvo et al., 2021).

Coupled hydrological-biogeochemical models has been used to perform predictions of land use alterations in surrounding watersheds and consequences on water quality (Fenocchi et al., 2020; Messina et al., 2020). In general, basin-scale water quality models require a large amount of data and extensive sets of parameters (Tang et al., 2019). Integrating geography information system (GIS) technologies also have been giving insightful qualitative answers for water resource management studies (Liu et al., 2018; Soares and Calijuri, 2021).

The Itupararanga reservoir is a large multipurpose reservoir built in the Southeast of Brazil in 1914. The reservoir is classified by its uses as "Class 2 freshwaters" (Brasil, 2005; Melo et al., 2019), which means the drinking water supply, after passing through a treatment plant; the protection of aquatic communities, recreational, irrigational, and fishing activities. The reservoir trophic state has changed over the years, currently showing meso-eutrophic characteristics, with high concentrations of nutrients (Cunha et al., 2017; Vargas et al., 2020). The literature has suggested that the main driver for the high trophic state, especially in the riverine zone is the nutrients released from the tributaries (Cunha et al., 2012; Frascareli et al., 2015) and there is a high relationship between nitrogen concentrations and phytoplankton growth, mainly cyanobacteria abundance (Beghelli et al., 2016).

Our hypothesis was that the release of allochthonous inorganic nutrients from the reservoir's tributaries due to land use changes is one of the main drivers of reservoir water quality deterioration. In this study, we aimed to assess the responses of dissolved oxygen and nitrate concentrations of the Itupararanga reservoir applying a biogeochemical model and a simple distributed basin load model. To do this, we evaluated three land use scenarios based on the basin transition potential to the 2050s.

2. METHODS

2.1 Study site

Itupararanga reservoir is a large lake built in 1914 in the Southeast of Brazil in the Alto Sorocaba basin to support multiple uses, mainly hydropower generation and drinking water supply for almost 1 million people. The reservoir surface area is 29.9 km² and a water depth range of 14.5-23 m (Barbosa et al., 2021).

The climate is of the Cwa type, according to the Köppen-Geiger classification, with distinct wet and dry seasons. The original vegetation is the semi-deciduous forest which is predominant in Brazil's Atlantic Forest. In the Alto Sorocaba basin, there is a preservation area called "APA of Itupararanga", which was created by São Paulo State Law nº10.100/1998 and altered by Law nº11.579/2003. The APA of Itupararanga has contributed to maintaining almost 41% of the forest formation in the basin land uses in 2019 according to land use land cover (LULC) data made available by MapBiomas v5.0 (Mapbiomas, 2020). On the other hand, agriculture is in second place with 40% occupation in the basin. Pasture (12%) and urban areas (3%) followed them.

The main human activities that have compromised the reservoir's water quality are the construction of subdivisions, such as farms and summer houses, intensive use of irrigation and pesticides, and the lack of land use zoning that disciplines the form of disorderly occupation (MANFREDINI, 2018). Another source of pollution in the Itupararanga reservoir is sewage discharge due to poor treatment mainly in Ibiúna, a small city located near the reservoir headwater that releases half of the sewage effluents without any treatment (FABH-SMT, 2018) in the tributary streams.

2.2 Database processing

All the processing of the physical variables required by the hydrodynamic model was assumed exactly the same as the previous application of GLM published by Barbosa et al. (2021). Details about the water quality concentration time-series, as well as all the assumptions made, and their processing are given in this section.

Using data from previous studies (Cunha, 2012; Rôdas, 2013; Garcia 2013), it was possible to calculate that the dissolved oxygen (DO) loads in the Sorocaba River upstream of the reservoir were statistically coincident (linear adjustment, r2 =0.85 (n=20)) with the sum of the flows and DO loads of the Sorocabuçu and Sorocamirim rivers measured ~ 3 km from the head of the Sorocaba River. Although upstream Sorocaba River receives effluents from the ETE Ibiúna, this has not sufficiently caused water quality deterioration due to the low flow.

We used flow data along the Sorocabuçu and Sorocamirim streams adopting studies carried out by Rôdas (2013) and Garcia (2013) from July 2011 to April 2012 to support the flow calculation per km in the streams through the equations of two exponential functions (adjustment = r2> 0.91, dry season and r2> 0.88, wet season). After calculating the correlation, we calculate an approximation factor to determine the flow values at the same point of the water quality gauge stations in each stream. We also filled in the gaps in the flow data through linear correlation between the available data and the affluent flow of the reservoir calculated by the water balance (r2 = 0.82).

Daily flows measured in the streams were also made available between December 2013 and December 2017 by two fluviometric monitoring stations operated by the Brazilian National Water Agency (ANA) located in the Sorocabuçu and Sorocamirim streams (62472800, 62473200).

The available water quality time-series was measured by the Environmental Company of the State of São Paulo (CETESB) in the Sorocabuçu, Sorocamirim and Una streams every two months since 2005 (SOBU02800, SOMI02850, BUNA02900). The three monitoring stations are located at the correspond sub-basins outlets where the main loads are released to the reservoir. We used 13 years of water quality data to estimate the long-term monthly geometric mean of concentrations based on a recent approach suggested by Isles (2020).

The location of the sampling sites and the monitoring stations are given in Figure 1: the green squares correspond to the 17 sampling sites measured at bimonthly time-step by Rôdas (2013) and Garcia (2013) and the red triangles refer to the 5 monitoring stations - monthly water quality time series (SOBU02800, SOMI02850, BUNA02900) and daily flows time series (62472800, 62473200).

