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**Synergistic interaction among reservoirs along a cascade system and
their response to the ongoing anthropogenic and climatic pressures:
evidence from deterministic hydrodynamic-biogeochemical modelling**

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Synergistic interaction among reservoirs along a cascade system and their response to the ongoing anthropogenic and climatic pressures: evidence from deterministic hydrodynamic-biogeochemical modelling

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Advisor: Prof. Titular Maria do Carmo Calijuri

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*To my husband Carlos, who lovely
encourages me everyday*

*To my parents, who supported me at all
steps of my education*

*All my love and gratitude
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RESUMO

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Em todo o mundo, reservatórios estão sendo construídos em sequência ao longo de grandes rios, formando sistemas em cascata com ambientes aquáticos interconectados. A compreensão dos processos físicos e biogeoquímicos em ambientes lênticos avançou nas últimas décadas, no entanto, evidências sólidas das interações entre reservatórios ao longo de um sistema em cascata permanecem insuficientes. Dessa forma, os principais objetivos da presente tese foram compreender a complexidade dos ecossistemas aquáticos interconectados e as respostas às contínuas pressões antrópicas e climáticas enfrentadas por seis reservatórios ao longo do Rio Tietê (Sudeste do Brasil). Há um grande interesse pela qualidade da água nesses reservatórios devido aos seus usos múltiplos. O modelo determinístico *General Lake Model* acoplado ao *Aquatic EcoDynamics* (GLM-AED) foi aplicado para simular os principais processos internos que afetam a qualidade da água nos reservatórios. A presente tese introduziu duas novas abordagens de modelagem: (i) uma estratégia de parametrização foi aplicada para realizar uma melhor estimativa de parâmetros potencialmente sensíveis para superar o desafio de explorar os processos hidrodinâmicos em dois reservatórios com ausência de medições de temperatura da água; e (ii) uma abordagem de modelagem sequencial que conecta os reservatórios, de forma que as alterações nas condições de contorno são propagadas de um corpo d'água para outro a jusante. O modelo foi então aplicado para (1) demonstrar os efeitos das mudanças climáticas sobre a hidrodinâmica do reservatório mais a montante no sistema ao longo de 26 anos (1993–2018). Os resultados indicaram que o reservatório experimentou um aquecimento significativo desde 1993 devido ao aumento da temperatura do ar e diminuição da velocidade do vento; (2) provar a interação sinérgica entre os reservatórios, desencadeando um efeito dominó ao longo do sistema em cascata, afetando assim a qualidade da água a jusante. Os resultados revelaram que a redução do aporte de fósforo no reservatório mais a montante resultou em maiores taxas de redução nos reservatórios a jusante, revelando a capacidade de atuarem como sumidouros de fósforo; e (3) testar cenários de métodos clássicos de restauração para orientar ações otimizadas em escala de bacia hidrográfica. Os resultados demonstraram que uma combinação de técnicas de mitigação na bacia hidrográfica com técnicas de restauração dedicadas ao reservatório mais a montante promoveria a recuperação da eutrofização não apenas no próprio reservatório, mas em todos os demais a jusante ao longo do sistema em cascata. As descobertas deste estudo são de grande interesse científico, pois fornecem um conhecimento profundo da limnologia física de reservatórios subtropicais, onde informações ainda são limitadas. Ademais, podem ser de interesse primário para os gestores de recursos hídricos, pois permitem a identificação do reservatório mais estratégico para dedicar ações de manejo visando estabelecer um programa de restauração eficiente em escala de bacia hidrográfica para garantir segurança hídrica para as gerações futuras.

Palavras-chave: ecossistema lêntico; qualidade da água; eutrofização; modelo GLM-AED; Rio Tietê.

ABSTRACT

SOARES, L. M. V. **Synergistic interaction among reservoirs along a cascade system and their response to the ongoing anthropogenic and climatic pressures:** evidence from deterministic hydrodynamic-biogeochemical modelling. Doctoral Thesis – São Carlos School of Engineering at University of São Paulo, São Carlos. 2021.

Reservoirs have been constructed in sequence along large rivers worldwide, forming cascade systems of interconnected aquatic environments. The general understanding of the physic and biogeochemical processes in lentic environments has improved over the last several decades, however, solid evidence of potential interactions among reservoirs along a cascade system remains unclear. Therefore, the main objectives of the present thesis were to comprehend the complexity of interconnected aquatic ecosystems and their response to the ongoing anthropogenic and climatic pressures faced by six reservoirs along the Tietê River (Southeast Brazil). There is a great interest in the water quality of these reservoirs in face of their multiple uses. The deterministic General Lake Model coupled to the Aquatic EcoDynamics (GLM-AED) was applied to simulate the major internal processes affecting water quality within the reservoirs. The present thesis introduced two novel model approaches: (i) a parameterization strategy was applied to accomplish a better estimation of potential sensitive parameters to overcome the challenge of exploring hydrodynamics in two reservoirs with a lack of measured temperatures; and (ii) a sequential modelling approach that fully links reservoirs' processes, in which alterations in the boundary conditions is propagated through one water body to the next. The model was then applied to (1) demonstrate the effects of climate change on the hydrodynamics of the uppermost reservoir in the system over 26 years (1993–2018). Results have indicated that the reservoir has experienced significant warming since 1993 related to increasing air temperature and decreasing wind speed; (2) prove a synergistic interaction among reservoirs triggering a domino effect along the cascade system, thus affecting the water quality further downstream. Results revealed that a reduction in phosphorus loads into the uppermost reservoir resulted in higher reduction rates in the downstream ones, revealing their capacity to act as a sink of phosphorus; and (3) test scenarios of classical restoration methods to provide guidance on optimised restoration efforts at a basin catchment scale. Results showed that a combination of on-land and in-lake restoration techniques devoted to the uppermost reservoir would promote restoration from eutrophication not only in the reservoir itself, but in all downstream ones along the cascade system. The present findings are of great scientific interest as they provide a deep understanding of the physical limnology of subtropical reservoirs, where information is still limited. Also, they may be of primary interest to water managers as it allows the identification of the most strategic reservoir to devote management actions for establishing an efficient restoration program at a catchment scale and ensure water security for future generations.

Keywords: lentic ecosystem; water quality; eutrophication; GLM-AED model; Tietê River.

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1

Introduction

1.1 General introduction

Reservoirs are artificial human-made water bodies created by impounded waters resulting from the construction of a dam across a river for the storage, regulation, and control of water. Historically, they have been built to attend to human needs for drinking water supply, hydropower generation, agricultural irrigation, fishery, flood regulation, and recreation. They can often be divided into three distinct zones: (1) riverine or lotic, where major tributaries enter and the river-like flowing condition is dominant, (2) transition, and (3) lacustrine or lentic, where a lake-like condition is dominant near the dam, supporting the notion that reservoirs are limnological intermediate systems between rivers and lakes. Reservoirs vary widely in morphometry, hydrology, and management objectives, but shares unique physical characteristics: long hydraulic residence time, relatively slow flow velocity, and development of vertical stratification. Those features often make internal chemical and biological processes significant along the water column, whereas these processes might be negligible in rapid-flowing rivers. Overall, reservoirs act as sinks of nutrients, sediments, toxins, and other substances originating from their catchment, and provide a favorable environment to promote algal growth.

Reservoirs can be built along a single river, forming a cascade system of hydrologically connected water bodies whose operation is interrelated toward fulfilling a common goal (Straškraba and Tundisi, 1999). This configuration is usually adopted for improving the efficiency of hydroelectric energy potential as numerous consecutive dams can better regulate the

flow regime and optimize the storage capacity. Several cascade systems of interconnected reservoirs have been constructed in sequence along large rivers worldwide, establishing a network of aquatic environments. The general understanding of the physic and biogeochemical processes in lentic environments has improved over the last several decades assisted by numerical models as a predictive tool widely used to describe ecosystem processes (Anagnostou et al., 2017; Costa et al., 2019; Janssen et al., 2015; Mooij et al., 2019; Vinçon-Leite and Casenave, 2019). However, solid evidence of potential interactions among reservoirs along a cascade system remains unclear (Miranda and Dembkowski, 2016), especially in the tropics (Winton et al., 2019).

To fully comprehend the complexity of interconnected aquatic ecosystems and their dynamic response to the ongoing pressures, six reservoirs along the Tietê River (Brazil) were selected as the study site. They are a remarkable example of multiple damming in a single river, having been created from the 1960s to 1990s for hydropower generation. There is a great interest in the water quality of these reservoirs due to their multiple uses, including navigation, drinking water supply, irrigation, fishery, flood regulation, and tourism. Despite their importance, the hydrodynamic and ecology of those reservoirs was never modelled before. This specific case study in the Tietê River's cascade system serves as a starting point to shed some light on the general mechanisms of downstream transport of energy, substances, and biota directly affecting water quality on the next reservoirs along the cascade system.

1.2 Study sites

Six reservoirs were built in the middle and lower reaches of the Tietê River in between 1964 and 1991 to meet the growing energy demand in the southeast region of the country: Barra Bonita, Álvaro de Souza Lima (Bariri), Ibitinga, Engenheiro Mário Lopes Leão (Promissão), Nova Avanhandava, and Três Irmãos reservoirs. It took advantage of the large river length (1150 km) and slope (860 m between the river's head and mouth). They are located in an important agricultural and industrial area in the São Paulo State, which gives a significant social and economic role to those reservoirs. Currently, they are intended for multiple uses in addition to hydroelectric power generation, including drinking water supply, irrigation, fish farming,

recreation, and tourism. Furthermore, they comprise the Tietê-Paraná navigation waterway, where large boats transport 6.5 million tons of cargo annually, mainly soy, corn, sand, and sugarcane.

The climate types in the reservoirs' catchments are (i) Cfa, humid subtropical climate without a dry season and hot summer, (ii) Cwa, humid subtropical climate with dry winter and hot summer, and (iii) Cwb, subtropical highland climate, with dry winter and warm summer (Figure 1.1a). There is a rainy period from October to March and a dry period from April to September. During dry months, the average rainfall is 276 mm, and during the rainy months is 1130 mm, reaching 1406 mm per year on average. The mean air temperature is 22.6 °C, with a minimum temperature of 14.0 °C in July and a maximum of 30.4 °C in October. The soil types in their catchments are: (i) eutrophic red-yellow argisol (27%), (ii) dystrophic red-yellow argisol (26%), (iii) dystrophic red latosol (23%), (iv) dystrophic red-yellow latosol (15%), (v) eutroferic red latosol (3%), (vi) dystroferic red latosol (2%), (vii) dystrophic Tb haplic cambisol (2%), (viii) ortic quartzarenic neosoil (1%), and (ix) dystrophic lithic neosoil (1%; Figure 1.1b). The following land uses are found in their catchments: (i) agricultural areas, mostly intensive sugarcane monoculture and citrus, (ii) urban areas, where more than 24 million inhabitants live in high-density regions, such as the São Paulo, Campinas, and Sorocaba Metropolitan Regions, (iii) pasture, (iv) forestry, (v) vegetation, and (vi) water bodies (Figure 1.1c).

