Ecological Modelling 476 (2023) 110227

Contents lists available at ScienceDirect

Ecological Modelling

journal homepage: www.elsevier.com/locate/ecolmodel

An integrated modeling approach to predict trophic state changes in a large Brazilian reservoir

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ARTICLE INFO

Keywords:
Climate change
Land Use and Land Cover changes
GLM-AED2
Water quality

ABSTRACT

Process-based ecological models have been used to study freshwater ecosystems and water quality on a broad scale. However, it is also of pivotal importance to incorporate watershed dynamics and nutrient releases in the downstream freshwaters. Integrated modeling approaches have been used to understand the combined effect of climate warming and land use and land cover (LULC) changes in lake ecosystems. Moreover, most basin-scale water quality models require many datasets and parameters to perform reliable simulations which contributes to reduce studies in poorly monitored basins, most of them located in the Global South. In this study, we developed a coupled hydrological-biogeochemical-ecological modeling framework forced by two regionalized climate models and three LULC change scenarios to forecast trophic state changes in a subtropical multipurpose reservoir for the decade 2050-2060. The projections indicated an average air temperature increase between 2°C and 3°C and a downward trend of the average rainfall and longwave radiation for the 2050s in comparison to the last decade. We found a pattern of 28% increase in total phosphorus (TP) and total chlorophyll-a (TChla) concentrations in the reservoir compared with the historical baseline. The climate warming projections along the 2059 projected LULC and basin's increased economic development scenarios have predicted trophic state index (TSI) shifts between mesotrophic and eutrophic conditions (53.3<TSI<57.7). On the other hand, one of the climate projections along the reduced deforestation scenario indicated a trend towards oligotrophication between 2054 and 2056, however higher phosphorus availability ($60 \mu g.l^{-1} < TP < 100 \mu g.l^{-1}$) and phytoplankton biomass ($50 \mu g.l^{-1} < TChla < 97 \mu g.l^{-1}$) would be expected for the entire decade compared to recent years. The proposed coupled modeling framework demonstrated the potential of open-source tools in water quality management studies, especially for poorly monitored basins, based on climate change trends and human pressure.

1. Introduction

The deterioration of water quality in freshwater ecosystems worldwide has been driven by several 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 (Teurlincx et al., 2019) taken in account the main ongoing problems (Downing, 2014), e.g., eutrophication (Liu et al., 2021), agriculture impacts (Lopes et al., 2020), overexploitation (Simonovic and Arunkumar, 2016), water withdrawal (Feldbauer et al., 2020) and climate change (O'Reilly et al., 2015; Woolway et al., 2020).

Climate change impacts on lakes and reservoirs have been extensively studied in the last years (Ladwig et al., 2018; Magee and Wu, 2017; Jeppesen et al., 2017; Sahoo et al., 2016). The increase in water temperatures, modification of stratification patterns and thermal regime are some of the consequences already observed (Paerl and Huisman, 2008, Moe et al., 2016). Changes in rainfall and climate patterns have been generating immediate responses in the biogeochemical and ecological dynamics of watersheds and lakes (Adrian et al., 2009). Disruption of biogeochemical cycles may impact the loading of dissolved organic matter and nutrients in the lake and affect the magnitude, variability and balance of in-lake metabolic processes (Brighenti et al.,

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https://doi.org/10.1016/j.ecolmodel.2022.110227
Received 21 June 2022; Received in revised form 17 October 2022; Accepted 16 November 2022
Available online 30 November 2022

2018) and increase eutrophication (Sinha et al., 2017). Thus, it has also driven the development, proliferation and maintenance of cyanobacteria blooms (Wells et al., 2015). Land use and land cover (LULC) changes have also driven eutrophication and have been investigated in order to improve water quality. On the other hand, even with the expected intensification of urbanization rate for the next decades, restoration efforts have shown to have effectiveness in the water quality control of some catchments (Fu et al., 2021).

The inference whether climate change or LULC changes are the most important drivers in water quality deterioration is not so straightforward. In this regard, integrated modeling approaches are important to advance our comprehension of how aquatic biogeochemical dynamics respond to meteorological conditions (Curtareli et al, 2015), human pressures (Munar et al 2018, 2019, Liu et al., 2015) and changing climate (Zhang 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). However, less than 5% of the modeling studies have tested coupled models to represent climate-catchment-lakes processes and only 6% have been conducted in Central/South America (Soares and Calijuri, 2021).

In the present study, we aimed to develop a coupled modeling framework based on open-source deterministic models and GIS tools to predict trophic state changes in a subtropical reservoir for the 2050s. We investigated how downscaled climate projections based on two regional climate models (RCM) along with three LULC change scenarios can facilitates our understanding of the combined effect of climate warming and landscape dynamics on the productivity of an aquatic ecosystem. Following this, we draw conclusions on the performance and potentialities of the models and also the implications of trends in water level and water quality for reservoir operation to prevent eutrophication and not impair the drinking water supply. The proposed integrated modeling approach facilitates our current comprehension of water quality management to incorporate climate change mitigation strategies to prevent the water crisis and control water quality and catchment zoning to protect threatened landscapes.

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 km^2 and a water depth range of 14.5-23 m (Barbosa et al., 2021).

The climate is of the Cwa type, characterized by winter precipitation of less than one-tenth of the amount in mid-summer and air temperatures above 22°C during the summer, according to the Köppen-Geiger classification. The wind fetch is 3.1 km. 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 n°10.100/1998 and altered by Law n°11.579/2003. The APA of Itupararanga has contributed to maintaining almost 41% of the forest formation in the basin land uses in 2019 according to 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. Driver historical dataset and data processing

The input data and the dataset required by calibration and validation of the coupled models were collected from several different sources, including government agencies, the private company that operates the dam and previous studies (Table S1). A first study simulated the thermal dynamics and water level changes in Itupararanga reservoir based on meteorological forcings, inflow and outflow and water temperature time-series (Barbosa et al., 2021). Those initial and boundary conditions were assumed to be exactly the same, however the water quality time-series of the tributaries and the reservoir were incorporated in the present study. Details on the water quality data processing and all the assumptions made are given below.