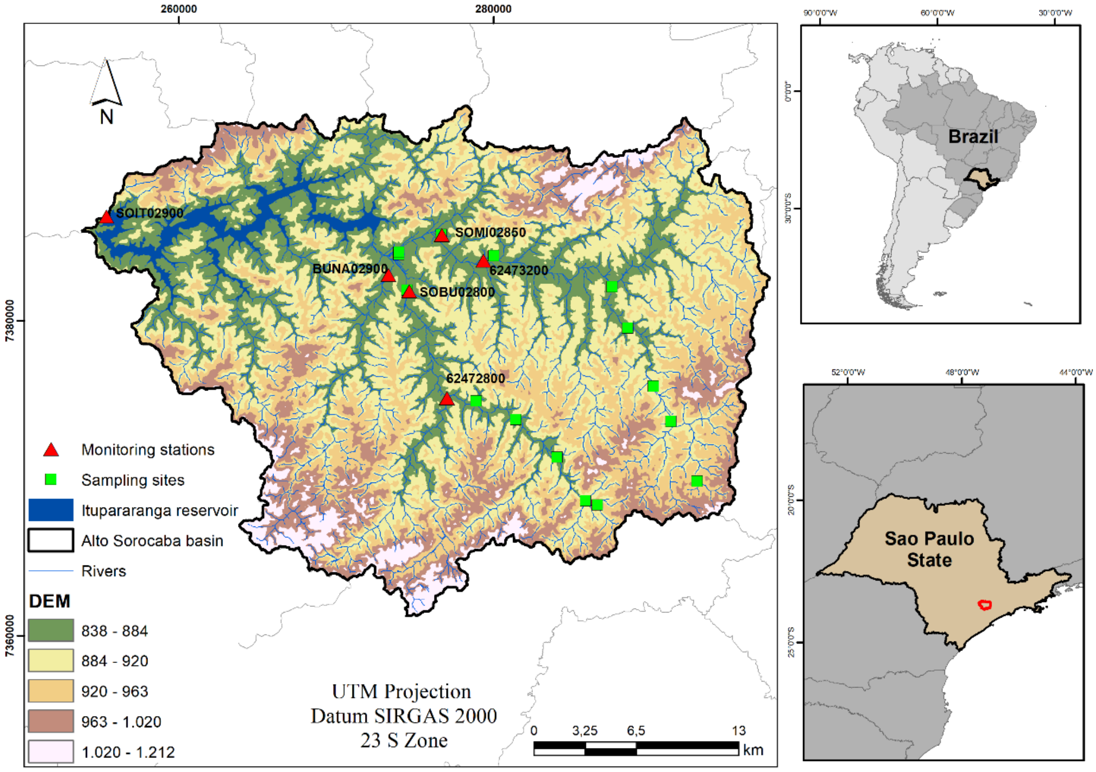

Figure 1: Sampling sites performed by Rôdas (2013) and Garcia (2013), and monitoring stations operated by CETESB and ANA.

We calculated a mass balance to determine the reservoir inflow concentrations (C_{Inflow}) using Eq 1:

$$(Q_{uçu} \text{ x } C_{uçu}) + (Q_{mirim} \text{ x } C_{mirim}) = (Q_{Inflow} \text{ x } C_{Inflow}) \quad (1)$$

Where: $Q_{uçu}$= Sorocabuçu stream flow, $C_{uçu}$= Sorocabuçu stream concentrations, Q_{mirim}= Sorocamirim stream flow, C_{mirim}= Sorocamirim stream concentrations, Q_{Inflow}= Reservoir inflow concentrations

The median values of reservoir inflow concentrations are shown in Table 1. As the water quality time-series by the CETESB did not have available data for particulate organic carbon (POC), organic nitrogen and all phosphorus and nitrogen pools, we had to estimate the required input data from the available biogeochemical time-series. As input for the GLM-AED2, 14 inflow time-series were used as follows: water temperature, pH, and concentrations of DO, DOC, POC, NH4, nitrate (NO3), DON, PON, FRP, ASRP, DOP, POP, and chlorophyll-a (Chla).

Table 1: Median values of inflow nutrient concentrations.

DO (mg.l^{-1})	**NO3 (mg.l^{-1})**	**PO4 (ug. l^{-1})**	**TN (mg. l^{-1})**	**TP (ug. l^{-1})**	**Chla (ug. l^{-1})**
5.66	0.57	21.7	1.16	55.8	4.6

We applied specific ratios to individual phosphorus forms based on Garcia (2013) and Rôdas (2013) measurements of the Sorocamirim and Sorocabuçu streams. The filterable reactive phosphorus (FRP), adsorbed soluble reactive phosphate (ASRP), dissolved organic phosphorus (DOP) and particulate organic phosphorus (POP) were estimated as median proportion of total phosphorus (TP). We also considered: DOP as the difference between the dissolved total phosphorus (DTP) and FRP concentrations and TP= FRP + ASRP + DOP + POP. The input Chla concentrations followed the same mass balance equation using a conversion factor of 50mgC.mgChla^{-1}.

2.3 Biogeochemical modeling

The General Lake Model (GLM) is a one-dimensional hydrodynamic model that calculates vertical profiles of water temperature, salinity, and density by representing upstream and downstream water flows, mixing, heating and surface cooling (Hipsey et al., 2017). The model can be coupled with the Aquatic Ecodynamics Modeling Library (AED2).

The AED2 comprises modules and algorithms that simulate water quality, aquatic biogeochemistry, and phytoplankton and zooplankton dynamics in lakes, reservoirs, and estuaries (Hipsey et al., 2013). The modules allow the simulation of carbon, nitrogen, phosphorus, dissolved oxygen, and silica cycles, as well as organic matter, phytoplankton and zooplankton through mass balance equations and functions related to internal nutrient cycling.

In the scope of the present section, the mass balance equations of dissolved oxygen (DO) and nitrate (NO3) concentration calculations are detailed below:

$$\frac{dO_2}{dt} = \pm f_{atm}^{O2} - f_{sed}^{O2} - \frac{f_{miner}^{DOC}}{X_{C:O2}^{miner}} - \frac{f_{nitrif}}{X_{N:O2}^{nitrif}} + \sum_a^{N_{PHY}} \left(\frac{f_{uptake}^{PHY-Ca}}{X_{C:O2}^{PHY}}\right) - \sum_a^{N_{PHY}} \left(\frac{f_{resp}^{PHY-Ca}}{X_{C:O2}^{PHY}}\right) - \sum_z^{N_{ZOO}} \left(\frac{f_{resp}^{ZOOz}}{X_{C:O2}^{ZOO}}\right) \quad (2)$$