Figure 1.1. a) Climate, b) soil, and c) land uses in the reservoirs' catchments.

1.3 Hypotheses

The following hypotheses were elaborated:

- The reservoirs' hydrodynamics are sensitive to alterations in meteorological conditions over the last decades as they are sentinels of climate change;
- There is an interaction among reservoirs along a cascade system, in a way that natural and anthropogenic pressures as well as restoration and management efforts affecting the water quality in any reservoir in the system will promote responses further downstream, affecting the state of the next water bodies.

1.4 Objectives

The main objectives of the present thesis were to improve the understanding of the current climatic and anthropogenic pressures faced by the reservoirs and to reveal the interconnection among them. The specific objectives were as follows:

- a. Application of a hydrodynamic model to simulate the vertical profile of water temperature in the six reservoirs, revealing their thermal regime;
- b. Assessment of water temperature trends and internal responses to climate forcing, envisioning potential driving factors explaining temporal thermal changes;
- c. Application of a biogeochemical model to better understand the role of nutrients and phytoplankton along the cascade system;
- d. Simulation of scenarios of classic restoration methods to assess the most efficient techniques to promote an overall improvement in water quality not only in one reservoir but in all water bodies along the cascade system.

1.5 Thesis outline

The present thesis is arranged in nine chapters, where the objectives are addressed by six chapters as draft manuscripts, following the structure below:

Chapter 2: Deterministic modelling of freshwater lakes and reservoirs: current trends and recent progress

The chapter gives an overview of the state of the art of deterministic models applied to lakes and reservoirs over the 2015–2020 period. The objective was to provide the recent developments in the field and the best practices to guide the modelling application presented in the next chapters.

Chapter 3: A parameterization strategy for hydrodynamic modelling of a cascade of poorly monitored reservoirs in Brazil

The chapter presents the application of the one-dimensional hydrodynamic General Lake Model (GLM) to hindcast multiannual temperature profiles for the six reservoirs along the cascade system over a period of eight years (2009–2016). To overcome the challenge of exploring hydrodynamics in two reservoirs with a lack of measured temperatures, a parameterization strategy was applied to accomplish a better simulation by the estimation of potential sensitive parameters through regression curves.

Chapter 4: Climate change enhances deepwater warming of subtropical reservoirs: evidence from hydrodynamic modelling

The chapter presents the hydrodynamic modelling of the uppermost reservoir along the cascade system, the one with more available in-situ data, over 26 years (1993–2018) to investigate its response to climate change in terms of warming trends, seasonal patterns, Schmidt stability, and the number of stratified days per year.

Chapter 5: Parameter sensitivity analysis for water quality modelling of subtropical reservoirs

The chapter provides the baseline simulation of the hydrodynamic model coupled to the biogeochemical Aquatic EcoDynamics library (GLM-AED) for three reservoirs along the

cascade system over a period of eight years (2009–2016). The focus was on a sensitivity analysis implemented to identify the most influential parameters in order to provide a detailed understanding of the governing ecosystem dynamics and guidance for model calibration.

Chapter 6: A sequential approach for modelling aquatic ecosystems in interconnected reservoirs along a cascade system

The chapter provides the GLM-AED model calibrated and validated to simulate biogeochemical processes for the six reservoirs along the cascade system over a period of eight years (2009–2016). A sequential approach was implemented to fully link reservoirs' processes along the system, taking into account the feedback from one water body to the next in order to better understand the role of water quality along the cascade system.

Chapter 7: Restoration from eutrophication in interconnected reservoirs: using a model approach to assess the propagation of water quality improvements downstream along a cascade system

This chapter presents the GLM-AED model as a tool to simulate scenarios of classic restoration practices to address eutrophication along the cascade system over a period of eight years (2009–2016). Each restoration scenario was propagated along the cascade system by using the sequential approach to reveal which restoration techniques are capable of promoting water quality improvements that are propagated to all downstream reservoirs along the cascade system.

Chapter 8: Concluding remarks and future directions

The chapter summarises the main results and draws suggestions and perspectives for further work.

Chapter 9: Publication list

The chapter provides the scientific publications produced from the thesis.

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2

Deterministic modelling of freshwater lakes and reservoirs: current trends and recent progress

Under review by Environmental Modelling & Software

Deterministic models have emerged as a widely accepted tool for investigations in lentic aquatic ecosystems. In this study, an extensive literature review is provided by an inventory of papers published over the last six years (2015–2020) to explore the recent progress of deterministic models applied to lakes and reservoirs. The current trends include the application of well-established models across broad ranges of time and spatial scales; an increasing interest for modelling the combined effects of climate change and eutrophication; the integration of lake, catchment and climate models, in addition to multi-model ensemble approaches; and the proliferation of high-frequency sensors and the usage of remote sensing images for model initialisation, forcing data inputs, and calibration and validation. It is expected that the emerging trends in modelling lakes and reservoirs can be of great use for future research prospects as a source of information for subsequent studies in the field.

Keywords: limnology, aquatic ecosystem, water quality, eutrophication, hydrodynamics, biogeochemistry.

2.1 Introduction

In the mid-twentieth century, when eutrophication became the major stressor of lakes and reservoirs worldwide (Vinçon-Leite and Casenave, 2019), the understanding emerged that inland waters are vulnerable to anthropogenic forcing (Gal et al., 2009). Preserving the integrity of aquatic ecosystems, as opposed to their passive exploitation, has been a growing goal, as aquatic ecosystems support economic activities, such as water supply for agriculture (Mereu et al., 2016) and drinking water (Jeppesen et al., 2015), hydroelectric power generation (Kobler and Schmid, 2019), and fishing (Makler-Pick et al., 2017). In addition, they provide ecosystem services, for example, by providing habitat for aquatic organisms (Schallenberg et al., 2013). To capture the ecosystem's response to anthropogenic stressors and pressures from climate change, affecting both developed and emerging countries, deterministic models emerged as a potential tool to explore the functioning of aquatic ecosystems at local, regional and global scales.

In an effort to obtain a greater understanding of the system behavior, lake models intend to achieve the following principles of (1) generality, by applying general equations and assumptions valid in a broad variety of sites, requiring few local adjustments; (2) accuracy, in which they reproduce the observed data with minimal errors; and (3) realism, in which they attempt to explain the dynamics of the real system in detail (Ganju et al., 2016). Deterministic lake models differentiate from statistical models in their capacity to simulate a system in terms of the processes acting on state variables. Statistical models, also called black box models or empirical models, are formulated as a direct mathematical relation between forcing and state variables, with no causality. Deterministic models, also referred to as mechanistic models or process-based models, are based on a set of differential equations that describe physical, chemical, and biological processes, i.e. the water column is represented as a compartment with different representations of boundary fluxes related to air-water exchanges, sediment-water exchanges, and inflows and outflows, providing the mechanisms underlying aquatic ecosystem processes.

Since the first lake models, their development and application have undergone substantial advances with increasingly predictive ability and now they can cover more than 100 state variables (Janssen et al., 2015). Lake models found widespread use for a wide range of time and spatial scales (Trolle et al., 2012) and have been applied for several purposes: (i) scientific,

aiming to advance theory by exploring ideas, demonstrating concepts, understanding the mechanisms that govern ecosystem functioning, and elucidating the relationships between internal processes and external forcing (Schmolke et al., 2010); (ii) methodological, intending to fill gaps in observations by extrapolating the range of historical temporal and spatial measurements (Janssen et al., 2015); (iii) decision-making to predict the interaction between management actions and ecosystem response and to estimate the effort required to avoid adverse conditions or to restore degraded systems (Hipsey et al., 2015); and (iv) synthesizing virtual experiments to manipulate conditions that would be too expensive, too time consuming or unethical to do in a real-world system (Peck, 2004).

Owing to the recognition of the contribution given by models to the study of spatio-temporal dynamics in lake ecosystems, several review articles have evaluated the development and application of models, in terms of diversity (Janssen et al., 2015), accuracy (Robson, 2014a), uncertainty (Uusitalo et al., 2015), complexity (McDonald and Urban, 2010), performance (Bennett et al., 2013), validation (Alexandrov et al., 2011), and applicability (Costa et al., 2019). A starting point review was conducted by Jørgensen (1995), which discussed the need for additional constraints to better represent the properties of ecosystems, the front line problem of modelling in the 1990s. More recently, overviews assessed the modelling of eutrophication and cyanobacteria harmful blooms in lake ecosystems (Bhagowati and Ahamad, 2019; Janssen et al., 2019; Roussio et al., 2020; Vinçon-Leite and Casenave, 2019), and the challenges to model water quality in the Anthropocene (Mooij et al., 2019).

However, most of these reviews were in the context of aquatic ecosystem models, applied not only to lakes and reservoirs, but also to rivers, estuaries, wetlands and oceans (*e.g.* Anagnostou et al., 2017; Brewer et al., 2018; Costa et al., 2019; De Goede, 2020; Robson 2014b), also including other modelling approaches, such as statistical and empirical models (*e.g.* Voinov et al., 2018). Considering that few reviews focused specifically on deterministic lake models, this paper provides an overview of the current generation of deterministic models applied to lakes and reservoirs by conducting an extensive literature review of papers published over the last six years (2015–2020). The aim of this study was to provide a comprehensive overview and novel insights of the recent progress in lake modelling in face of the rapid developments in the field. The in-

depth analysis of the state of the art is expected to encourage modellers' future works and to assist water managers towards a sustainable management of water resources.

2.2 Historical trajectory of deterministic lake models

Historically, lake ecosystem models have been developed to address questions concerning water quality degradation, mostly related to eutrophication, nutrient cycling, dissolved oxygen concentration, chlorophyll-a concentration (Hipsey et al., 2015), and fish habitat, by investigating oxygen, temperature, and, later on, light (Chang et al., 1992). The first empirical equations that related loads to concentrations, the precursors of lake ecosystem models, were developed in the early 1970s to describe eutrophication processes for environmental management purposes based on the scientific insight of the work of Vollenweider (1968) that provided algorithms to calculate nutrient retention in lakes. From the late 1970s to the mid-1980s, models were based upon ecological knowledge and, despite their qualitative or semi-quantitative prediction capacity, they could be used as prognosis tool in limnology, being applied to environmental management (Jørgensen, 1995). During the 1990s and 2000s, modelling experienced rapid growth determined by the advances in technological and computational progress, providing greater processing speed and memory, data storage at a lower cost, and better graphic properties, which ultimately allowed more complexity and greater use of 3D models (Robson, 2014a). At that time, there was a tendency for each research group to develop their own models instead of applying previously existing models (Jørgensen, 2010).