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 location of the sampling sites and the monitoring stations are given in Fig. 1. 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).

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

$$\left(Q_{u\c{c}u} \text{ x } C_{u\c{c}u}\right) + \left(Q_{mirim} \text{ x } C_{mirim}\right) = \left(Q_{Inflow} \text{ x } C_{Inflow}\right) \tag{1}$$

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

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 estimated the required input data from the available biogeochemical time-series. We applied specific ratios to individual phosphorus forms based on Garcia (2013) and Rôdas (2013) measurements of the Sorocamirim and Sorocabuçu streams. Organic nitrogen was calculated as the difference between the Total Kjeldahl nitrogen (TKN) and ammonium (NH4) concentrations. We considered that the organic nitrogen concentrations would be higher in the particulate organic nitrogen (70%) than in the dissolved organic

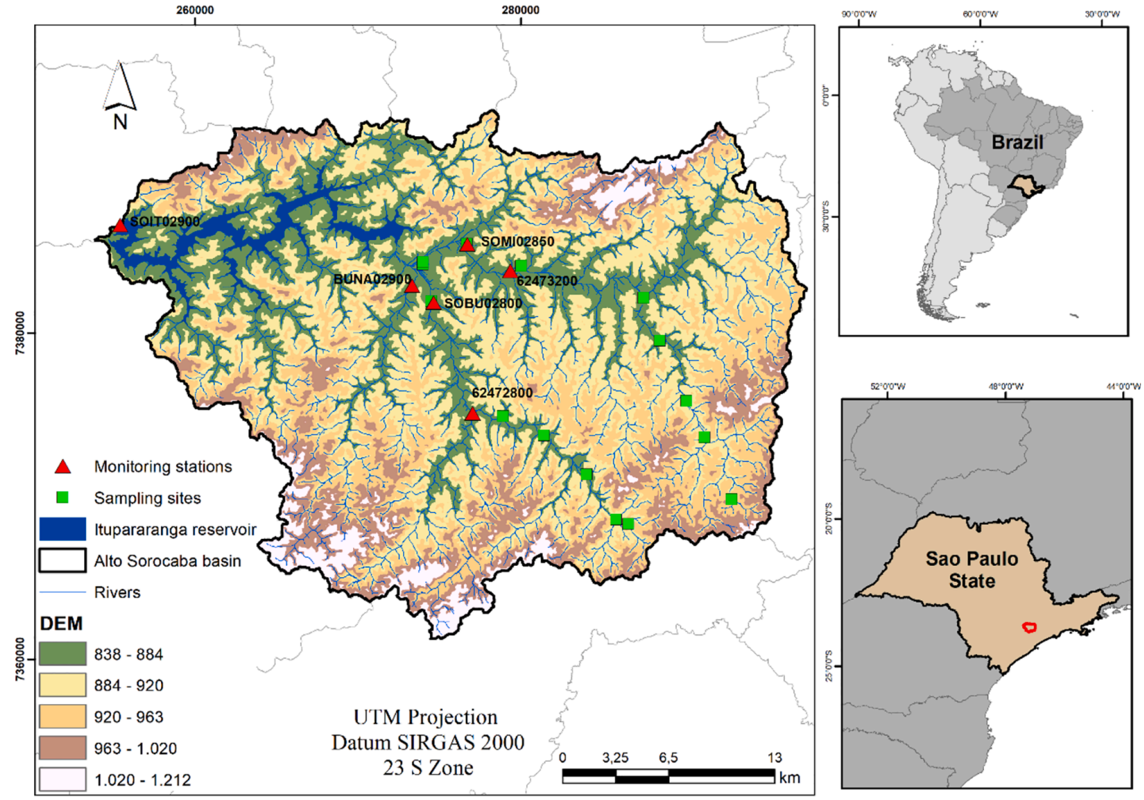

Fig. 1. Sampling sites performed by Rôdas (2013) and Garcia (2013), and monitoring stations operated by CETESB and ANA. Green squares correspond to the 17 sampling sites measured at bimonthly time-step by Rôdas (2013) and Garcia (2013) and red triangles refer to the 5 monitoring stations - monthly water quality time series (SOBU02800, SOMI02850, BUNA02900) and daily flows time series (62472800, 62473200).

nitrogen (30%), based on the stream's features. The filterable reactive phosphorus (FRP), adsorbed soluble reactive phosphate (ASRP), dissolved organic phosphorus (DOP) and particulate organic phosphorus (POP) were estimated as proportions of total phosphorus (TP). We also considered: DOP as the difference between the dissolved total phosphorus (DTP) and FRP concentrations. The input total chlorophyll-a (TChla) concentrations followed the same mass balance equation using a conversion factor of 50mgC.mgChla^{-1}. The median values of reservoir input concentrations are in Error.

2.3. Climate projections

We have chosen two global climate models (GCMs) regionalized for South America by the ETA Model (Chou et al., 2014) to compare the future climate projections and their impacts on the water quality of the Itupararanga reservoir.

The first GCM used in the present study was the Model for Interdisciplinary Research on Climate, version 5 (MIROC5). The MIROC5 is a Japanese coupled ocean-atmosphere model of resolution of about 150 km in horizontal and 40 levels in vertical. The other GCM chosen was the Hadley Centre Global Environmental Model (HadGEM2-ES), a British GCM with 60 levels of vertical resolution. Both RCMs have 20 km of resolution and cover South America, Central America and Caribbean. The Eta-HadGEM2-ES and the Eta-MIROC5 have similar model components (e.g., atmosphere, aerosol, land surface, Flato et al., 2013), however the first one has already proved to be more sensitive to greenhouse gas (GHG) emissions than the ETA nested in MIROC5 (Chou et al., 2014).

The radiative forcing scenarios (RCP) chosen was 8.5 W.m-^{2} (RCP 8.5). Our choice was based on RCP 8.5 to be the best match out to mid-century greenhouse gases emissions and stated environmental policies as reported by Schwalm et al. (2020).