Where: f_{atm}^{O2}=atmospheric O2 exchange, f_{sed}^{O2}=sediment O2 demand, $\frac{f_{miner}^{DOC}}{X_{C:O2}^{miner}}$=O2 consumption by mineralization of DOC (bacterial respiration), $\frac{f_{nitrif}}{X_{N:O2}^{nitrif}}$= O2 consumption by nitrification, $\sum_a^{N_{PHY}} \left(\frac{f_{uptake}^{PHY-Ca}}{X_{C:O2}^{PHY}}\right)$=O2 production by photosynthesis, $\sum_a^{N_{PHY}} \left(\frac{f_{resp}^{PHY-Ca}}{X_{C:O2}^{PHY}}\right)$=O2 consumption by phytoplankton respiration, $\sum_z^{N_{zoo}} \left(\frac{f_{resp}^{ZOOz}}{X_{C:O2}^{ZOO}}\right)$=O2 consumption by zooplankton respiration.

$$f_{sed}^{O2} = f_{max}^{O2} \frac{O_2}{K_{sed}^{O2} + O_2} (\theta_{sed}^{O2})^{T-20} \left(\frac{\widehat{Az}}{dz_z}\right) \quad (3)$$

Where: $\widehat{Az} = \frac{A_z^{ben}}{Az}$ and dz_z $is\ the\ thickness\ of\ the\ z^{th} layer/cell$

$$\frac{dNO_3}{dt} = -f_{sed}^{NO3} + f_{nitrif}^{NH4} - f_{denit}^{NO3} - \sum_a^{N_{PHY}} [p_{NO3}^a\ x\ f_{uptake}^{PHY\_Na}] \quad (4)$$

Where: f_{sed}^{NO3}=sediment flux, f_{nitrif}^{NH4}=nitrification, f_{denit}^{NO3}=denitrification, $\sum_a^{N_{PHY}}$ $[p_{NO3}^a\ x\ f_{uptake}^{PHY\_Na}]$=uptake from the phytoplankton community

2.3.1 Calibration and validation

The model parameters were calibrated following the bottom-up principle: firstly, the water level and water temperature were previously calibrated as described in Barbosa et al. (2021), and then the parameters regarding the concentrations of DO and NO3. Due to the low water quality data availability compared to the water level and water temperature historical time-series, the chosen calibration and validation period were shorter for the present study compared to the previous one. Firstly, we used 3 months (Jan 2009 to March

2009) to spin up the model. Then, we performed 936 days (April 2009 to Dec 2011) for the calibration and 784 days (Jan 2017 to Feb 2019) for the validation.

A global sensitivity analysis based on the Morris Method (Morris, 1991) was performed to identify the most sensitive parameters for the predictions of DO and NO3. After that, an automatic calibration was performed using the derivative-free, optimization algorithm (CMA-ES; Hansen, 2016) with 100 iterations aiming to reduce the root mean square error (RMSE) followed by a manual calibration to ensure that the model was not reproducing unreal biogeochemical parameter combinations. A similar sensitivity analysis and calibration approach was conducted by Ladwig et al. (2020).

The model parameters were manually changed aiming to sequentially optimize goodness-of-fit (GOF) metrics focusing on reproducing DO and NO3 concentrations of the dry and wet periods. As the observed NO3 concentrations in the reservoir did not show a significant temporal fluctuation pattern during the calibration and validation periods, we focused on representing mainly the long-term median concentration. As the purpose of this study was to simulate future scenarios and represent the likely alterations and quantify them based on a historical baseline scenario, we did not focus on capturing nitrate peaks during the calibration process. Furthermore, we chose to simulate nitrate dynamics in the Itupararanga reservoir, despite the few available data for nitrate calibration (n=15) and validation (n=7). We do not consider that a major concern for our purposes, given the same context as above.

We calculated five GOF metrics (RMSE, the Pearson correlation coefficient (r), mean absolute error (MAE), the Nash–Sutcliffe model efficiency coefficient (NSE) and the Kling-Gupta efficiency (KGE)) to compare model outputs regarding the surface and epilimnion concentrations and measured data using the hydroGOF package for R. (Zambrano-Bigiarini, 2017). We chose to simulate the surface and epilimnion layers, since the DO and NO3 concentrations were found in higher proportion in the epilimnion (<6.5m, 72% of the time-series) compared to the hypolimnion (28%). The target of calibration was to maximize the r and reduce the RMSE values for each variable. A similar approach was performed by Fenocchi et al. (2019).

2.4 Basin distributed load modeling

The focus of the basin distributed load simulation was to estimate the annual released load of TN and TP in the Itupararanga reservoir considering the nutrients load generated by different types of land use and land cover. We adopted the methodology developed by Anjinho et al. (2021) based on the export coefficient modelling approach (Johnes, 1996) implemented in GIS to quantify TN and TP loads and concentrations in the tributaries of the Itupararanga reservoir. This method combines nutrient export coefficients and a simple flow model to quantify TN and TP annual mean concentrations.

The digital elevation model (DEM) of the Alto Sorocaba basin was used in QGIS 3.4 software to generate flow direction and surface runoff accumulated per pixel. We adopted 13.5 m^3. s-1 as the long-term mean daily inflow in the reservoir (Barbosa et al., 2021) to simulate the accumulated long-term mean annual flow per pixel for each upstream. We used the regionalization method based on a basin yield that assumes the existence of a proportional linear relationship between drainage area and streamflow to simulate distributed flow in the basin. Thus, we divided the long-term mean daily inflow by the total number of pixels in the basin (m3 s−1 pixel−1) and the flow accumulation algorithm was used to determine the model of mean annual accumulated inflow.

The mean annual TN and TP loads were simulated based on the export coefficients established in the Mathematical Model of Correlation between Land Use and Water Quality (MQUAL), v. 1.5 (SMA, 2010) that were developed for the Guarapiranga Basin located also in São Paulo State and presenting a similar LULC to the Alto Sorocaba Basin (Table 2). We used the LULC GEOTiff data published by the MapBiomas project (MapBiomas, 2020) to determine the specific areas of the basin (km^2) covered by each LULC to calculate the nutrient export coefficient regarding each of them. Load values were converted from $kg.km^{-2}.y^{-1}$ to $kg.pixel^{-1}.y^{-1}$ and then the flow accumulation algorithm was used to generate the accumulated nutrient load model.

Table 2: MQUAL 1.5 export coefficients (SMA, 2010; Anjinho et al., 2021).