More recently, however, rather than using independently developed models directed to a specific set of questions, investigators are focusing on widely applicable and well-established open-source models (Frassl et al., 2019), covering a wide range of lake characteristics in terms of morphology, geographical location and hydrological features. This emerging trend can be seen as an organised effort to avoid 'reinventing the wheel', as suggested by Mooij et al. (2010), and to go into more depth in terms of development tasks, taking advantage of the existing models to modify and combine the strengths of them. Additionally, from the beginning of the 2010s, the scientific community organised itself in interdisciplinary collaborative networks in order to accelerate advances in the modelling of lake ecosystems through the sharing of data, methods and

experiences. The collaborative networks, together with the increasing resolution and quality of field data, boosted the development, performance, transparency and reliability of models in predicting lake systems on a global scale (Weathers et al., 2013). The representation of lake ecosystems has become more complex after incorporating the concept of environmental integrity, which also considers the ability of ecosystems to maintain their ecological function (Hipsey et al., 2015). The models have been increasingly applied to encompass regional or continental aspects, resulting in their application in different environmental and geographical conditions (Janssen et al., 2015).

2.3 Model typology

Deterministic lake models can be classified according to their (i) variation on time, as static or dynamic, (ii) dimensionality, from 0D to 3D, and (iii) components of the ecosystem, including hydrodynamic module, nutrients module and biological module. Static models are based on a steady state assumption. They are suited when a static situation is sufficient to give a proper description of an ecological system, relying in a reduced applicability. On the other hand, dynamic models are based on ordinary or partial differential equations to describe processes over time. Most of the eutrophication models in the early development stage were static types, but rapid development in dynamic modelling has been observed since the 2000s, resulting in less than 2% of static models publication in Ecological Modelling from 2000 to 2006 (Jørgensen, 2008).

Models vary in spatial dimension according to the water body's features and targeted processes. Zero-dimensional or box models assume a complete mixed water body with no spatial variation, being suited for small lakes or ponds. One-dimensional models simulate the spatial change over a single dimension, either horizontally (length) or vertically (depth) averaged, being able to represent a narrow estuary or a small but well-stratified lake, respectively. Two-dimensional models, which are more rarely used, simulate spatial variations in the lateral and longitudinal directions (width and length) or in vertical and longitudinal directions (depth and length). They are most suited for large but shallow lakes or deep but narrow lakes. Three-dimensional models simulate changes in all three spatial domains (width, length, and depth),

being adequate for deep and large lakes and reservoirs. 3D models are the most physically realistic representation for a water body, providing the most detailed assessment of the studied processes. Justifiable simplifications should always be considered to balance problem, ecosystem, and knowledge, not making the model more complex than the data set can support (Jørgensen, 1995). Ultimately, the selection of a model's dimension must be bound by the research question, the ecosystem, and the data. Besides, the availability of resources, such as computing and manpower, govern which dimension can be supported. For example, the simulation of climate change effects on a water body over a 100-year period would be a difficult task using a 3D model in terms of computational costs and time constraints. In addition, model outputs would have a high level of uncertainty. Rather, a 1D model may perhaps provide just as valuable and as accurate outputs at a lower time and cost.

According to the objective of the modelling, i.e. the problem to be assessed, different components should be represented. Hydrodynamic models are based on well constrained equations to simulate the physical environment, such as the water level, water velocity, temperature, salinity, ice, and photosynthetically active radiation. The nutrients module and biological module are often simulated by ecological models. They cover a wide range of components, including nutrient cycles, oxygen balance, and biological communities.

2.4 Review of papers published over the last six years

The present review performed a compilation of modelling studies written in English over the last six years (2015–2020). The research was conducted on November 2020 in the following databases: Scopus, Web of Science, and Google Scholar. The selection of models was based on the most widely referenced deterministic models in recent years (Gaudard et al., 2019; Janssen et al., 2015; Mooij et al., 2010) applied to lakes and reservoirs and currently under use worldwide, for example by the Inter-Sectoral Impact Model Intercomparison Project (ISIMIP). They consist on an inventory of seventeen hydrodynamic, water quality and ecosystem models: (1) Aquatic EcoDynamics (AED; Hipsey et al., 2013), (2) Arctic Lake Biogeochemistry Model (ALBM; Tan et al., 2017, 2015), (3) CE-QUAL-W2 (Environmental and Hydraulics Laboratories, 1986), (4) Computational Aquatic Ecosystem DYNamics Model (CAEDYM; Hipsey et al., 2005),

(5) Delft3D-FLOW (Deltares, 2021a) and/or its water quality model (Delft3D-WAQ; Deltares, 2021b), (6) DYnamic REservoir Simulation Model (DYRESM; Antenucci and Imerito, 2000) and/or its water quality module (DYRESM–WQ), (7) Ecopath with Ecosim (EwE; Christensen et al., 2000), (8) Estuary, Lake and Coastal Ocean Model (ELCOM; Hodges and Dallimore, 2007), (9) Freshwater Lake Model (FLake; Mironov, 2008), (10) General Lake Model (GLM; Hipsey et al., 2019, 2017, 2014), (11) General Ocean Turbulence Model (GOTM; Burchard et al., 1999), (12) LAKE (Stepanenko et al., 2016), (13) MINLAKE (Riley and Stefan, 1988), (14) MyLake (Saloranta and Andersen, 2007), (15) PCLake (Janse and Van Liere, 1995), (16) Phytoplankton RespOnses To Environmental CHange (PROTECH; Elliott et al., 2010), and (17) Simstrat (Goudsmit et al., 2002).

The search term was taken as the exact name of each model, resulting in 479 peer-reviewed publications. From those, we selected the ones that simulated at least one of the key variables that represent either the hydrodynamics or the water quality, including (Ji, 2007, p. 5): water temperature, salinity, velocity, sediment, toxics, dissolved oxygen, algae, and nutrients. Also, only the studies that presented a case study of real lakes or reservoirs were considered in the present study, resulting in 328 papers. Modelling of virtual systems, bays, lagoons, estuaries, and ponds were not included, as well as thesis and conference papers. A full-text assessment was conducted to support the discussion of the state-of-the-art of deterministic models regarding the following topics: (1) global distribution of model applications, (2) temporal and spatial domains, (3) state variables, (4) stressors of the aquatic ecosystem, (5) coupled models, (6) ensemble modelling approach, (7) frequency of field measurements, (8) use of technological devices, (9) prediction accuracy, and (10) methodological procedures.

2.4.1 Geographical distribution

The most studied lakes during the 1970s and the 1980s were mainly located in North America, while in the 1990s, modelling works were increasingly carried out on lakes from Western Europe (Vinçon-Leite and Casenave, 2019). From 2015 to 2020, investigations were conducted in lakes and reservoirs from more than 45 countries (Figure 2.1). The continents where lake ecosystem models began to be applied still top the list of study areas. Indeed, the most studied lakes and reservoirs are situated in Europe (34%, mostly in Germany, Switzerland, and

Italy) and North America (23%, in the United States and Canada). However, a clear dissemination has been observed beyond temperate countries. There was a significant increase in the number of studies carried out in Asia (20%, in Bangladesh, India, Philippines, Russia, Singapore, South Korea, Taiwan, and especially in China) and in Middle East (9%, in Iran, Israel, Lebanon, Turkey, and Turkmenistan). Indeed, 45 studies (out of 328) were applied to Chinese lakes and reservoirs, such as Lake Taihu, for which models were developed to predict and warn against future algal blooms (Hu, 2016).

Figure 2.1. Global distribution of study sites of lake ecosystem modelling from 2015 to 2020.

In parallel, only 6% of the studies was conducted in Central/South America (Brazil, Chile, Colombia, and Mexico), 5% in Africa (Congo, Egypt, Ethiopia, Ghana, Kenya, Morocco, and Tunisia), and 3% in Oceania (New Zealand and Australia). Although progress has been made towards a greater geographic distribution of the places where the studies were conducted, additional efforts are still needed for further studies in Africa and South America, due to the small number of published articles on lake modelling in these continents.

2.4.2 Expanding temporal and spatial domains

Typically, traditional environmental approaches have focused on understanding processes that operate on a temporal scale convenient for human observation, ranging from about an hour to

a year or two (Rose et al., 2016a). Long-term studies are expanding observations to decades or longer mostly to assess policy and management issues, which are often influenced by environmental factors acting in various temporal scales. Indeed, mid or long-term modelling is required for assessing ecosystem evolution in response to local and global changes, such as (i) climate change: 104-year in Fish Lake (USA; Magee et al., 2018); 57-year in Lake Chaohu (China; Zhang et al., 2020); 40-year in Lake Langtjern (Norway; Couture et al., 2015); and 34-year of Lake Nam Co (China; Huang et al., 2017), (ii) urbanisation: 60-year in Lake Chaohu (China; Kong et al., 2017a); and 25-year in Lake Dianchi (China; Li et al., 2019), and (iii) contamination: 60-year in Lake Chaohu (China; Kong et al., 2017b). Besides, over longer time-scales, models are used to capture long-lasting responses to management practices and restoration efforts. For instance, the simulation of scenarios for reduction of phosphorus load into Lake Mendota (USA) over a 37-year period provided the required reduction to alleviate oxythermal stress, and the associated economic cost (Magee et al., 2019). This latter is an example of how the temporal expansion provided by modelling approaches has the advantage of testing management strategies in face of long-term responses.

In the 328 published articles, simulations covered a period of 191 years, from 1911 to 2101 (Figure 2.2). Most of them were focused on the years from 1990 to 2020, on average each year over this period was assessed by 77 studies, aiming at understanding processes, such as extreme events, and at simulating management strategies for operation optimisation, pollution, water abstraction, and anoxia. Studies that applied models for hindcasting purposes for the period from the 1910s and 1990s (on average each year over this period was assessed by 14 studies) were focused mostly on the impacts of human disturbances on the ecosystem, especially eutrophication and regime shifts. Hindcasting studies for the period prior to the 1950s focused mostly on the long-term alterations in thermal regimes. The projection studies covered the period from the present until 2101, on average each year over this period was assessed by 21 studies, aiming at predicting future climate and land use scenarios and their influences on aquatic ecosystems.

The spatial scale, historically focused on single study sites, increasingly includes research across many sites. Indeed, 53 over 328 studies (16%) covers regional or continental aspects, which enables a more contextual understanding of hydrodynamics (Bruce et al., 2018), gas

emissions (Guo et al., 2020), response to extreme events (Woolway et al., 2020), and effects of climate change (Almeida et al., 2015; Hansen et al., 2017; Maberly et al., 2020; Woolway et al., 2017). Efforts have been made to identify universal descriptors of processes, similarity in emergent behaviors, and how water quality pathways vary across geomorphologic and climate gradients (Hipsey et al., 2015). For example, Winslow et al. (2017) modeled the response of 10,774 lakes to changing climate drivers to give managers insight on individual lakes. Similarly, Rose et al. (2016b) modeled the thermal characteristics of 1,894 temperate lakes in the USA to investigate how water clarity can influence the response of both surface and bottom water temperatures to climate change.