The time-series of climate projections were bias-corrected to adjust historical data and correct the future projections using 1-decade data as control period (2009–2018). Details of the bias correction procedure are given in Barbosa et al. (2021).

2.4. Hydrological modeling

The Soil Moisture Accounting Procedure (SMAP) was used to simulate the future inflow in the Itupararanga reservoir. The SMAP model is based on a simple structure of reservoirs to represent the basin storage and water flow and uses the Soil Conservation Service (SCS, 1964) method to predict runoff (Lopes and Braga, 1982). The model input data are the total precipitation and evaporation heights on a daily time step, the drainage area, and the initial conditions of the basin.

We used 1000 days (June 23, 2010- June 23, 2013) for the calibration and 700 days (June 29, 2016- Sept 07, 2018) for the validation of the model. The statistics metrics used to assess the model performance were the percent bias (PBIAS) (Gupta et al., 1999) which measures the average tendency of the simulated data to be larger or smaller than their observation, and the Pearson correlation coefficient (r). We stopped the calibration efforts when the model was able to achieve a range of PBIAS considered satisfactory ($\pm 15 < \text{PBIAS} < \pm 25$) according to Moriasi et al. (2007), and we were able to identify good agreement between simulated and observed discharge by visual inspection.

After the calibration and validation of the SMAP model, we have estimated future daily discharges from January 2050 to December 2059 using the Eta-HadGEM2-ES and Eta-MIRO-C5 projections for air temperature and evaporation. Model outputs were used as input to the distributed load basin model and the lake ecosystem model.

2.5. Water temperature prediction using Air2stream

The Air2stream is a model to predict stream water temperature as a function of daily air temperature and flow discharge time-series (Toffolon and Piccolroaz, 2015). The model is based on a lumped heat budget that considers an unknown volume of the river reach, its tributaries considering both surface and subsurface water fluxes, and the heat exchange with the atmosphere (Toffolon and Piccolroaz, 2015).

The model calibration consists of identifying the set of parameters that solve an optimization problem to reduce the error between simulated and observed water temperatures. The calculation is a Monte Carlo based optimization procedure. The Particle Swarm Optimization (PSO) was our chosen optimization algorithm, which is implemented in the code with 500 iterations using the Crank Nicolson method to solve the model equation.

After manually testing each version of the model and quantifying the minimum value for the objective function based on RMSE metric, we have chosen the 5-parameter version as the best option for our calibration. We have calibrated the air2stream model using the daily air temperature, the reservoir daily inflow and the water temperature time-series from 2009 to 2013 and we have validated from 2014 to 2019. The mean absolute error (MAE) and r were calculated to assess the model performance to fit observation and simulation.

We have implemented the open-source code in R environment to run the model and visualize outputs. Thus, using the calibrated and validated model, we made predictions of future water temperatures upstream of the Itupararanga reservoir using air temperature projections from Eta-HadGEM2-ES and Eta-MIROC5 climate models and also future flow discharges using the calibrated and validated SMAP model.

2.6. Prediction of TN and TP upstream loads

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 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.

The digital elevation model 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 ($m^3 s^{-1} pixel^{-1}$) 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 S3). 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.

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:

$$C_a = \left(\frac{L_a}{Q_a}\right).\ 10^3 \quad (2)$$

Where: Ca: average annual TN and TP concentration (mg l^{-1}); La: accumulated TN and TP load (kg $year^{-1}$); Qa: mean annual flow (m^3 $year^{-1}$)

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.

2.7. Catchment transition potential modeling and land use changes scenarios for the 2050s

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 Flow chart for the MOLUSCE methodology is shown in Fig. 2. 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 module analyzes the transitional potential to predict LULC patterns in the future using the cellular automaton model (Burnham, 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 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, 1977, 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 (Molusce scenario). The Molusce scenario was used as a first scenario for future modification actions in the basin. 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 1). The three LULC scenarios were considered to evaluate likely future impacts on the upstream nutrient's concentrations in the Itupararanga reservoir.

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 NO_3 inflow and FRP concentrations by the increased or decreased proportions based on the baseline values in the biogeochemical model.

Thus, this modeling approach was used to simulate future nutrients

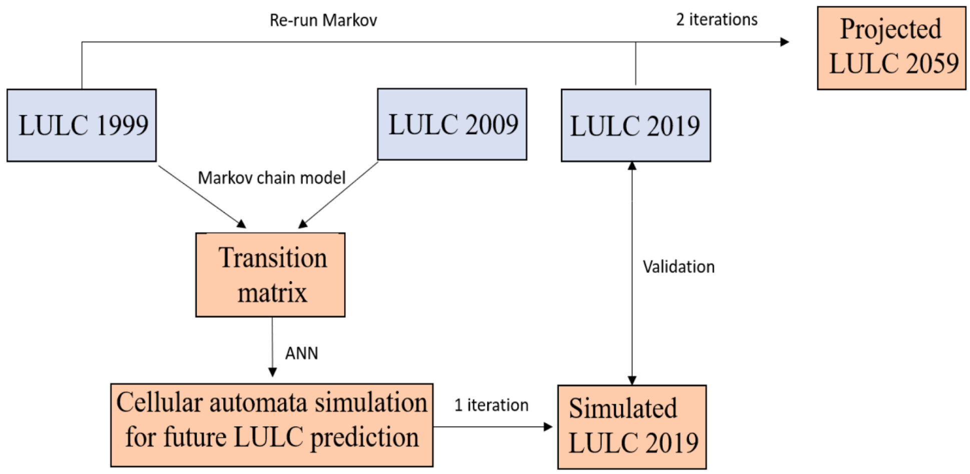

Fig. 2. Flow chart for the MOLUSCE methodology. Pink boxes refer to the MOLUSCE outputs.

Table 1
LULC scenarios 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

loads in the reservoir based on the three LULC future scenarios and the future daily discharges from the two climate models. We have calculated the long-term average discharge of the Eta-HadGEM2-ES and Eta-MIROC5 projections for 2050s to use in the estimation of TP and TN loads in the same future period. We have performed the estimation using each LULC area and its respective export coefficient divided for the two future long-term average discharge to find the average annual nutrient concentrations upstream of the reservoir.