LULC	**TP LOAD ($KG\ KM^{-2}Y^{-1}$)**	**TN LOAD ($KG\ KM^{-2}Y^{-1}$)**
AGRICULTURE	126.29	1076.75
FOREST FORMATION	14.24	219
PASTURE	10.22	182.5
RURAL AREA	18.25	328.5
SILVICULTURE (FOREST PLANTATION)	14.24	219
URBAN AREA	12.41	465.01

The average annual nutrient concentration upstream of the Itupararanga reservoir was calculated by combining the results of the calculations above, according to the following equation:

$$C_a = \left(\frac{L_a}{Q_a}\right).10^3 \tag{5}$$

Where: Ca: average annual TN and TP concentration (mgL−1); La: accumulated TN and TP load (kg year−1); Qa: mean annual flow (m3 year−1)

In order to assess the model performance, we performed a double validation approach which consisted of using the long-term historical time-series of flows (Q), TP and TN in the first step (Validation 1) for the three streams' monitoring stations: 12 years for the Sorocamirim stream, 8 years for the Sorocabuçu stream and 13 years for the Una stream; and the second step (Validation 2) was to validate it considering eight monitoring stations in the Sorocamirim and Sorocabuçu streams from 2011 to 2012 (Garcia, 2012; Rôdas, 2012) aiming to evaluate the model performance at the spatial scale. Thus, we used the Pearson (r) and Spearman (r2) correlation and the percent bias (PBIAS) metrics to evaluate the validation analysis.

2.5 Transition potential modeling of the Alto Sorocaba catchment

We used LULC maps for 1999 and 2009 (MapBiomas, 2020) to calculate the transition matrix between 1999 and 2019. We performed a cellular automata simulation using artificial neural networks (ANN) to predict the Alto Sorocaba basin LULC for 2019 using the “Module for land use scenarios” plugin (MOLUSCE) in QGIS 2.18 (Sherman et al., 2016).

The module can use ANN, Multi Criteria Evaluation (MCE), Weights of Evidence (WoE) and Logistic Regression (LR) methods to model LULC transition potential. The ANN method is a learning algorithm which analyzes the accuracy on training and validation sets of samples based on neighbor pixels and three learning parameters. The MOLUSCE module analyzes the transitional potential to predict LULC patterns in the future using the cellular automaton model (Burnham et al., 1973). The model integrates the spatial rules of cellular automaton with the transition of the Markov chain (CA-Markov) to simulate maps based on two images from different dates. The Ca-Markov is a stochastic model that reproduces changes in LULC by transition and information matrix based on the current state. The MOLUSCE methodology framework is shown in detail in Figure 02.

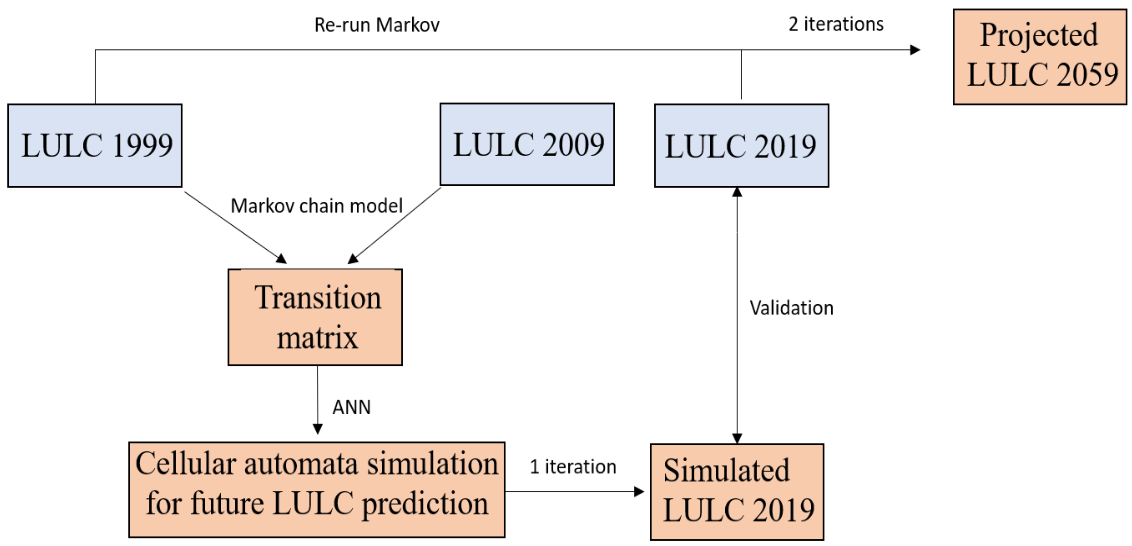

Figure 2: Flow chart for the MOLUSCE methodology. Pink boxes refer to the MOLUSCE outputs.

The model performance was calculated to validate the simulated LULC compared to the observed LULC for 2019 (Mapbiomas, 2020). Thus, the r and r2 coefficients and the Kappa overall coefficient (K) were used to measure the agreement between the observed and predicted LULC. The K statistics represent the total accuracy of the number pixel that was correctly classified between the reference map and the simulated map and the accuracy of the classification (Landis and Koch, 1997, Mienmany, 2018).

When the model was able to generate the acceptable validation result, we re-ran the CA-Markov model considering the step size as 20 years with 2 iterations to perform a LULC projection for 2059.

2.5.1. Land use scenarios for the 2050s

Three land use scenarios were considered to evaluate likely future impacts on the DO and NO3 concentrations in the Itupararanga reservoir.

The potential transition scenario (MOLUSCE) was used as a first scenario for future modification actions in the basin. The other two scenarios were formulated based on the simulated LULC for 2059 considering the increase in preservation areas, focusing on the restoration of permanent preservation areas, and reducing agricultural uses (Green Scenario) and increased economic development of the basin focusing on agriculture, pasture, soy and urbanization (ED scenario) (Table 3).

Table 3: Percentage of changes regarding the MOLUSCE scenario.