Figure 2.2. Temporal scale covered by modelling studies published from 2015 to 2020.

2.4.3 A variety range of variables of interest

Water temperature was the most studied variable (in 71% of the studies; Table 2.1). However, 50% of these references did not focus on the modelling of temperature only, but on the representation of the physical habitat and thermal structure of aquatic systems as a compulsory step for modelling biogeochemical processes. The other state variables of the hydrodynamic component were water circulation (7%; e.g. Amadori et al., 2018; Gasca-Ortiz et al., 2020; Kranenburg et al., 2020; Liu et al., 2018; Ndungu et al., 2015) and salinity (1%; e.g. Elsaheed et al., 2020; Sabeti et al., 2017).

Table 2.1. State variables addressed in modelling studies from 2015 to 2020, the percentage of studies that covered each variables, and some references.

State variable	Percentage of studies	References
Temperature	71%	Almeida et al., 2015; Piccioni et al., 2021; Shatwell et al., 2019; Soares et al., 2020
Salinity	1%	Elsaeed et al., 2020; Sabeti et al., 2017
Circulation	7%	Gasca-Ortiz et al., 2020; Kranenburg et al., 2020; Ndungu et al., 2015
Phosphorus	24%	Brett et al., 2016; Dehbalaei et al., 2016; Kim et al., 2019; Messina et al., 2020
Nitrogen	21%	Kong et al., 2019; Liu et al., 2019; Moridi, 2018; Ziaie et al., 2019
Dissolved oxygen	27%	Luo et al., 2018; Snortheim et al., 2017; Weber et al., 2017
Carbon	6%	Edlund et al., 2017; Guseva et al., 2020; Iakunin et al., 2020; Kiuru et al., 2018
Methane	1%	Guo et al., 2020; Guseva et al., 2016; Schmid et al., 2017; Stepanenko et al., 2016
Sediments	1%	Huang et al., 2016; Zhang et al., 2015a
Contaminants	2%	Organic compounds: Aboutalebi et al., 2017; Afshar et al., 2017; Amirkani et al., 2016; Hydrocarbons: Kong et al., 2017b; Metal: Torres et al., 2016
Phytoplankton	38%	Chen et al., 2016; Fadel et al., 2019; Gray et al., 2019; Vinçon-Leite et al., 2017
Zooplankton	15%	Banerjee et al., 2016; Dalton et al., 2016; Kerimoglu et al., 2017
Macrophytes	8%	Bulat et al., 2019; Coppens et al., 2020
Fish	13%	Bhele et al., 2020; Cremona et al., 2018; Goto et al., 2020

Total phosphorus (24%), total nitrogen (21%), and their constituents were largely studied, which can be attributed to their role in eutrophication. Dissolved oxygen was also extensively studied (27%), mostly to assess issues concerning hypoxic conditions in deep lakes and reservoirs. In addition, carbon (6%), methane (1%), sediments (1%), and contaminants (2%), including organic compounds, hydrocarbons, and metal, were simulated geochemistry state variables.

The ecosystem was represented mostly in terms of phytoplankton, which was the interest of 125 modelling studies out of 328 (38%), aiming at a better understanding of phytoplankton dynamics and the processes that control its excessive biomass. From those 125 studies, 64 of them (51%) represented the phytoplankton as multiple functional groups rather than simulating the total biomass, which relies on the representation of different morphological, physiological, and ecological characteristics. The functional grouping offers an intuitively approach that accounts for different patterns of specialism, considering that the external forcing and the internal environment may profoundly modulate the signals of each group (Shimoda and Arhonditsis, 2016). When the objective of the simulation relies on the total concentration of chlorophyll-a, for example, for assessing the trophic status of a water body, the simulation of the total biomass as

one group is sufficient. Otherwise, when the composition of the biomass, the competitive interactions between different groups for resources, such as light and nutrients, or succession dynamics are important for the ecosystem, the simulation of multiple groups is a valuable approach. From 2015 to 2020, phytoplankton community was represented as two (Cui et al., 2016; van der Linden et al., 2015; Zamani et al., 2016), three (Brett et al., 2016; Brito et al., 2018; Chen et al., 2016), four (Gray et al., 2019; Khatun et al., 2020; Soullignac et al., 2019), five (Dalton et al., 2016; Tesfaye and Wolff, 2018), and seven (Wang et al., 2019b; Zhu et al., 2020) taxa. Among the phytoplankton groups, cyanobacteria has gained an increased interest due to the worldwide occurrence of their blooms and the associated public health concerns (*e.g.* Fadel et al., 2017; Silva et al., 2019).

Furthermore, few studies went into more depth concerning the specialisation and simulated phytoplankton species. For example, Fadel et al. (2017) simulated the succession of cyanobacterial blooms of two different species in a hypereutrophic reservoir for early warning systems and management scenarios; Bracht-Flyr and Fritz (2016) simulated the timing and distribution of two diatom species in Crevice Lake, the USA; Radbourne et al. (2019) assessed the effects of changes in external nutrient loads on the seven most abundant phytoplankton species in Rostherne Mere lake, England; and Elliott et al. (2016) investigated how eight phytoplankton species may adapt in response to potential future changes in air temperature and future load in Lough Neagh lake, Ireland.

Zooplankton was also the target variable of some studies (15%) mainly focused on the eutrophication and the impact of regime shifts. Moreover, from the 49 studies that have simulated zooplankton, 30 of them (61%) represented zooplankton by groups. For instance, three zooplankton groups (predatory zooplankton, herbivorous zooplankton, and micro-zooplankton) were simulated in Lake Kinneret, Israel (Makler-Pick et al., 2017); two groups (herbivores and carnivores) were simulated in Lake Bourget, France (Kerimoglu et al., 2017); and also two groups (cladocerans and copepods) were simulated in Lough Leane lake, Ireland (Dalton et al., 2016).

The dynamics of macrophytes (8%), and fishes (13%) were also simulated to represent food-web dynamics. Macrophytes were simulated in a recent investigation that studied how they can affect flow dynamics by increasing flow resistance (Bulat et al., 2019). Fish communities

were also simulated in an investigation focused on the impact of the total external nutrient load on the dynamics of Lake Taihu, China (Janssen et al., 2017). The models selected for the present review analysis provided a comprehensive overview of the most investigated state variables. However, as some of the models are not able to simulate zooplankton, macrophytes or fishes, we recognise that the percentages presented above might be biased and should be interpreted with caution.

2.4.4 Modelling combined effects of climate change and eutrophication

Several threats to the health of aquatic ecosystems were assessed by modelling studies. As expected, climate change and eutrophication were the major concerns, covering 29% and 14% of the published studies, respectively (Figure 2.3). The impacts of eutrophication and climate change are closely related and, therefore, some studies (3%) have investigated their combined effect. Different approaches were adopted to investigate the combined effects of both climate change and eutrophication: (i) using regional climate models as input to the lake model to assess changes in atmospheric forcing variables, mainly in air temperature and precipitation. For instance, Chang et al. (2015) have found that the intensified thermal stratification caused by the rising water temperature resulted in a higher risk of algal blooms and eutrophication in the Hsinshan Reservoir, Taiwan; (ii) coupling lake model with catchment model to account for projected changes in runoff and nutrient loads. The study by Me et al. (2018) indicated that polymictic lakes may be particularly vulnerable to eutrophication associated with climate change due to increased internal nutrient loading, while changes in external loads will have lesser relative impact; and (iii) using a sensitivity procedure by applying incremental perturbations in the forcing variables to disentangle the effects of changes in individual physical drivers in a present day simulation. Gray et al. (2019) conducted systematic and independent changes in water temperature and mixed depth in Blelham Tarn lake, England, whilst keeping other variables constant, revealing that each change result in impacts that can act synergistically on phytoplankton biomass. Similarly, Rolighed et al. (2016) simulated multiple combinations of increasing air temperatures and reduced external nutrient loads, which reveals that in a future warming scenario, a nutrient load reduction of as much as 60% would be required to achieve summer chlorophyll-a level similar to those of the present-day in Lake Søbygaard, Denmark.

Figure 2.3. Aquatic ecosystem stressors addressed in modelling studies over the 2015–2020 period.

Considering that the effects of climate change on lakes and reservoirs have great ecological significance because they can affect ecosystem's biogeochemistry and ecology, modelling the simultaneous impacts of climate change and eutrophication in a lake system produce model results physically based on climate forcing that can be used as a proxy for future planning. While a rich literature now exists documenting the interactions between climate change and eutrophication, this field is currently under development since many physiological attributes of the phytoplankton are likely to be differentially impacted, therefore there is still a lack of accurate predictions at a species-level and further consequences we might expect with a changing climate (Burford et al., 2020). The interactions between climate change and greenhouse gas emissions via direct temperature effects are also an emerging topic in the field (Bartosiewicz et al., 2019).

Moreover, increasing interest for modelling the impact of other issues was observed related to climate on aquatic ecosystems, such as extreme weather events (*e.g.* Chen et al., 2020; Soares et al., 2019), regime shifts (*e.g.* Kong et al., 2017a), and variations in evaporation rate

(e.g. Helfer et al., 2018). In addition, the biomass and spatial distribution of fish populations in face of unsustainable fishery was assessed in previous studies (e.g. Bhele et al., 2020; Clancey et al., 2017; Goto et al., 2020; Tesfaye and Wolff, 2018). Some importance was given to the modelling of other threats related to pollution (e.g. Eilers et al., 2016), including nutrient loads from different land uses (e.g. Mueller et al., 2019) and erosion (e.g. Sadeghian et al., 2017). Owing to the strong impact on trophic webs and aquatic organisms, and the implications for human health, the simulation of contaminants, including organic compounds (e.g. Amirkani et al., 2016) and hydrocarbons (e.g. Kong et al., 2017b), has emerged in some investigations. Finally, operational strategies of lakes and reservoirs were assessed (e.g. Carr et al., 2020), for instance for optimum water abstraction (e.g. Lindenschmidt et al., 2019) and for hypoxia avoidance (e.g. Weber et al., 2017), both in terms of quantitative and qualitative impacts on aquatic ecosystems.

2.4.5 Coupled models for an interdisciplinary link between catchment, lake and climate

Coupling models, i.e., the output from one model as input for the other, enables the assessment of the potential for synergistic or antagonistic interactions between forcing variables and internal processes. This approach has gained prominence since the 2000s (Jørgensen, 2010) for predictions of lake ecosystems across a variety of scientific disciplines. Hydrodynamic models coupled to biogeochemical models have been increasingly applied. For example, the DYRESM was used coupled to the CAEDYM biogeochemical model, as well as GLM used coupled to the AED biogeochemical model (Table 2.2).