2.8. Lake Ecosystem modeling

The vertical one-dimensional model GLM-AED2 which couples hydrodynamic, biogeochemical, and ecological processes in lakes was used to simulate TN, TP and TChla in the Itupararanga reservoir.

The TN and TP concentrations are based on the sum of nitrogen and phosphorus pools considering dissolved, particulate, organic and inorganic forms, as well as internal nitrogen and phosphorus stores in phytoplankton community Eq. (3) and (4).

The TChla concentrations are calculated as an indicator of phytoplankton abundance (Equation 5) using a carbon mass balance equation based on processes of uptake, excretion, mortality, respiration, and vertical movement in the water column (Equation 6). Grazing was not taken into account in the model equations as we did not have available zooplankton data.

$$TN = NO_3 + NH_4 + DON + PON + \sum_{a}^{N_{PHY}} PHY_{Na} \tag{3}$$

$$TP = PO_4 + PO_4^{ads} + DOP + POP + \sum_{a}^{N_{PHY}} PHY_{Pa} \tag{4}$$

$$TChla = \sum_{a}^{N_{PHY}} PHYa_{Xc:Chla}\, PHY_{Ca} \tag{5}$$

$$\frac{dPHY_{Ca}}{dt} = +f_{uptake}^{PHYCa} - f_{excr}^{PHYCa} - f_{mort}^{PHYCa} - f_{resp}^{PHYCa} - f_{set}^{PHYCa} \tag{6}$$

Where: f_{uptake}^{PHYCa}= function of uptake (C, N, P), f_{excr}^{PHYCa}= function of excretion, f_{mort}^{PHYCa}= function of mortality, f_{resp}^{PHYCa}= function of respiration, f_{set}^{PHYCa}= function of vertical movement (settling or migration).

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 TP, TN and TChla. We performed 3 months (Jan 2009 to March 2009) to spin up the model, 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 TP, TN and TChla. 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. This sensitivity analysis and calibration followed the same approach described in Ladwig et al. (2020).

The model parameters were manually changed aiming to sequentially optimize goodness-of-fit (GOF) metrics focusing on reproducing those concentrations of the dry and wet periods. As the observed TP, TN and TChla 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 peaks during the calibration process.

We calculated five GOF metrics (the mean absolute error (MAE), the Nash–Sutcliffe model efficiency coefficient (NSE), the Kling-Gupta efficiency (KGE), r and RMSE) to compare model outputs regarding the TP and TN surface, epilimnion and hypolimnion concentrations and measured data using the hydroGOF package for R. (Zambrano-Bigiarini, 2017). We have calibrated and validated the TChla concentrations for the surface and epilimnion layers. The target of the calibration was to represent the median values in order to simulate their future trends and be able to calculate the trophic state changes over the years.

When the ecosystem model was able to capture the median, maximum and minimum concentrations of TP, TN and TChla, we performed simulation of future scenarios using the output of the hydrological model and the distributed basin load model, and also took into account the future prediction of two climate projections and three LULC scenarios.

2.9. Coupled hydrological-hydrodynamic-ecological models

We performed simulation of future scenarios using the output of the hydrological model and the distributed basin load model, and also took into account the future prediction of two climate projections and three LULC scenarios. We used a coupled modeling framework to assess a total combination of six scenarios (Fig. 3, Table 2).

The previously presented calibrated and validated models were used to perform analysis of water quality and water level in the Itupararanga reservoir based on future projections of climate data and LULC for 2050s. We have used observed time-series of water level and TP and TChla concentrations as baselines to compare likely changes based on the proposed scenarios. To assess the future consequences on the water quality of Itupararanga reservoir, we have also calculated the trophic state index for tropical/subtropical reservoirs (TSI_{tsr}) proposed by Cunha et al. (2013). The TSI_{tsr} takes in account the annual geometric mean concentrations of TP and TChla Eqs. (7)-(9).

$$TSI_{tsr} = \frac{TSI(TP)_{tsr} + TSI(TChla)_{tsr}}{2} \tag{7}$$

$$TSI(TP)_{tsr} = 10\left[6 - \left(\frac{-0.27637 lnTP + 1.329766}{ln2}\right)\right] \tag{8}$$

$$TSI(TChla)_{tsr} = 10\left[6 - \left(\frac{-0.2512 lnTChla + 0.842257}{ln2}\right)\right] \tag{9}$$

Where: $TSI(TP)_{tsr}$= Trophic state index for tropical/subtropical reservoirs regarding the TP concentrations, $TSI(TChla)_{tsr}$= Trophic state index for tropical/subtropical reservoirs regarding the TChla concentrations, TSI_{tsr}= Trophic state index for tropical/subtropical reservoirs.

3. Results

3.1. Models performance

The SMAP model was used to simulate daily flows upstream from the Itupararanga reservoir. The values of the calibrated parameters are shown in Table S4 in the Supplementary material. The hydrological model reasonably represented seasonality differences and captured flow peaks from the daily observed rainfall and evaporation data (Fig. 4). The PBIAS metric was 19% and r=0.52 in the calibration period and PBIAS=4% and r=0.69 in the validation one.

The air2stream model was used to simulate the daily temperatures of the headwater of the Itupararanga reservoir as shown in Fig. 5. Simulated water temperatures were similar to observed water temperatures in the calibration (MAE=-0.039, r=0.88, RMSE=1.11°C) and validation (MAE= -0.011, r=0.95, RMSE=0.89°C) periods.

The distributed load modeling was able to represent the Q and concentrations of TP and TN along the Itupararanga headwaters compared with the reference values from Moriasi et al. (2007) highlighted in Table 3. 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

Table 2
Models and input and output data for each of them used for the scenario's simulation from 2050 to 2059.