Scenario	Percentage of changes	LULC
Green	+30%	Forest formation
	-25%	Agriculture
	-5%	Pasture
ED	-30%	Forest formation
	+15%	Agriculture
	+5%	Pasture
	+5%	Soy
	+5%	Urban area

The inflow mean TP and TN concentrations were accounted for in each scenario and those concentrations were compared to the baseline period (2009-2011 and 2017-2019). Thus, we altered the NO3 inflow and FRP concentrations by the increased or decreased proportions based on the baseline values in the biogeochemical model. This modelling approach aimed to take into account the influence of the LULC changes in the water quality of the Itupararanga reservoir.

3. RESULTS

3.1 Biogeochemical simulations

The input time-series concentrations show that overall, the pH values and DO concentrations represented peaks at the beginning of the dry season (June). On the other hand, peaks of TN concentrations were at the end of the dry season (September). The TOC and TP concentrations followed the expectations with higher values in the wet season due to the watershed runoff increase (Figure S1, Supplementary material).

The biogeochemical sensitive parameters and their respective values calibrated in the present study are compared with the reference values and shown in Table S1. Overall, the biogeochemical modeling showed good fit criteria compared with the observations for simulation of the DO concentrations (Table 4). The DO simulation was able to catch the small changes between wet and dry season, especially in the calibration which has a longer period of simulation compared to validation (Figure 3).

On the other hand, the simulated NO3 concentrations presented reasonable fit criteria. Although the NO3 validation showed RMSE and r values much lower than the calibration (Table 4), the performance metrics are similar with range values from previous studies (0.05 mg. l^{-1}<$RMSE_{NO3}$< 1.2 mg. l^{-1}, Ladwig et al., 2018; Weng et al., 2020) and the model also represented the median values of the observations in both simulation periods (Figure 3).

Table 4: Performance metrics of the DO and NO3 calibration and validation

	Depth	Calibration						Validation					
		n	**RMSE**	**r**	**MAE**	**NSE**	**KGE**	**n**	**RMSE**	**r**	**MAE**	**NSE**	**KGE**
DO	**Surface**	43	1.06	0.73	0.74	-0.1	0.53	15	1.81	0.36	1.24	-7.1	-0.86
	Epilimnion	43	1.09	0.75	0.82	-0.1	0.55	15	2.04	0.43	1.53	-2.2	0.02
NO_3	**Surface**	42	0.04	0.45	0.03	0.4	0.36	7	0.08	-0.03	0.07	-0.0	-0.04
	Epilimnion	42	0.04	0.38	0.03	0.4	0.32	7	0.13	-0.03	0.09	-0.1	-0.14

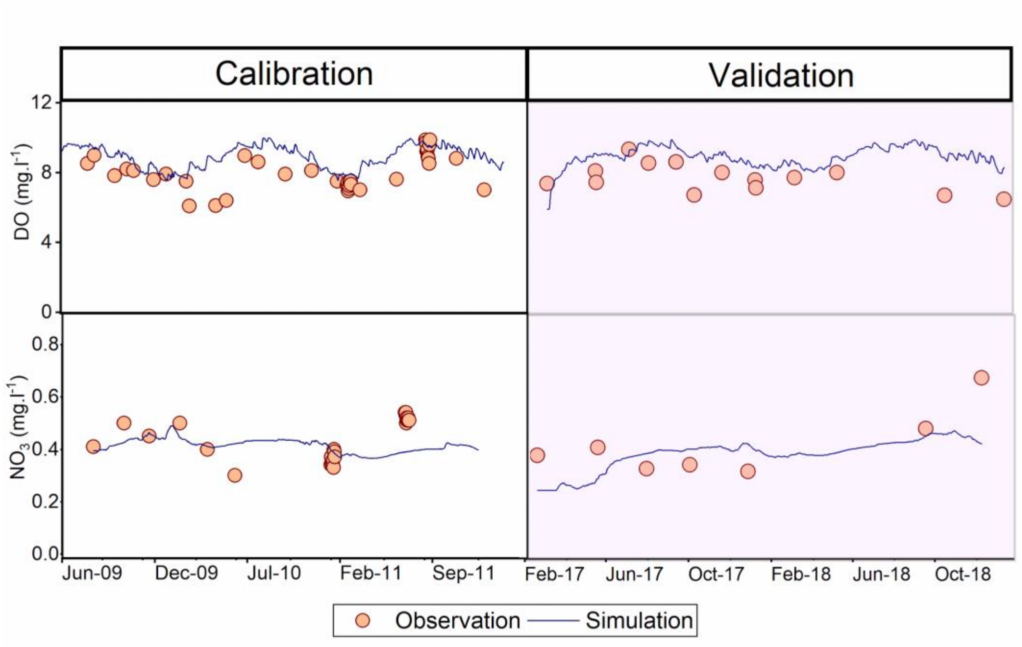

Figure 3: Comparison between observed and simulated DO and NO3 concentrations.

3.2 Distributed load and transition potential modeling of Itupararanga reservoir

The distributed load modeling was able to represent the flows (Q) and concentrations of TP and TN along the Itupararanga headwaters compared with the reference values from Moriasi et al. (2007) highlighted in Table 5.

Validation 1 represented the model performance at temporal scale considering the long-term historical time-series of Q, TP, and TN and validation 2 considered mainly the spatial scale using the time-series from Rôdas (2012) and Garcia (2012). Although the TP simulations in validation 02 showed an unsatisfactory fit compared to the observed data, these measurements only performed between 2011 and 2012 may not be representative of the long-term average pattern of TP concentrations observed and validated in the first stage of the experiment (Validation 01).

Table 5: Results for the distributed load modeling

	r			PBIAS			R2		
	Q	TP	TN	Q	TP	TN	Q	TP	TN
Validation 01	0.99	0.95	-0.40	-7.83	14.66	17.49	1.00	0.89	0.16
Validation 02	0.99	0.11	0.66	-10.37	-70.24	19.87	0.98	0.01	0.44

Very good	Good	Unsatisfactory

The validation results of the transition potential for the Alto Sorocaba basin in 2019 using 1999 and 2009 LULC data according to each land use/land cover are presented in Table 6 in relation to the total area (km²) of the Alto Sorocaba basin.

Table 6: Validation of the transition potential in 2019 (km²).