Moreover, using catchment models to generate boundary input conditions for lake models has been a tendency to assess the nutrient loadings and to coordinate environmental strategies. For instance, SWAT (Soil and Water Assessment Tool) was coupled to CE-QUAL-W2, to DYRESM-CAEDYM, and to GLM-AED and PCLake; SWMM (Storm Water Management Tool) was coupled to DYRESM-CAEDYM; MARINA (Model to Assess River Inputs of Nutrients to seAs) was coupled to PCLake; SimplyP was coupled to MyLake; and finally, INCA (Integrated Catchment Model) was coupled to PROTECH (Table 2.2). In addition, some tools have been developed to improve the coupling of lake and catchment models, such as the plugin SWAT2lake (Molina-Navarro et al., 2018) and the Water Ecosystems Tool (Nielsen et al., 2017).

Table 2.2. Coupled models adopted in modelling studies from 2015 to 2020, the percentage of studies that applied this approach, and some references.

Coupled models	Percentage of studies	References
Hydrodynamic-Biogeochemical	19%	GLM-AED: Farrell et al., 2020; Fenocchi et al., 2020; DYRESM-CAEDYM: Hamilton et al., 2015; Takkouk and Casamitjana, 2015; ELCOM-CAEDYM: Curtarelli et al., 2016; Karatayev et al., 2018; DYRESM-WQ: Hamilton et al., 2018; Magee et al., 2018; Delft-WAQ: Guénand et al., 2020; Han et al., 2016; GOTM-PCLake: Andersen et al., 2020; Chen et al., 2020; GLM-PCLake: Rolighed et al., 2016
Catchment-Lake	8%	SWAT-CE-QUAL-W2: Park et al., 2018; Shabani et al., 2017; SWAT-DYRESM-CAEDYM: Me et al., 2018; SWAT-GLM-AED and SWAT-PCLake: Bucak et al., 2018; SWMM-DYRESM-CAEDYM: Silva et al., 2019; MARINA-PCLake: Li et al., 2019; Wang et al., 2019a; SimplyP-MyLake: Messina et al., 2020; INCA-PROTECH: Crossman et al., 2019; Crossman and Elliott, 2018
Climate-Lake	16%	Bueche and Vetter, 2015; Hallnan et al., 2020; Kobler et al., 2019
Climate-Catchment-Lake	4%	Coppens et al., 2020; Couture et al., 2018; Mack et al., 2019; Messina et al., 2020; Moe et al., 2016

Some published articles combined climate models and lake models in order to project future climate-change impacts on water quality (*e.g.* Bueche and Vetter, 2015; Hallnan et al., 2020; Kobler et al., 2019). Additionally, the complex task of coupling climate, catchment and lake models was the focus of some studies (*e.g.* Coppens et al., 2020; Couture et al., 2018; Mack et al., 2019; Messina et al., 2020; Moe et al., 2016) as climate and land-use change drive a suite of stressors that can pose additive, antagonistic or synergistic effects (Birk et al., 2020). For instance, Bucak et al. (2018) linked catchment model outputs to two lake models, and tested the scenarios of five General Circulation Models to assess the effects of climatic and land use changes on phytoplankton and water quality of Lake Beysehir, Turkey. Me et al. (2018) combined a catchment model with a lake water quality model to simulate future climate projections of the trophic state of Lake Rotorua, New Zealand, to better understand the potential for synergistic or antagonistic interactions between regional climate change and nutrient load reductions.

2.4.6 *Multi-model ensemble improving robustness and reliability*

As predicted by Janssen et al. (2015), multi-model ensembles are becoming more common since the first implementation of phytoplankton ensemble modelling revealed a superior

prediction accuracy than any of the individual models (Trolle et al., 2014). Indeed, 19 studies out of 328 (6%) applied ensemble models to compare different dimensions and pathways for representing processes in order to improve the robustness and to account for structural uncertainty, thereby improving the reliability of the outcomes. For example, Kobler and Schmid (2019) found that the mean output of the model ensemble of a two-dimensional model (CE-QUAL-W2) and three one-dimensional models (GLM, Simstrat and MyLake) was able to better reproduce observed ice thickness and ice cover duration than individual model projections in Sihlsee reservoir, Switzerland. Mi et al. (2019) also adopted an ensemble approach to provide more reliable outputs than individual simulations from CE-QUAL-W2 and GLM models, aiming to elucidate the response of winter stratification to future-climate warming combined with different water withdrawal elevations in the Rappbode Reservoir, Germany. The multi-model ensembles applied to a given problem were able to elucidate the strengths and weaknesses of each model, which can benefit researchers for model selection and help developers to enhance the models in the future.

2.4.7 Using high-frequency in-situ measurements

High-frequency sensors monitor the physical, chemical or biological environment by collecting in-situ data at time intervals between seconds and hours through an autonomous equipment to provide data in real-time. There has been a major proliferation of their use to undertake observations for (i) model performance assessment, (ii) model forcing data, and (iii) model calibration and validation. Indeed, from the 328 published studies, 63 of them (19%) used high-frequency sensors for measurements at a time scale from seconds to hours. For example, water column carbon dioxide concentration measurements were performed with a 1-minute time resolution in Lake Kuivajärvi, Finland (Kiuru et al., 2018).

High-frequency measurements realistically capture the ecosystem state when a phenomenon occurs at short-term scales and also provide more reliable data by calculating time-averaged values, thus bridging the gap of discrete traditional manual samplings and ultimately enhancing the development of deterministic models. While manual water sampling is time-consuming, costly and often lacks the appropriate sampling frequency (Marcé et al., 2016), high-frequency sensors can be used in remote locations and severe conditions where conventional

measurements would be complicated. Limitations are most regard to vulnerability to third party action, such as vandalism and robbery, incrustation of solids and micro-organisms, occasional failures in the systems, and maintenance issues that causes gaps in time series data. A transition from manual sampling to high-frequency technologies as a standard tool in water quality monitoring is currently an ongoing trend not only in developed countries. Indeed, although the majority of high-frequency studies were undertaken in Europe and North America, as previously identified by Meinson et al. (2016), the rapid proliferation of such sensors are currently allowing its widespread use in the Middle East, South America, and Africa (Figure 2.4).

Figure 2.4. Countries where high-frequency sensors were used for measurements in published studies from 2015 to 2020.

2.4.8 Using remote sensing data

Remote sensing monitoring relies on optically active constituents of chlorophyll-a, total suspended solids, coloured dissolved organic matter, and water clarity at surface of inland waters (Topp et al., 2020). Satellite remote sensing is increasingly being used in recent years due to cost-efficient data acquisition to complement traditional measurements, thus promoting the development of deterministic lake models by data collection and processing and/or algorithm calibration and validation. Remote sensing is a promise tool for bridging the gap of the often poor spatial characterisation of lakes and reservoirs provided by traditional monitoring as satellite

images retrieve information from the entire aquatic system surface, achieving a large-scale spatial resolution, including for remote and inaccessible locations. Limitations of remote sensing data are mainly attributed to the inherent high dependency of image accuracy on weather conditions, since cloudiness can impair image visualisation, and the large temporal scales with relatively infrequent return periods, which make them more suited to detecting long-term changes as opposed to daily or weekly variation (Topp et al., 2020). Also, it is quite difficult to capture coincident field and satellite observations necessary for model applications when *in-situ* monitoring is taken at low frequencies. Although the use of satellite image requires quite a high level of technical skills (Voinov et al., 2018), new generation of satellites (Salmaso et al., 2018) is helping a broader implementation of satellite image as a data source for modelling applications.

Remote sensing is a contemporary trend in the field. From 328 studies, 30 of them (9%) took advantage of the combining *in-situ* water analysis, deterministic modelling, and remote sensing for investigating biogeochemical processes or for calibration and validation purposes. For example, satellite images were applied to characterise physical and biological patterns in surface conditions of lakes and reservoirs, in terms of sediments (*e.g.* Sadeghian et al., 2017; Zhang et al., 2015a), allocthonous particles (*e.g.* Nouchi et al., 2019), inundation area (*e.g.* Zhang et al., 2015b), surface temperature (*e.g.* Baracchini et al., 2020; Kirillin et al., 2017; Lazhu et al., 2016; Maberly et al., 2020; Thiery et al., 2015; Woolway et al., 2020), ice albedo, cover area, and duration (*e.g.* Lang et al., 2018; Su et al., 2019; Woolway and Merchant, 2019), water surface elevation (*e.g.* Ottlé et al., 2020), light extinction coefficient (*e.g.* Zolfaghari et al., 2017), and chlorophyll-a concentration (*e.g.* Soullignac et al., 2018).

2.4.9 Simulation accuracy

The physical structure of the hydrodynamic variables follows well-understood physical laws, resulting in a relative accurate and precise prediction (Figure 2.5). For instance, in the studies published from 2015 to 2020, the median coefficient of determination of water temperature and level were 0.94 and 0.99, respectively, (*e.g.* Chang et al., 2015; Clancey et al., 2017; Hallnan et al., 2020; Kim et al., 2019; Mi et al., 2020; Zhao et al., 2020). On the other hand, given the inherent complexity of chemical and biological processes, which requires more assumptions and simplifications than hydrodynamic models (Robson, 2014a), the level of

prediction of the chemical and biological state variables is expected to be lower than predictions of the hydrodynamic variables. In fact, model performance has reduced considerably moving from physical to biochemical variables. The median of the coefficient of determination of the chemical and biological variables varied between 0.30 and 0.61 (*e.g.* Brett et al., 2016; Bucak et al., 2018; Crossman and Elliott, 2018; Farrell et al., 2020; Lodhi et al., 2019). In addition, the median coefficient of determination of total nitrogen and nitrate ($R^2 = 0.61$ for both) achieved better prediction capacity than ammonium ($R^2 = 0.35$; *e.g.* Andersen et al., 2020; Chen et al., 2020; Cui et al., 2016; Snorheim et al., 2017), which can be attributed to its more reactive nature, since ammonium can be both assimilated and nitrified, and is produced by decay or organic matter, thereby resulting in a much shorter turnover time in water.

Figure 2.5. Coefficient of determination for hydrodynamic, chemical, and biological state variables in published studies from 2015 to 2020.

Note: WT: water temperature; WL: water level; DO: dissolved oxygen; NH₄: ammonium; NO₃: nitrate; TN: total nitrogen; PO₄: filterable reactive phosphorus; TP: total phosphorus; chl-a: chlorophyll-a.

Surprisingly, chlorophyll-a concentration by groups presented higher median coefficient of determination ($R^2 = 0.54$; *e.g.* Cui et al., 2016; Fadel et al., 2017; Mi et al., 2020) than the total chlorophyll-a concentration ($R^2 = 0.43$; *e.g.* Couture et al., 2018; Mack et al., 2019; Rolighed et al., 2016), in contrast to previous expectations (Shimoda and Arhonditsis, 2016). When simulated as the total concentration, it was expected that models exhibited higher accuracy as measured chlorophyll-a concentration provides a bulk proxy for phytoplankton biomass, with no group or species differentiation. Otherwise, when chlorophyll-a is simulated at sub-group level, model output is compared with chlorophyll-a concentration that is estimated from the count of the number of cells pertaining per each group. However, the chlorophyll-a content per cell presents substantial variations depending on several environmental conditions, such as season, nutrient

availability, light, and cell position in the water column (Rigosi et al., 2010), thus tending to result in poorer performance metrics. Although in some cases the predictive capacity of chlorophyll-a concentration was low, the models generally succeeded to capture seasonal and inter-annual trends, and the pattern of phytoplankton succession.