Model type	Model name	Input data (Number of time-series)	Output data (Number of time-series)
Hydrological	SMAP	Projected rainfall (2) Projected evaporation (2)	Simulated discharge (2)
Thermodynamic	Air2stream	Projected air temperature (2) Simulated discharge (2)	Inflow water temperature (2)
Catchment	Distributed load model	Simulated average discharge (2) TP and TN loads based on the three projected LULC (3)	TN and TP concentrations (6)
Hydrodynamic-ecological	GLM-AED2	Projected meteorological data (2) Simulated water temperature (2) Simulated TN and TP loads (6)	Water quality features (6) Water level changes (2)

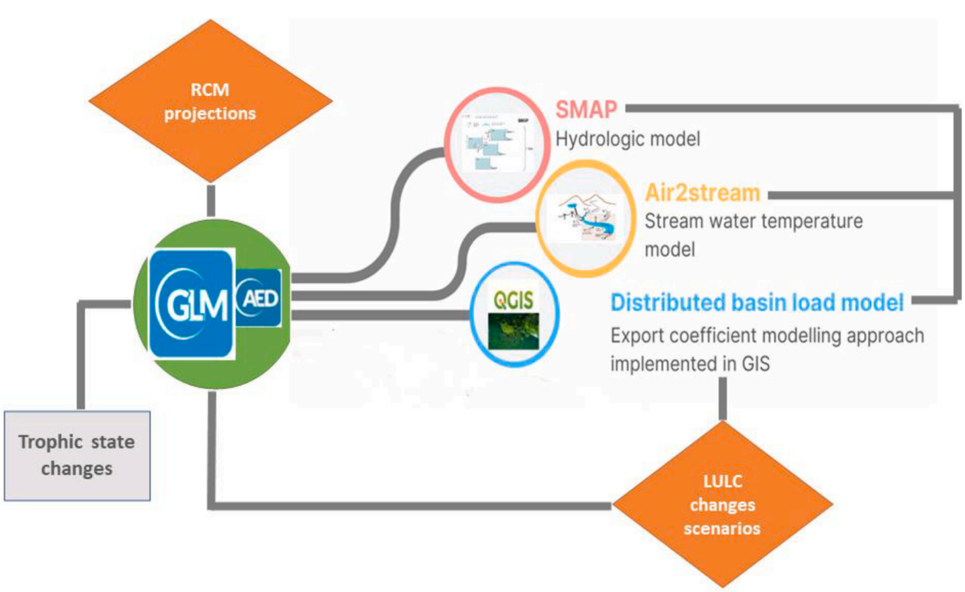

Fig. 3. Methodological framework. Process-based models as circles, input data as diamonds and output as rectangle.

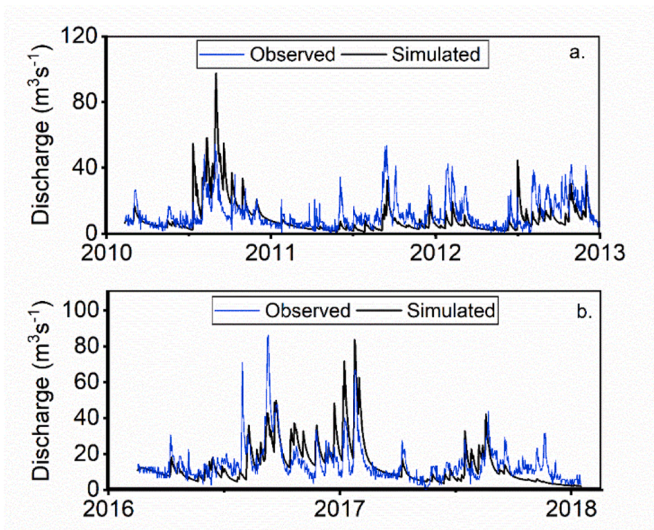

Fig. 4. Comparison between: a. calibration and b. validation results of the SMAP model.

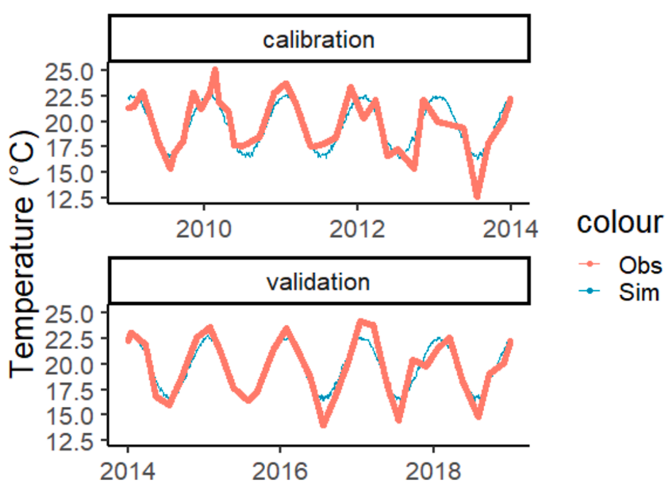

Fig. 5. Comparison between observed and simulated water temperatures for the calibration and validation periods.

experiment (Validation 01).

The validation results of the transition potential for the Alto Sorocaba basin in 2019 using 1999 and 2009 data according to each LULC are presented in Table S5 in relation to the total area (km^2) of the Alto Sorocaba basin. Overall, the model had a satisfactory performance (r=0.99, r2=0.99, K=0.73) to represent the LULC evolution in the basin (Fig. S1) despite underestimating forest plantation, urban, soybean and other temporary crops areas. The built scenarios related to the 2019 baseline are shown in Figure 6.

An automatic and manual calibration was performed to identify suitable values of the most sensitive parameters for the predictions of TP, TN and TChla in the GLM-AED2. Thirty-seven parameters were identified through the sensitivity analysis. They are related to oxygen and carbon mineralization dynamics, nitrification and denitrification processes, phosphate and DOP fluxes and growth, light, respiration, nitrogen and phosphorus of the phytoplankton. A list of the sensitive parameters and a comparison between the calibrated values and the literature range values is shown in Table S6 in the Supplementary material.