Class	Observed	Simulated
Forest Formation	380.42	382.39
Forest Plantation	19.17	4.07
Pasture	107.04	121.48
Sugar Cane	0.11	0.10
Mosaic of Agriculture and Pasture	344.67	365.87
Urban Infrastructure	30.81	20.43
Other Non-Vegetated Areas	1.50	1.35
Rocky Outcrop	0.04	0.02
River, Lake and Ocean	24.22	24.43
Perennial Crop	0.01	0.00
Soybean	4.26	0.39
Other Temporary Crops	21.60	12.87

Overall, the model had a satisfactory performance (r=0.99, r2=0.99, K=0.73) to represent the LULC evolution in the basin despite underestimating forest plantation, urban, soybean and other temporary crops areas. The simulation of the transition potential of the Alto Sorocaba basin in 2059 shown in Figure 4 and the built scenarios related to the 2019 baseline are shown in Figure 5.

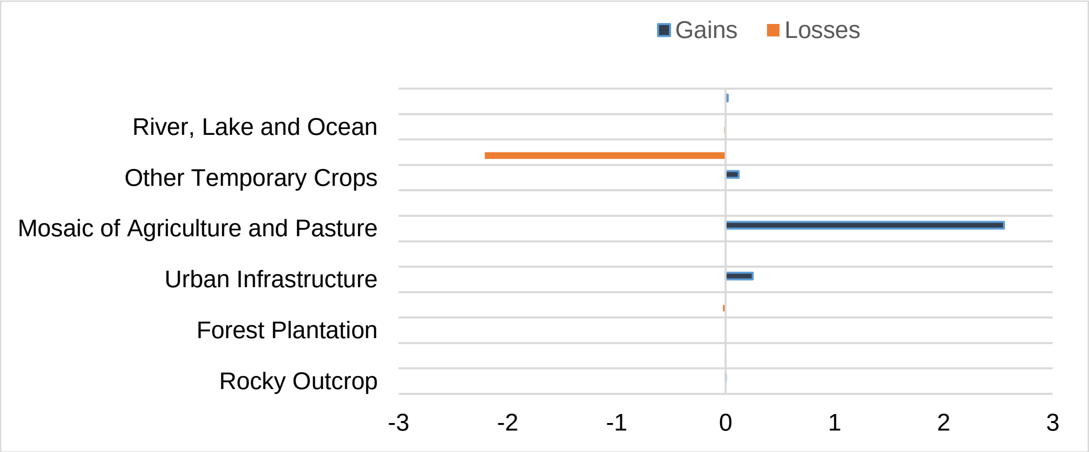

Figure 4: Comparison (%) of gains and losses for the Alto Sorocaba basin between the historical baseline LULC and simulated LULC for 2059.

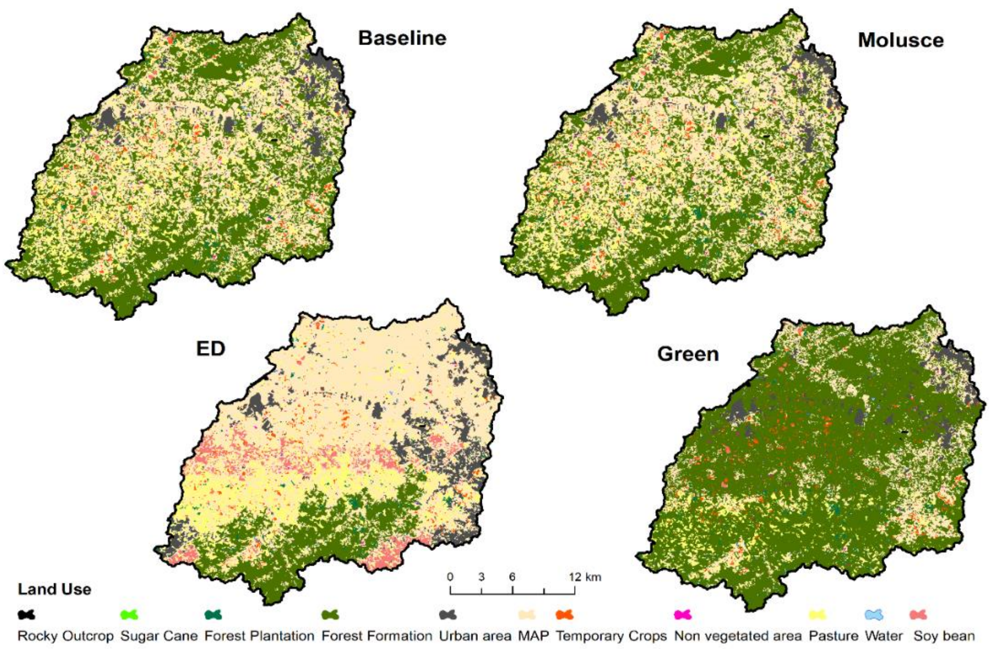

Figure 5: LULC scenarios used in the present study compared to the 2019 baseline.

3.3 Changes in DO and NO3 concentrations under three land use scenarios

The DO concentrations from the three scenarios slightly changed compared to the historical baseline (2009-2011 and 2017-2019), as shown in Table 7 and Figure 6a. As expected, the mean DO concentration decreased in the MOLUSCE and ED scenarios due to an increase in O2 consumption by nitrification. On the other hand, changes in inflow NO3 and PO4 concentrations led to a greater influence on the NO3 simulations in the reservoir, which may be associated with the greater impact of allochthonous loads in the reservoir due to changes in land use (Figure 6b). The simulated Chla concentrations for each scenario were shown to be influenced by such changes of the inflow dissolved nitrogen and phosphorus concentrations (Figure 6c).

Table 7: Mean and standard deviations of the DO and NO3 simulations.