Current model applications proved that the incorporation of phytoplankton functional groups achieved better predictive capacity than for phytoplankton as total biomass. Moreover, a distinctly higher performance was found when compared to the $r^2 = 0.28$ for aggregated phytoplankton and to the median r^2 varying from 0.07 to 0.53 for different functional groups reported by modelling studies from 1980 to 2012 (Shimoda and Arhonditsis, 2016). Given the currently increasing cyanobacteria blooms globally (Huisman et al., 2018), models have focused on modelling the functional characteristics of dominant species (Hu et al., 2019). Improvements in cyanobacteria field data acquisition and modelling approaches may explain an overall better accurate prediction ability, robustness and reliability in recent studies: (i) in situ fluorescence and pigment analytical analysis to estimate phycocyanin, a specific pigment of cyanobacteria, which can provide better estimates of biomass, biovolume or cell density of this group (Fadel et al., 2017; Mi et al., 2020); (ii) the coupling of hydrodynamic-ecological lake model (Cui et al., 2016); and (iii) the combination of an atmospheric-land-lake modelling approach (Bucak et al., 2018). The simulation of phytoplankton towards specialisation into groups or species seems to be a future tendency, further supported by other recent monitoring technologies, such as high-frequency buoys and remote sensing, and other modelling approaches, such as ensemble models. Performance metrics of the prediction accuracy of modelling other levels of biodiversity, such as bacteria, zooplankton, macrophytes and fish, are rarely reported, which can be attributed to the lack of a detailed knowledge of the aquatic ecology of the study sites and the long-term presence of ecological monitoring.

2.4.10 Towards a systematic methodological protocol of good practices

Recognising the need to establish good modelling practice was already claimed by different authors (Arhonditsis et al., 2006; Hipsey et al., 2020; Schmolke et al., 2010; Shimoda and Arhonditsis, 2016), highlighting the importance of critical methodological steps, such as sensitivity analysis, calibration, validation, and assessment of goodness-of-fit. The adoption of

calibration and validation procedures is in the pathway to no longer be the exception, but the rule in modelling studies of lakes and reservoirs, as the majority of them applied those procedures (Figure 2.6). Some studies did not calibrate the model because the processes and the parameters are well established; instead, they performed a validation or performance assessment (*e.g.* Cardoso-Mohedano et al., 2019; Hamilton et al., 2018; Soullignac et al., 2018). Regarding the validation procedure, 174 over 328 studies (53%) performed this methodological step. However, the present analysis revealed some methodological inconsistency regarding the absent consensus in terms of terminology. For instance, the terms model evaluation (*e.g.* Couture et al., 2015) and validation (*e.g.* Buccola et al., 2016) were used for the same procedure.

Figure 2.6. Percentage of studies that applied a) sensitivity or uncertainty analysis, b) calibration, c) validation, and d) goodness-of-fit metrics in published studies from 2015 to 2020.

There is an increasing portion of the reviewed papers that performed the sensitivity analysis (34%) compared with the 27.5% identified by Shimoda and Arhonditsis (2016). Sensitivity analysis is an important tool for investigating the role of model components by computing the influence of input factors on model outputs, ultimately being useful for scientific discovery, dimensionality reduction, identification of processes, parameters and scales that dominantly control a system, and decision support (Razavi et al., 2021). In general, the analysis can be referred to as ‘Local Sensitivity Analysis’ by conducting a one-at-a-time method that assesses the model output change against variations of a single input, while keeping all others fixed at their initial values, or as ‘Global Sensitivity analysis’ taking into account the joint interaction among input factors when they vary simultaneously within their perturbation range, producing an overall response on the model outputs (Koo et al., 2020). Although the implementation of sensitivity analysis is showing an increasing trend, it should be carefully

evaluated as the local approach is the most largely used technique (Ferretti et al., 2016), including for complex and non-linear models, in circumstances where it has been criticised for providing only a limited indication of model behavior (Saltelli et al., 2019).

Statistics metrics to quantify model performance have been more used than in the 2000s, when few studies published the error between simulated and observed values of the variable of interest (Rigosi et al., 2010). Indeed, 64% of the studies clearly exhibited the statistics metrics of performance to evaluate the goodness-of-fit (Table 2.3). The widely applied metrics were, in the descending order of importance: (1) root mean squared error (RMSE), (2) mean absolute error (MAE), (3) coefficient of determination (R^2), (4) bias, the average difference between simulation and observation data, (5) Nash-Sutcliffe Efficiency (NSE), (6) mean error (ME), (7) Pearson correlation coefficient (r), (8) standard error, (9) percentage of error, (10) Spearman's rank correlation coefficient (ρ), (11) mean absolute percentage error (MAPE), (12) model efficiency (MEFF), and (13) Kling-Gupta Efficiency (KGE).

Table 2.3. Goodness-of-fit (GOF) metrics used to assess model performance in modelling studies from 2015 to 2020, the percentage of studies that used each metric, and some references.

GOF metrics	Percentage of studies	References
RMSE	55%	Brett et al., 2016; Carr et al., 2020; Lee et al., 2018
MAE	23%	Buccola et al., 2016; Liu et al., 2019; Noori et al., 2015
R^2	19%	Kim et al., 2019; Lodhi et al., 2019; Mesquita et al., 2020
Bias	13%	Helfer et al., 2018; Me et al., 2018; Shabani et al., 2017
NSE	11%	Magee and Wu, 2017; Mi et al., 2020; Park et al., 2017
ME	6%	Cui et al., 2016; Prats and Danis, 2017; YoosefDoost et al., 2020
r	6%	Feldbauer et al., 2020; Silva et al., 2019
Standard error	3%	Choulga et al., 2019; Han et al., 2016; Kienel et al., 2017
Error (%)	2%	Andersen et al., 2020; Chen et al., 2016; Wilson et al., 2020
ρ	2%	Farrell et al., 2020; Magee et al., 2019
MAPE	1%	Fadel et al., 2017; Mellios et al., 2015
MEFF	0.3%	Bruce et al., 2018
KGE	0.3%	Ladwig et al., 2020

Most of the studies applied the combination of at least two metrics, enhancing a comprehensive evaluation of models by minimizing potential inconsistencies arising from human judgment (Bennett et al., 2013). Some studies exhibited solely a visual performance analysis (*e.g.* Abed et al., 2019; Haddad et al., 2015; Moridi, 2018), which is adequate only for highly complex situations or when data are scarce or unreliable. In an effort to make models more transparent,

future model development should aim to incorporate automatic goodness-of-fit metrics calculation using software tools, as proposed by Alexandrov et al. (2011).

2.5 Summary and conclusions

Deterministic lake models have undergone a continuous refinement since their development, triggered by trends in science, technology and society, to accomplish the difficult task to predict ecosystem behavior. There is significant ongoing effort to address the challenges pointed out by previous reviews, for instance, in terms of a better collaboration between the scientific community and the use of multi-model ensemble. In an overall conclusion from the literature published over the last six years, (1) model applications across broad ranges of time (from months to decades) and spatial (local, regional and continental) scales, covering multiple study sites, are an increasing trend over the last few years (Figure 2.7a); (2) phytoplankton biomass have been consistently simulated as functional groups or species (Figure 2.7b) supported by improved prediction accuracy than its simulation as the total biomass, which can be considered as the major advance in the past few years; (3) novel modelling approaches, such as coupling models (Figure 2.7c) and multi-model ensemble (Figure 2.7d) were envisioned in the past and now are gaining importance to account for structural uncertainty and to improve the reliability of the model outcomes; (4) the proliferation of high-frequency sensors (Figure 2.7e) for sub-hourly field measurements and the usage of satellite remote images (Figure 2.7f) has been overcoming the challenge to be used in developing countries, thus finding global application for improving data acquisition for model initialisation, forcing data inputs, calibration, and validation; and (5) there is still a considerable gap for modelers to adopt a systematic protocol of good practices.

Figure 2.7. Temporal evolution over the 2015–2020 period of a) modelling multiple study sites, b) modelling groups of phytoplankton, c) coupling models, d) multi-model ensemble, e) high-frequency monitoring, and f) use of remote sensing.

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3

A parameterization strategy for hydrodynamic modelling of a cascade of poorly monitored reservoirs in Brazil

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The scarcity of long time-series of water temperature for tropical reservoirs, usually available at a low frequency of measurements, represents a serious constraint for the understanding of their thermal behavior. Hydrodynamic models become a powerful tool for that understanding through a qualitative approach. In this study, the one-dimensional General Lake Model (GLM) was applied to hindcast multiannual temperature profiles of a cascade system of six reservoirs located in southeast Brazil over a period of eight years. The model parameters were calibrated and validated by field data for four reservoirs. To overcome the challenge of exploring hydrodynamics in two reservoirs with a lack of measured temperatures, a parameterization strategy was applied to accomplish a better simulation by the estimation of potential sensitive parameters through regression curves. It is expected that this approach can be extended to other tropical reservoirs whenever field data is not available for the calibration procedure.

Keywords: thermal dynamics, stratification, one-dimensional vertical model, GLM, low-latitude reservoirs.

3.1 Introduction

The number of man-made lakes has increased continuously, mainly after the 1950s, and currently accounts for 6% of the total inland water surface area (Downing et al., 2006). The growing need for water has resulted in the construction of reservoirs beyond Europe and the United States, in several low-latitude countries. According to the International Commission on Large Dams, there are 59,000 reservoirs of more than 15 m depth, and more than half of them (53%) are located in China, India, Brazil, and South Africa (ICOLD, 2019). Nowadays, reservoirs are highly valued as they serve multiple purposes and provide numerous ecosystem services, such as fishery, flood control, recreation, nutrient uptake, sediment stabilisation, and navigation (Schallenberg et al., 2013), beyond the historical uses for water supply and hydropower generation. They make a significant contribution to the efficient management of finite water resources that are subject to large seasonal fluctuations.

Compared to lakes, reservoirs have been poorly documented. In the tropics, it is in part because they are located far from the most active research centers, causing a corresponding gap in limnological investigations. As a result, 41% of the 54 most-large low-latitude reservoirs have not yet been subject to basic limnological studies (Winton et al., 2019). Low-latitude reservoirs often lack long-term series of temperature profiles, an easily measurable *in-situ* data. Many reservoirs, including the current study site, only have reliable data sets for irregular periods.