The GLM-AED2 was able to simulate median and mean values of TP, TN and TChla concentrations in the reservoir (GOF metrics in Table S7). The simulated TP and TN concentrations were better represented in the epilimnion (TP: $5 \mu g.l^{-1} < RMSE < 9 \mu g.l^{-1}$, TN: $110\ mg.l^{-1} < RMSE < 170 mg.l^{-1}$) compared to the hypolimnion (TP: RMSE=9 $\mu g.l^{-1}$, TN: RMSE=250$\mu g.l^{-1}$). On the other hand, the simulated median of the TChla concentrations was slightly overestimated, as well as the simulated maximum and minimum concentrations (Fig. 7). Our calibration approach aimed to reproduce essential patterns instead of seemingly exact numerical values, as suggested by Jachner et al. (2007) for ecological simulations.

3.2. Climate projections and water level trends

The meteorological forcing data projected for 2050-2059 by two RCMs have shown significant differences for longwave radiation, air temperature and rainfall in comparison with the historical baseline period (Table 4). Although both models taken in account the 8.5 $W.m^{-2}$ radiative forcing scenario, the ETA-MIROC5 model has indicated to be less sensitive to GHG emissions compared with the Eta-HadGEM2-ES projections. The British model predicts increase of 4% of shortwave radiation and 9% of wind speed and decrease of 2.6% of air relative humidity for the 2050s.

We have used the SMAP model with the calibrated parameters to predict future daily flows upstream from the Itupararanga reservoir based on the two RCMs projections. Mainly due to the downward trend in both rainfall projections, in comparison to the long-term annual flow (13.53 $m^3.s^{-1}$), the flows would decrease ~18% (11.06 $m^3.s^{-1}$) in the ETA-MIROC5 projections and ~57% (5.86 $m^3.s^{-1}$) in the Eta-HadGEM2-ES climate projections (Fig. S2). Such a reduction in inflows and the air temperature increase would directly influence the water table in Itupararanga reservoir, leading to a water level decrease for the 2050s. The median water level of the Eta-HadGEM2-ES and Eta-MIROC5 projections are going to be 18m and 13.8m, which means a reduction of 10% and 31% compared to the median water level observed between 2009 and 2018 (20m).

3.3. Trophic state changes for the 2050s

The trends in the TP and TChla concentrations for each simulated scenario are shown in Fig. S3. Overall, there is a pattern of increase in such concentrations in 28% compared with the baseline. The trophic state index (TSI) was calculated for each year in the 2050s considering all the six simulated scenarios (Fig. 8, Table S8). As noted earlier, the Eta-HadGEM2-ES climate projections tend to be more significant and have direct consequences on reservoir productivity. The simulated TSI values showed shifts from mesotrophic to eutrophic state ($53.6 < TSI < 57.7$) and from oligotrophic to eutrophic state ($52.4 < TSI < 57.7$), respectively, for Eta-HadGEM2-ES and Eta-MIROC5 along LULC change scenarios.

The Eta-MIROC5 projections along the green scenario, which considers a reduction in deforestation, predicted decrease of the TP and TChla median concentrations between 2054 and 2056 towards an oligotrophication trend ($52.4 < TSI < 52.8$). However, higher phosphorus availability ($60\ \mu g.l^{-1} < TP < 100\ \mu g.l^{-1}$) and phytoplankton biomass ($50 \mu g.l^{-1} < TChla < 97\ \mu g.l^{-1}$) are expected for the 2050s in comparison to recent years. On the other hand, the main consequences of the Eta-HadGEM2-ES projections along economic development scenario were the trophic state increase in the reservoir ($55.8 < TSI < 57.7$), remaining eutrophic from 2050 to 2059.

4. Discussion

4.1. Evaluation of model's performance and reproducibility

The simulated daily upstream flows were considered satisfactory for calibration and in very good agreement for validation according with

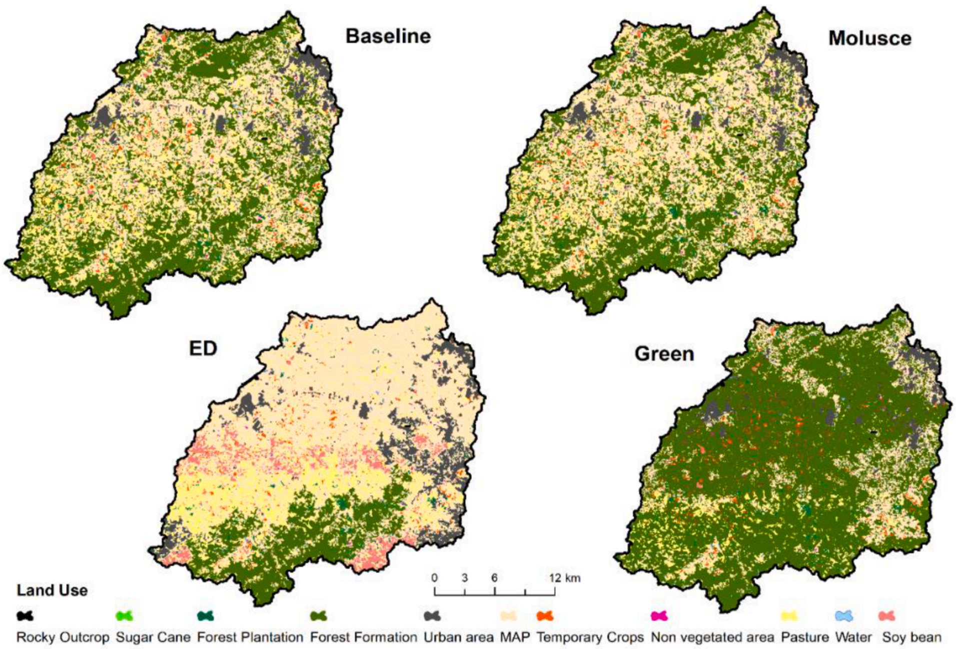

Fig. 6. LULC scenarios compared to the 2019 baseline upstream of the reservoir.

Table 3
Validation results for the distributed load modeling compared to the reference values from Moriasi et al. (2007).