Scenario	DO concentration (mg. l-1)	NO3 concentration (mg. l-1)
Baseline	8.87 (0.38)	0.38 (0.05)
MOLUSCE	8.45 (0.90)	0.44 (0.06)
Green	8.98 (0.38)	0.09 (0.03)
ED	8.45 (0.90)	0.74 (0.09)

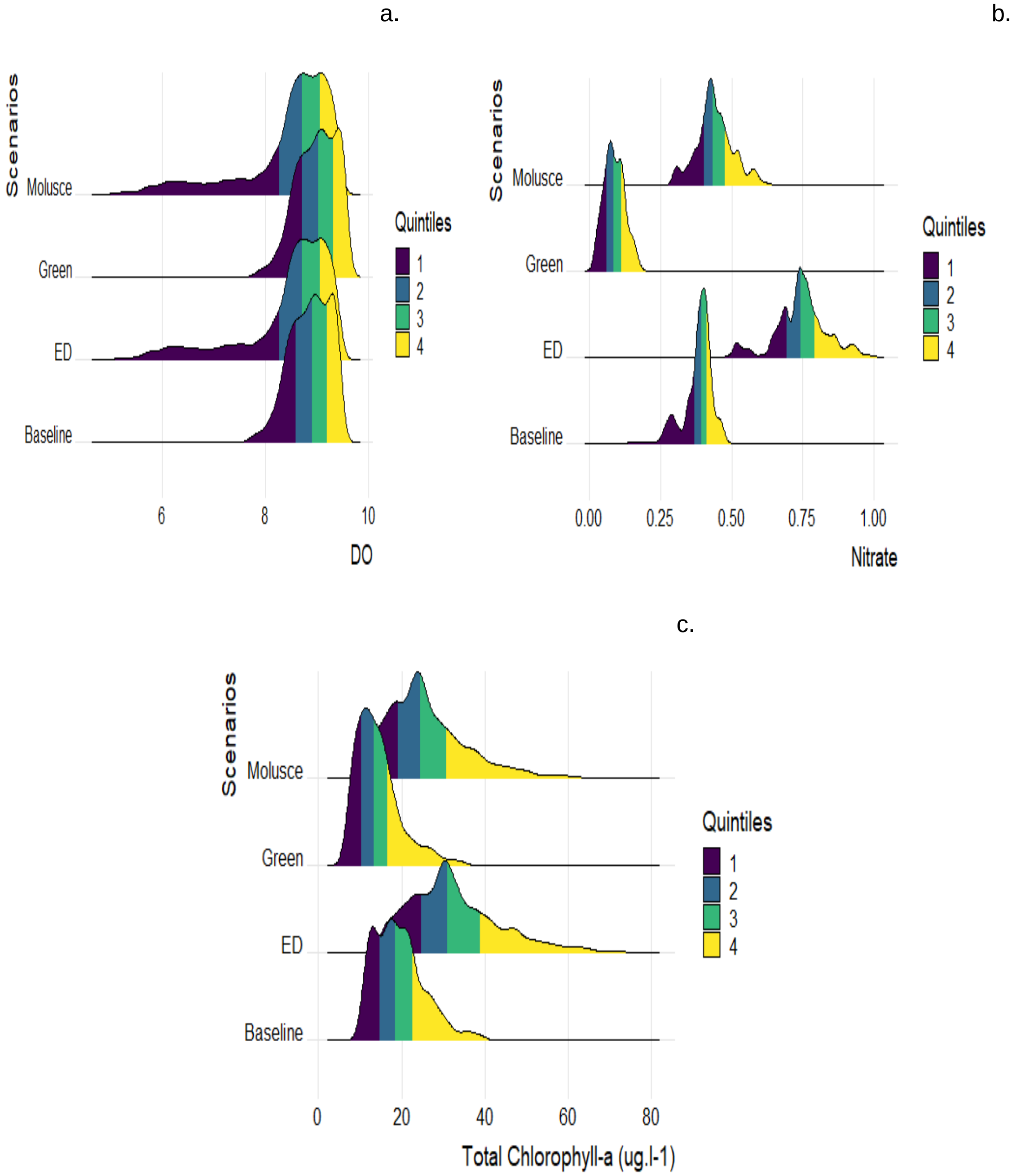

Figure 6: Quintiles based on the kernel density estimation (KDE) for a. DO, b. NO3 and c. Chla concentrations in each simulated scenario.

4. DISCUSSION

4.1. Performance of models

The biogeochemical modeling was able to represent the average DO and NO3 concentrations on the Itupararanga reservoir. Model performance metrics for 936 days of calibration and 784 days of validation showed similar results along the surface and epilimnion depths with values in the range of previous studies

($0.96 mg.l^{-1} < RMSE_{DO} < 3.6$ $mg.l^{-1}$, Burger et al., 2008; Farrell et al., 2020; 0.05 $mg.l^{-1} < RMSE_{NO3} < 1.2$ $mg.l^{-1}$, Ladwig et al., 2018; Weng et al., 2020).

The GLM-AED2 was also able to represent and capture seasonal variations in the dissolved oxygen simulations. The temporal fluctuation of nutrient concentrations and phytoplankton biomass in tropical and subtropical lakes is mainly driven by hydrological patterns, especially at the beginning of the wet season when more nutrients loads are released to the water bodies. Biotic and abiotic alterations in those ecosystems are stronger than in temperate regions (Lewis, 1978). On the other hand, since the observed NO3 concentrations did not show any clear seasonal pattern, the focus in the calibration was to represent the median values for the calibration and validation periods. A similar approach was taken by Ward et al. (2020).

The distributed modeling validations of TN and TP concentrations along the Alto Sorocaba Basin based on the nutrient loads exported from the catchment (Johnes, 1996) can highlight the potentialities of this GIS approach to assess the LULC impacts on the streams and the Itupararanga reservoir. The simulated TP and TN concentrations in the watercourses showed good fit criteria compared with the reference values from Moriasi et al. (2007). Another recent study applied a catchment-scale nutrient model with a similar modeling fit compared to the results shown in Table 5 (Messina et al., 2020).

Despite the good results generated by this modeling approach in the present and previous studies (Anjinho et al., 2021; Lima et al., 2016), it represents the dynamics of nutrients in rural basins more effectively than in urban ones due to a poor performance in the simulation of nutrient concentrations from point source pollution. Since the Alto Sorocaba Basin has less than 10% of the urban area in the total catchment area, we did not consider point sources as sewage treatment plants in the basin for our simulations. Another limitation of this approach is considering only the conservative nutrient transport that does not take into account the temporal and spatial transformations of TN and TP concentrations in watercourses (Lima et al., 2016).

4.2. LULC changes in the last two decades and projections for 2050s

We have analyzed LULC changes in the Alto Sorocaba basin comparing the last two decades (1999 and 2019) based on data from the MapBiomas project (2020). It can be observed that the pasture areas reduced 50% of their area in that period, but the agricultural areas increased significantly focusing on sugarcane, which grew three times, and soybeans, which grew five times its area, in addition to forest plantation areas (which grew four times their previous percentage of area). The observed LULC changes were similar to the spatial pattern already highlighted for Brazil in the past decades (Miccolis et al., 2014).