In such context, hydrodynamic models are fundamental tools to support the comprehension of lake's dynamics since they can simulate and predict multiannual cycles of water temperature, providing additional information to field measurements on mixing extent and stratification periods. They simulate the vertical thermal dynamics which have important implications for the biogeochemical and ecological cycles, including renewal of dissolved oxygen in the hypolimnion, the release of nutrients from the sediments, as well as the control of timing, magnitude and composition of phytoplankton blooms (Cao et al., 2016). Therefore, given the paramount importance of the thermal structure for lentic aquatic ecosystems, for both field biologists interested in ecosystem ecology and engineers charged with the management of reservoirs, hydrodynamic models have become more abundant and sophisticated since the early models developed in the 1970s (Imberger, 1985). They have been used for various purposes, such as to evaluate the response to different wind conditions (Mi et al., 2018), to evaluate the impacts

of storm water runoff on lake ecosystems (Silva et al., 2019), to select the withdrawal depth (Kerimoglu and Rinke, 2013) and to forecast the mixing regime under climate change scenarios (Fenocchi et al., 2018).

It is expected that as the population grows, simultaneous competing water uses in addition to increased nutrient loading will intensify anthropogenic pressures on low-latitude reservoirs, increasing their vulnerability globally (Folke et al., 2004). Hence, the understanding of their thermal behavior is essential to assist in planning mitigation and adaptation strategies. In this context, the main objective of this study was to deepen the knowledge on the thermal behavior across six reservoirs using them as representative of the sub-tropical ones by applying the well-established 1D hydrodynamic model GLM over an 8-year period (2009–2016). The specific aims were as follows: (1) to simulate multiannual cycles of the thermal behavior; (2) to perform a sensitivity analysis of parameters and variables influencing water level and water temperature; (3) to calibrate and validate the model for simulating both the water temperature and the water balance; and (4) to provide an experimental calibration strategy for two reservoirs lacking water temperature data to illustrate how hydrodynamic modelling can provide surrogates for missing data. We expect that the results provide useful guidance for modelling efforts of poor monitored reservoirs, especially in low-latitude countries.

3.2 Materials and Methods

3.2.1 Study site

The study site is located in southeast Brazil and comprises a sub-tropical cascade system along the Tietê River, composed by the following six reservoirs, from upstream to downstream: Barra Bonita (BB), Bariri (BA), Ibitinga (IB), Promissão (PR), Nova Avanhandava (NA) and Três Irmãos (TI). The reservoirs were built from 1964 to 1991, and they were hydrologically and operationally connected through the cascade for attending the common goal of electricity generation, taking advantage of the cumulative effect of flow regulation to attend country demand. Nowadays, the reservoirs are intended for multiple uses (see Table A.1 in Appendix A). This cascade system was chosen because it is composed of reservoirs representing many others of

tropical regions, where water temperature is warm throughout the year. In addition, the reservoirs have a varied range of morphometric features, such as mean depth from 8.6 m to 17.2 m, surface area from 45 km² to 654 km², and volume from 0.61×10⁹ m³ to 11.46×10⁹ m³ (Table 3.1). High-resolution meteorological stations are situated near them, gauged inflows and outflows are available, and water quality stations are available for some reservoirs (Figure 3.1).

Table 3.1. Physical characteristics of each reservoir.

Reservoir	Elevation (m)	Mean depth (m)	Surface area at crest (km ²)	Maximum volume (10 ⁹ m ³)	Residence time (days)	Wind fetch (km)	Latitude	Longitude
BB	451.5	10.2	272	2.98	139	9.3	20°31'11"S	48°32'04"W
BA	427.5	8.6	45	0.61	17	3.8	22°09'14"S	48°45'13"W
IB	404.0	8.6	94	0.98	25	5.5	21°45'30"S	48°59'29"W
PR	384.0	12.0	538	7.41	160	13.1	21°17'51"S	49°46'47"W
NA	358.0	13.0	195	2.72	54	7.9	21°07'02"S	50°12'05"W
TI	328.0	17.2	654	11.46	442	14.4	20°40'10"S	51°17'57"W

Note: Wind fetch (F) was calculated from surface area (A_s) as $F = \sqrt{A_s/\pi}$ (Hipsey et al., 2019).

Figure 3.1. Cascade system location and its monitoring stations. Each reservoir is associated with a two-letter code: Barra Bonita (BB), Bariri (BA), Ibitinga (IB), Promissão (PR), Nova Avanhandava (NA), and Três Irmãos (TI).

Land use in their catchment basin is characterised by urban areas with more than 24 million inhabitants (IBGE, 2019) and intensive agriculture, mainly sugarcane (Camara and Caldarelli, 2016). The climate in the region is sub-tropical (Köppen, 1948) with a rainy season from October to March and a dry season from April to September. The mean annual rainfall from 1981 and 2010 was 1,406 mm, the mean air temperature was 22.6 °C, with a minimum of 14.0 °C in July and a maximum of 30.4 °C in October (INMET, 2019).

3.2.2 Hydrodynamic model description

The hydrodynamic one-dimensional General Lake Model (GLM, v. 2.2.0, Hipsey et al., 2019) was applied to predict the thermal structure of each reservoir. GLM was selected mainly because of its good performance documented in several investigations all around the world (e.g. Bruce et al., 2018; Bueche et al., 2017). The model assumes that horizontal gradients are negligible and it computes the vertical profiles of temperature, salinity, and density over time in lentic water bodies such as lakes, reservoirs, mining pit lakes, wastewater ponds, and urban wetlands, whether shallow and well mixed or deep and stratified. GLM simulations are based on parameterizations of mixing processes, surface dynamics, energy budget, and water balance. The algorithms are based on equations defined by Hamilton and Schladow (1997) and by Imberger and Patterson (1981).

The occurrence of thermal stratification and vertical mixing processes is based on the energy balance between the kinetic energy and the internal potential energy of the water body. The model assumes the occurrence of mixing whenever available kinetic energy exceeds the potential energy required to keep stratification. The available kinetic energy is calculated from wind stirring, shear production between layers, convective overturn, and Kelvin-Helmholtz billowing. The mixing process ends when the internal kinetic energy is insufficient to overcome the stored potential energy. Then, the thermal stratification process begins (Hipsey et al., 2019).

3.2.3 Required input data for modelling

GLM requires the following site information as input data: morphometry, meteorological time-series, and hydrological time-series. Obtaining and processing of input data required by GLM is described in the following paragraphs.

(i) The hypsographic curve of each reservoir was provided by bathymetric surveys from previous studies. A comparative plot of the hypsographic curves for all reservoirs shows diversity in reservoir size and volume (Figure 3.2).

Figure 3.2. Hypsographic curves for all reservoirs.

(ii) High-resolution meteorological data from terrestrial-based stations were available. Hourly measurements of air temperature, wind speed, solar radiation, air relative humidity, and rainfall were obtained from five monitoring stations operated by the National Institute of Meteorology (INMET, 2020; red markers in Figure 3.1, Table A.2 in Appendix A). The meteorological variables were measured as required by GLM: air temperature, air relative humidity and wind speed were measured 10 m above ground; solar radiation and rainfall were measured at the ground. Wind direction, although not required by GLM, is presented in Figure A.1 in Appendix A.

For PR and NA reservoirs, meteorological data were obtained from one station, the closest one to both reservoirs. The missing values (Table A.3 in Appendix A) of air temperature, solar radiation, and air relative humidity were filled by linear regression with data from the meteorological station with the highest correlation coefficient (Table A.4 in Appendix A). When data was not available for both stations, remaining data gaps were filled by the linear regression with the station of the following highest correlation coefficient and then successively. In face of the weak linear correlation between measured data in different meteorological stations regarding wind speed ($r < 0.54$) and rainfall

($r < 0.27$), the missing data were filled by linear interpolation. When data gaps were longer than ten consecutive hours, instead of using the linear interpolation method, gaps were filled by the mean monthly value. Cloud cover data was not available and it was estimated by GLM based on the Bird Clear Sky insolation model (Bird, 1984), which compares the measured and theoretical clear-sky solar irradiance in order to approximate the cloud cover fraction.

(iii) Daily hydrological data has been provided by the National Water Agency (ANA, 2018). Gaps in daily inflow and outflow volume were rare (less than 0.6% of total data), and they were filled by linear interpolation. Inflow temperature data was measured every two months by the Environmental Company of the State of São Paulo (CETESB, 2019) for all reservoirs (yellow circles in Figure 3.1), except for IB. For this reservoir, data from BA was adopted. Inflow temperature was then converted into daily frequency through linear regression between bi-monthly inflow temperature and minimum air temperature (BB, BA, PR and TI), mean air temperature (IB) and maximum shortwave radiation (NA). The meteorological variable used in the linear regression was selected from the highest correlation coefficient with bi-monthly inflow temperatures (r values between 0.56 and 0.91; see Figure A.2 in Appendix A). As inflow salinity is not monitored, it was estimated from electrical conductivity data. Due to its low value (below 0.2 g kg^{-1}), a constant value was assumed for the entire simulation period. Figure A.3 in Appendix A presents monthly means and range of input data for the six reservoirs. The description of the applied input data is summarised in Table 3.2.

3.2.4 Required in-situ data for modelling

The vertical profile of temperature and salinity in the reservoir, as well as Secchi depth and water level, are also required for parameterization, setting initial conditions and performing model assessment.

Table 3.2. Summary of input data type, frequency and source in each reservoir.

Input data	Type of data	Frequency	Provided by
<i>(i) Morphometry</i>			
Elevation x area	Digitised	Once	Previous studies
<i>(ii) Meteorology</i>			
Air temperature	Gauged	Hourly	(INMET, 2020)
Wind speed	Gauged	Hourly	(INMET, 2020)
Solar radiation	Gauged	Hourly	(INMET, 2020)
Air relative humidity	Gauged	Hourly	(INMET, 2020)
Rainfall	Gauged	Hourly	(INMET, 2020)
Cloud cover	Estimated by GLM	Hourly	Not available
<i>(iii) Hydrology</i>			
Inflow discharge	Gauged	Daily	(ANA, 2018)
Inflow temperature	Gauged/Estimated	Every two months	(CETESB, 2019)
Inflow salinity	Gauged/Estimated	Every two months	(CETESB, 2019)
Outflow discharge	Gauged	Daily	(ANA, 2018)

(i) The vertical profile of water temperature in the middle of the reservoirs' bodies was measured every two months as follows (see purple triangles in Figure 3.1): (a) for BB, it was measured by CETESB (2019), in 1 m depth steps down to the bottom; (b) for IB, it was measured by the National Institute of Space Research (Cairo, 2015), continuously from surface until 2 m above the bottom, from November 2013 to September 2014; and (c) for PR and TI, it was measured only at the surface by CETESB.

(ii) The electrical conductivity was measured every two months only at surface for BB, PR and TI, and along the water column for IB reservoir.

(iii) Secchi depth was measured every two months for BB (CETESB, 2019) and IB (Cairo, 2015), and twice a year in 2008 and 2009 for PR and TI (Santos, 2010).

(iv) The water level of all six reservoirs was daily gauged by ANA (2018).

For BA and NA reservoirs, there was no field data available for the simulation period. The description of the field data applied for initial conditions and modelling assessment during calibration and validation is summarised in Table 3.3.