	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 (green) — Good (blue)

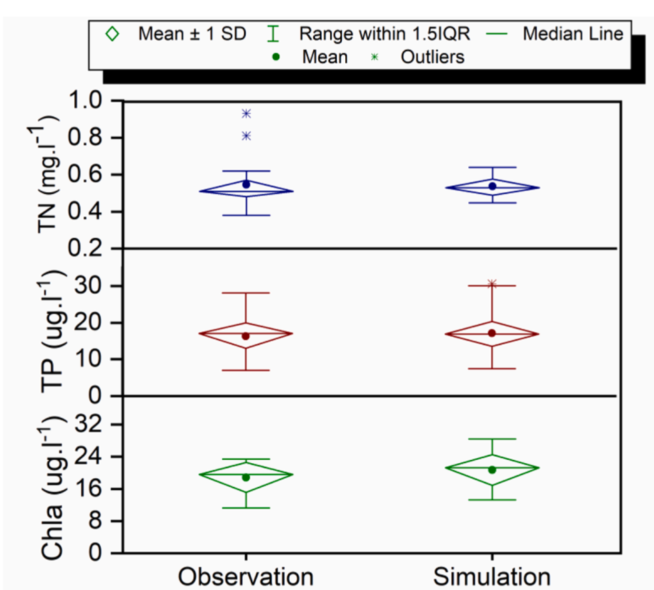

Fig. 7. Diamond plots of the simulated and observed TN, TP and TChla concentrations.

Moriasi et al., 2007. Likewise, the predictions of stream water temperature by Air2stream are in the range found in previous studies using the model (0.86°C<RMSE<1.52°C, Fenocchi et al., 2017; Toffolon and Piccolroaz, 2015). The simulated upstream TP and TN concentrations 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 this study (Messina et al., 2020).

The validations of TN and TP distributed modeling 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. 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).

The results of the basin transition potential simulation have shown satisfactory performance based on r and r2 values (>0.9) and very good agreement (K=0.73) between the reference map and the simulated map according to Landis and Koch (1977).

Since the TN, TP and Chla concentrations of the Itupararanga

Table 4
Mean and standard deviations of meteorological inputs. SW: shortwave radiation, LW:longwave radiation, AT: air temperature, RU: air relative humidity, WS: wind speed, Ra: rainfall

Source	Time range	SW ($W.m^{-2}$)	LW ($W.m^{-2}$)	AT (°C)	RU (%)	WS ($m.s^{-1}$)	Ra ($mm.\ d^{-1}$)
Gauged	2009-2018	214(76.5)	367(19.8)	21(3.3)	75(9)	2.2(1.0)	3.2(8.8)
Eta-HadGEM2-ES -RCP8.5	2050-2059	224(59.9)	360(29.0)	24(3.8)	73(16)	2.4(0.8)	1.8(6.0)
Eta-MIROC5 -RCP8.5	2050-2059	213(61.0)	334(33.3)	23(3.6)	75(11)	2.2(0.8)	2.9(8.2)

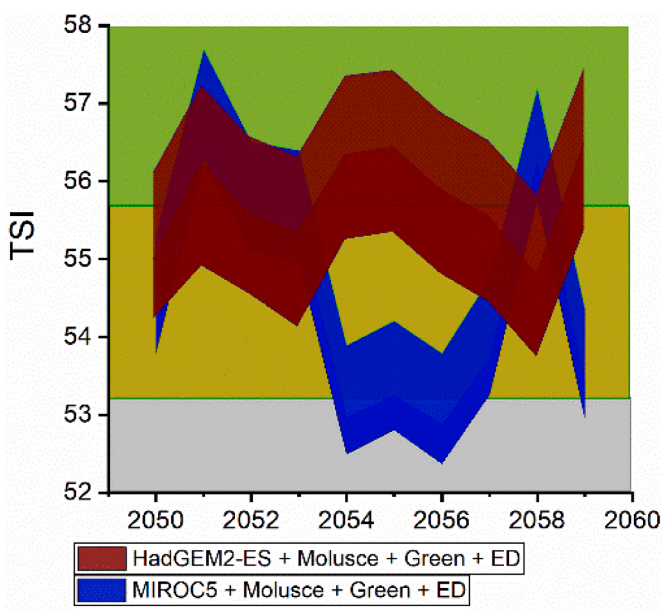

Fig. 8. Projections of the trophic state index (TSI) based on climate projections and LULC change scenarios. Background colors refer to the trophic state: gray – oligotrophic, yellow – mesotrophic, green – eutrophic.

reservoir did not show any clear seasonal pattern, the simulation efforts focused to represent the median values for the calibration and validation periods. A similar approach was taken by Ward et al. (2020). The hydrodynamic-ecological model was able to represent the median concentrations on the Itupararanga reservoir. The PBIAS values for the TP, TN and TChla simulations were considered good and very good (PBIAS$<\pm40$) according to the classification given by Darko et al. (2019) and Moriasi et al. (2007). A recent study found a similar range and the same trend for the TP and TN simulations using the GLM-AED2 (Farrell et al., 2020).

4.2. *Trophic state changes for the 2050s under climate change and LULC scenarios*

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 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).

As expected, the Eta-HadGEM2-ES projections has shown intensified climate trends compared to the Eta-MIROC5, however both RCMs predicted climate warming and rainfall decrease during the 2050s. The Eta-HadGEM2-ES predicted fall of 43% of the average precipitation compared to the measurements gauged from 2009 to 2018. Likewise, Sarmento et al. (2013) have predicted rainfall decrease for the tropical South America based on the IPCC projections for this century. Those trends of rainfall decrease have also impacted the reservoir volume. The downward trend of the water level in the Itupararanga reservoir have also found in Barbosa et al. (2021) for the last years of this decade.

Some studies have been highlighted the consequences of previous drought periods in the water quality of tropical and subtropical lakes and reservoirs (Brasil et al., 2016; da Costa et al., 2016; Tundisi et al., 2015). 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).

Although a previous study has indicated that N is not a limiting factor for the phytoplankton development in Itupararanga reservoir (Cunha et al., 2017), we recognize that a more extensive dataset would be necessary to reveal further differences in the potential shifts in nutrient limitation.Total phosphorus has been well established as a predictor of phytoplankton in lakes, especially in the Itupararanga reservoir (Beghelli et al., 2016; Melo et al., 2019). Recently, it has been reported that TP have nearly equal importance to that of climate in predicting water quality in lakes on a global scale (Shuvo et al., 2021). Itupararanga reservoir has already been reported as nutrients sink (Cunha, 2012) and also it has shown to have high sedimentation rate which contribute to release in the outflow a higher quality of the water (Melo et al, 2019).