The APA Itupararanga has favored environmental conservation in the Alto Sorocaba basin to remain at ~ 41% of the basin's total area in native forest areas and its percentage of area has not changed in recent years, as shown by the comparison of spatial analysis. The potential LULC conditions in 2059 were projected based on catchment changes over 20 years, highlighting the increase in agricultural areas and the decrease in pasture areas in line with the changing trends of LULC observed in previous decades. This open source GIS technique has been widely used to assess and predict LULC changes from small (Satya et al., 2020) to large areas (Fernandes et al., 2020).

Taniwaki et al. (2013) suggested that exposed bare soil, agriculture without the protection of riparian zones and urbanization were the most significant drivers of water quality degradation and reflected major damage to the Itupararanga reservoir in 2010. The low availability of NO3 concentrations and the phosphorus limitation in the Itupararanga reservoir has proven to have significant effects on cyanobacteria biomass, especially *R. raciborskii*, and toxin levels measured in the reservoir surface waters (Machado et al., 2021, under review). Recently, Melo et al. (2019) observed that urban areas are mostly responsible for the deterioration of the water quality that supplies the Itupararanga reservoir, however, the authors identified that agricultural areas are the main contributors to the input of TN and TP near the dam.

4.3 Novel open science framework based on coupled models

This novel modeling framework presented was aimed at coupling watershed hydrological and biogeochemical process-based modeling to assess impacts of the catchment LULC changes on the downstream reservoir. This approach is suitable for poorly monitored basins which have a few available water quality data and can be used to analyze overall responses of water quality to changes in external nutrient loads, given a historical baseline. Most basin-scale water quality models require many datasets and parameters to perform reliable simulations (Tang et al., 2019).

The results of coupling hydrological models and aquatic ecosystems, such as hydrodynamic models (Munar et al., 2018, 2019) have highlighted their potential as management tools to understand and predict actions that cause future impacts on aquatic ecosystems. Remote sensing techniques applied to limnology studies have also been expanded to simulate watershed features and likely LULC changes over the years (Curtarelli et al., 2015; Lins et al., 2018; Ma et al., 2016).

We assess water quality changes focusing on reservoir DO and NO_3 concentrations in response to the proposed scenarios based on land use forecasts for 2059. The first scenario was simulated based on the potential LULC conditions for the Alto Sorocaba basin in 2059 and the second and third ones took into account an increase in green areas and an increase in economic development of the Alto Sorocaba basin. The results of the basin transition potential simulation show that even though the K coefficient value (K=0.73) corresponds to a moderate agreement between the reference map and the simulated map (Mienmay, 2018), the r and r^2 values (>0.9) have shown satisfactory performance.

The simulated scenarios were able to indicate future biogeochemical changes in the Itupararanga reservoir and also the water quality deterioration in an environmental degradation scenario (ED). A 31% increase in NO_3 and FRP concentrations in the inflow in the ED scenario compared to the MOLUSCE scenario has led to an increase in O_2 consumption by nitrification and a decrease in the DO concentrations. On the other hand, in the green scenario, a 64% decrease in input NO_3 and FRP concentrations compared to the MOLUSCE scenario can have led to a decrease in O2 consumption by nitrification and an increase in DO concentrations. Likewise, a 4% increase in the same concentrations in the MOLUSCE scenario performed similarly.

Despite the fact that the simulated DO and NO3 concentrations in the Itupararanga reservoir were in agreement with the Brazilian environmental law (BRASIL, 2005), based on the kernel density estimation (KDE) (Figure 6c), the average chlorophyll-a concentrations would be above the limit (<30ug.l) in the ED scenario which may indicate alterations in the trophic dynamics of the reservoir. Higher Chla concentrations were expected in such a scenario compared to the others, mainly because phosphorus is the final limiting nutrient for primary production in (sub)tropical freshwaters (Quinlan et al., 2020). However, the high potential for NH4 and NO3 uptake by cyanobacteria throughout different periods of the year has been reported in the Itupararanga reservoir (Cunha et al., 2017), mainly driven by the N availability and high water temperatures. It is also important to consider warming air temperatures and other climate change projections to assess the likely consequences for reservoir water quality, as suggested by Barbosa et al., (2021).

5. CONCLUSION

The present study aimed to simulate future LULC scenarios in the Itupararanga reservoir based on likely conditions of LULC in 2059 and two hypothetical conditions considering an increase in preserved areas (green) and another accounting for the increase in economic development activities focusing on agricultural and urbanized areas.

Thus, we calibrated and validated a biogeochemical model focusing on dissolved oxygen and nitrate concentrations to simulate their responses from the LULC scenarios. Even if DO and NO3 concentrations did not increase above the limits allowed by Brazilian legislation for all scenarios, Chla concentrations would increase significantly, which could pose a serious threat to the use of the Itupararanga reservoir as a source of water supply. The coupling modeling was also able to represent the importance of forest formation lands in the reservoir water quality improvement (green scenario). We did not assess the management characteristics in relation to exposed soil and agriculture without riparian protection in detail in the present study, however, we suggest that these characteristics should be considered in future studies on LULC scenarios in the Itupararanga reservoir.

The modeling framework proposed based on the coupling watershed load and biogeochemical lake model was able to represent the responses of water quality changes in the reservoir due to the LULC changes. This novel modeling framework can be a valuable tool to guide water resources management considering future pressure on freshwater due to population growth and intensive agricultural practices for human consumption.

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SOFTWARE AVAILABILITY

Instructions to download and install the GLM-AED2 model and the QGIS MOLUSCE Plugin can be found at:

- GLM-AED2: https://aed.see.uwa.edu.au/research/models/aed/download.html

-QGIS MOLUSCE Plugin: https://qgis.org/en/site/forusers/download.html and https://plugins.qgis.org/plugins/molusce/ (Last access: 2021-08-18)

The basin distributed load approach is a GIS implementation of commonly used simple nutrient loading equations and can be run in any GIS software. Detailed instructions are provided in Anjinho et al., 2021.

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