Recent studies have compared the effects of climate change and LULC in watersheds and lake ecosystems (Bucak et al., 2018; Comte et al., 2021; Messina et al., 2020; Motew et al., 2019; Zipper et al., 2018; Pace et al., 2021). Climate have shown a stronger influence in surface water quality of Yahara Watershed, USA, than land use on three water quality indicators (Motew et al., 2019). The authors have also highlighted that the land use effects were significant and local management plays a key role in future outcomes, independent from the role of climate.

Despite the previous identified lack of a relationship between TChla and TP concentrations (Beghelli et al., 2016), Itupararanga reservoir has been classified with mesotrophic conditions in the lacustrine zone (Cunha, 20120). For the 2050s, the simulated scenarios showed shifts from mesotrophic to eutrophic state and from oligotrophic to eutrophic state. As expected, there was an increase in the trophic state in the ED scenario along climate projections. Such high productivity is related to the increase in the impervious areas in the watershed and greater release of external loads in the reservoir compared to the current LULC. Previous studies have identified increase in the TSI values in dry periods in the Itupararanga reservoir mainly due to the land use in the Alto Sorocaba basin (Cunha et al., 2017; Pedrazzi et al., 2013). Likewise, Itupararanga reservoir has been identified as having external nutrient loads more significant than internal turnover (Cunha, 2012; Cunha et al., 2017). Sarmento et al. (2013) considering climate change consequences in large tropical lakes mainly driven by internal loads indicates oligotrophication rather than eutrophication as a result of the increased water column stability.

Management strategies and catchment-scale ecological restoration are needed to mitigate the climate change impacts in the water quality of Itupararanga reservoir. In a eutrophication scenario, advanced water treatment may be necessary, as suggested by Beghelli et al. (2016). However, water resources management efforts must be done to control agricultural lands without environmental protection actions in the Alto Sorocaba basin and also change the reservoir operation to save water for drinking water supply and protection of the aquatic ecosystem. Investments in source control (e.g., biogas digester, fermentation bed, rural population benefited by sewage treatment facilities) have shown stronger impact on water quality in rivers of China than investments in restoring sinks (e.g., ecological forest, surface flow wetlands, dredging of contaminated sediment) (Fu et al., 2021).

4.3. *Framework based on coupled open-source models*

The proposed modeling framework aimed at coupling simple process-based models and GIS techniques to assess impacts of the catchment LULC and climate change on the Itupararanga 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 and climate, given a historical baseline.

The results of coupling hydrological models and aquatic ecosystems, such as hydrodynamic models have highlighted their potential as management tools to understand and predict actions that cause future impacts on aquatic ecosystems (Munar et al., 2018, 2019, Zhang et al., 2019). 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 highlighted the uncertainty in the model's processes and compared the prediction outputs with the historical TP, TN and TChla measurements in the Itupararanga reservoir to give insights to the water quality management. Our coupled modeling approach are not suitable for short-term forecasting purposes due to the LULC changes scenarios take into account only historical trends beside dynamic land processes or human interventions. It is also important to perform forecasts using several meteorological driver data. Quantifying the contribution of different sources of uncertainty in the model prediction is crucial for ecological forecasting. Several studies have proposed novel uncertainty quantification processes (Thomas et al., 2020; Khatami et al., 2019; Huang, 2015), however less than 50% of recent papers have included uncertainty in their forecast outputs (Lewis et al., 2022).

5. Conclusion

The current study developed an integrated modeling approach forced by two regionalized climate models and LULC change scenarios to perform forecasting of trophic state in a subtropical reservoir for the 2050s and to compare the outputs with the historical observations. We have chosen open-source tools implemented in R and GIS to foster the reproducibility of the modeling approach. The contribution of uncertainties in the models' processes was also taken into account in the modeling framework. We also proceed to data processing and gap filling to reduce the uncertainty of driver data and initial conditions. However, we did not perform uncertainty quantification from different sources in each model. Our main goal was to simulate trophic state predictions and compare those results with historical observations to provide insights for water management.

The two RCMs forced by the greenhouse gases representative concentration pathway of 8.5 W.m-^{2} showed rainfall and longwave radiation decrease and air temperature increase in the studied basin. Overall, the outcomes of the climate model projections along the LULC change scenarios suggest water quality deterioration due to increase of TP and TChla concentrations and shifts of the reservoir trophic state from oligo-mesotrophic to eutrophic state. Due to climate and LULC changes trends, we suggest installation of advanced water treatment plants and management efforts to control agricultural lands without environmental protection actions in the basin in the near future. The proposed modeling framework can be a valuable tool to guide water resources management in poorly monitored basins considering climate warming and future pressures on freshwater due to population growth and intensive agricultural practices for human consumption.

Software availability

Instructions to download and install the SMAP, Air2stream, GLM-AED2, and the QGIS MOLUSCE Plugin can be found at:

-SMAP: http://www.labsid.eng.br/software.aspx?id=1

-Air2stream: https://github.com/marcotoffolon/air2stream

- 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.

CRediT authorship contribution statement

Carolina Cerqueira Barbosa: Writing – original draft, Writing – review & editing, Conceptualization, Methodology, Software, Visualization. **Maria do Carmo Calijuri:** Supervision, Resources, Writing – review & editing, Writing – original draft. **Phelipe da Silva Anjinho:** Writing – review & editing, Methodology, Visualization. **André Cordeiro Alves dos Santos:** Writing – review & editing, Data curation.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

Acknowledgements

This work was supported by the doctoral scholarship provided by the Coordination for Improvement of Higher Education Personnel (CAPES). The authors declare no conflicts of interest. Two anonymous reviewers have provided valuable suggestions for improving this manuscript.

Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.ecolmodel.2022.110227.

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