Table 3.3. Summary of field data type, frequency, source, and depth of measurement in each reservoir.

Field data	Type of data	Frequency	Provided by	Vertical Resolution
<i>(i) Vertical profile of water temperature</i>				
BB	Measured	Every two months	(CETESB, 2019)	1 m interval
IB	Measured	Every two months	(Cairo, 2015)	Continuously
PR, TI	Measured	Every two months	(CETESB, 2019)	At surface
BA, NA	Not available	Not available	Not available	Not available
<i>(ii) Salinity</i>				
BB	Estimated	Every two months	(CETESB, 2019)	At surface
IB	Estimated	Every two months	(Cairo, 2015)	Continuously
PR, TI	Estimated	Every two months	(CETESB, 2019)	At surface
BA, NA	Not available	Not available	Not available	Not available
<i>(iii) Secchi depth</i>				
BB	Measured	Every two months	(CETESB, 2019)	-
IB	Measured	Every two months	(Cairo, 2015)	-
PR, TI	Measured	Twice a year	(Santos, 2010)	-
BA, NA	Not available	Not available	Not available	-
<i>(iv) Lake level</i>				
BB, BA, IB, PR, NA, TI	Gauged	Daily	(ANA, 2018)	-

3.2.5 Modelling setup and baseline simulations

The GLM simulations were conducted at an hourly time step. A baseline simulation was run for nine years from 2008 to 2016 and a generic model parameterization (Table 3.4) was set according to Hipsey et al. (2019). The period of simulation was run from the first day with field measurements for BB, PR, and TI reservoirs. For the other reservoirs, the first day of simulation was set as 1st January 2008. The initial temperature and salinity profiles in the reservoir were taken as follows: for BB, the vertical profile was taken from field measurements in the first simulation day; for PR and TI, the initial condition was set only at the surface; for BA, IB, and NA, both temperature and salinity were set only at the surface as the mean value computed from the measured values in the other reservoirs.

The light extinction coefficient (K_W) was determined for BB, IB, PR, and TI reservoirs from the mean value of measured Secchi depth ($\overline{SD}$) and assuming $K_W = 1.7/\overline{SD}$ according to Poole and Atkins (1929). For BA and NA, the light extinction coefficient was set as 0.2 m^{-1} (Table 3.4). The initial conditions for each reservoir are summarised in Table 3.5. The software R 3.4.0 (R Core Team, 2017) was applied to simulate and analyze modelling results using the packages GLMr (Hipsey et al., 2014) and glmtools (Read et al., 2014).

Table 3.4. Initial values of GLM parameters for the baseline simulation (Hipsey et al., 2019).

Symbol	Description	Initial value	Calibration range
K_W	Light extinction coefficient (m^{-1})	0.2	-
C_K	Mixing efficiency for convective overturn	0.20	0.10–0.30
C_W	Mixing efficiency for wind stirring	0.23	0.11–0.35
C_S	Mixing efficiency for shear production	0.30	0.15–0.45
C_T	Mixing efficiency for unsteady turbulence	0.51	0.25–0.77
C_{KH}	Mixing efficiency for Kelvin-Helmholtz turbulent billows	0.30	0.15–0.45
C_{HYP}	Mixing efficiency for hypolimnetic turbulence	0.50	0.25–0.75
ce	Bulk aerodynamic coefficient for latent heat transfer	0.0013	0.0007–0.0017
ch	Bulk aerodynamic coefficient for sensible heat transfer	0.0013	0.0007–0.0020
cd	Bulk aerodynamic coefficient for transfer of momentum	0.0013	0.0006–0.0034

Note: The initial value of the light extinction coefficient was only applied when Secchi measurements were not available.

Table 3.5. Initial conditions for the baseline simulation adopted for each reservoir.

Reservoir	Simulation first day	Water temperature and salinity	Light extinction coefficient
BB	15 th January 2008	Measured vertical profile	Calculated
BA	1 st January 2008	Estimated at surface	0.2 (Hipsey et al., 2019)
IB	1 st January 2008	Estimated at surface	Calculated
PR	12 th February 2008	Measured at surface	Calculated
NA	1 st January 2008	Estimated at surface	0.2 (Hipsey et al., 2019)
TI	12 th February 2008	Measured at surface	Calculated

3.2.6 Sensitivity analysis

A sensitivity analysis was applied for the baseline simulation to reduce the effort of the model calibration process. The one-at-a-time method was adopted, through which the model was first run with the initial parameter values (Table 3.4) and then by successive runs in which every parameter value was either increased or decreased by $\pm 10\%$ of initial values while holding constant the remaining parameters. The sensitivity of water level to ten parameters presented in Table 3.4 was evaluated for all reservoirs, and the sensitivity of water temperature was evaluated only for those with available data (BB, IB, PR, and TI) at all available depths. Given the uncertainties in wind speed and hydrological data, wind speed factor was included in the sensitivity analysis with a range of $\pm 30\%$, and inflow and outflow factors were included with a range of $\pm 10\%$. The objective was to account for the distance between meteorological station and reservoirs as well as wind sheltering effects, and to account for groundwater inflows, smaller tributaries or seepage.

The normalised sensitivity index (SI) was calculated for each selected parameter according to:

$$SI = \frac{\Delta Y/Y}{\Delta X/X} \quad (3.1)$$

where Y is the model performance for the reference value X of the parameter, which has a variation ΔX generating a model performance variation ΔY . The model performance was assessed through the root mean square error (RMSE):

$$RMSE = \sqrt{\frac{\sum_{i=1}^N (S_i - O_i)^2}{N}} \quad (3.2)$$

where N is the number of observations, O_i and S_i are the “ i^{th} ” observed and simulated data, respectively.

3.2.7 Calibration and validation

A calibration procedure was performed to simultaneously optimise both water level and temperature for the reservoirs with measured field data (BB, IB, PR, and TI). For BB, PR, and TI reservoirs, a 5-year calibration period was determined from the first day of the baseline simulation to 31st December 2012. For IB reservoir, the simulation was calibrated from 1st November 2013 to 18th September 2014. For BA and NA, due to the lack of measured field data, the model was calibrated only regarding water level for the period from 1st January 2008 to 31st December 2012. The initial conditions were set as the same adopted for the baseline simulation. The first year of simulation (2008) was considered as a warm-up period to avoid uncertainties related to the initial conditions, thus it was not included in the performance assessment.

The automatic calibration procedure was executed using the package glmGUI (Poschlod et al., 2018), which implements the brute-force method for all possible combinations and permutations of the selected parameters to gradually improve them until the simulation results reached the lowest deviations between simulated and measured water level and water temperature. The selection of parameters to be calibrated was based on the sensitivity analysis. Parameters with $SI > 0.01$ were calibrated to optimise both water level and temperature

simultaneously. The initial values of mixing parameters were tested for a percentage range of $\pm 50\%$, considering that those values can be significantly different in a tropical region from the initial ones, usually estimated in a temperate zone (Table 3.4). The surface transfer coefficients were calibrated for ranges experimentally determined in previous studies (Brutsaert, 1982; Xiao et al., 2013): $0.7\text{--}1.7 \times 10^{-3}$ for the latent heat transfer coefficient (ce), $0.7\text{--}2.02 \times 10^{-3}$ for the sensible heat transfer coefficient (ch), and $0.6\text{--}3.4 \times 10^{-3}$ for the momentum coefficient (cd) (Table 3.4). The calibration range for wind factor was set between 0.7 and 1.3 ($\pm 30\%$), and for inflow and outflow factors was set between 0.9 and 1.1 ($\pm 10\%$).

The best-fitted model of water level and temperature was validated using the calibrated parameter values and an independent set of data for a 4-year period from the first day with field measurements in 2013 to 31st December 2016 for BB, PR and TI reservoirs. The initial conditions in these reservoirs were taken from field measurements in the first simulation day. The validation of water temperature was not performed for IB reservoir due to the absence of data beyond the dataset applied for the calibration. In this manner, for BA, IB and NA, the model was validated only regarding water level for the period from 1st January 2013 to 31st December 2016. A summary of the periods applied for calibration and validation for each reservoir is presented in Table 3.6.

The objective function used for both calibration and validation procedures was the RMSE. The model performance was also assessed through the linear correlation coefficient (r) computed from simulated and measured water level and water temperature and the RMSE normalised by the data range (nRMSE) in order to standardise comparisons among reservoirs. The abovementioned error metrics were calculated as follows:

$$r = \frac{\sum_{i=1}^N (S_i - \bar{S})(O_i - \bar{O})}{[\sum_{i=1}^N (S_i - \bar{S})^2 \sum_{i=1}^N (O_i - \bar{O})^2]^{1/2}} \quad (3.3)$$

$$nRMSE = \frac{RMSE}{O_{max} - O_{min}} \quad (3.4)$$

where N is the number of observations, O_i and S_i are the “ith” observed and simulated data, $\bar{O}$ and $\bar{S}$ are the mean observed and simulated data, and O_{max} and O_{min} are the maximum and minimum observed data, respectively.

Table 3.6. Simulation periods for calibration and validation regarding water level and temperature.

Reservoir	Calibration	Validation
BB	From 15 th Jan 2008 to 31 st Dec 2012	From 29 th Jan 2013 to 31 st Dec 2016
IB	From 1 st Jan 2008 to 31 st Dec 2012*	From 1 st Jan 2013 to 31 st Dec 2016*
	From 1 st Nov 2013 to 18 th Sep 2014	
PR	From 12 th Feb 2008 to 31 st Dec 2012	From 28 th Jan 2013 to 31 st Dec 2016
TI	From 12 th Feb 2008 to 31 st Dec 2012	From 26 th Feb 2013 to 31 st Dec 2016
BA, NA	From 1 st Jan 2008 to 31 st Dec 2012*	From 1 st Jan 2013 to 31 st Dec 2016*

Note: * only regarding water level.

3.2.8 Parameterization strategy for non-monitored reservoirs

Since there is no field data for the calibration procedure of water temperature for BA and NA, linear regression curves were constructed aiming at the estimation of the most sensitive parameters, as indicated in the sensitivity analysis. A linear correlation analysis was performed between the calibrated parameter values for BB, IB, PR, and TI, and their morphometric and meteorological variables. The following variables were selected based on their physical relationship with model parameters as reported in previous studies: (i) mean wind speed computed from 2008 to 2016, considering the calibrated wind factor (m s^{-1}), (ii) fetch (F, km), calculated from surface area (A_s) as $F = \sqrt{A_s/\pi}$ (Hipsey et al., 2019), (iii) mean depth (m), (iv) surface area (km^2), and (v) perimeter (km) as measure of reservoir's size.

Wind speed data and reservoir morphometric characteristics such as, mean depth, surface area, perimeter and fetch, are in general easily obtained and are available for the reservoirs of this study. Furthermore, their relationship with hydrodynamic processes in lentic systems was extensively presented in previous studies (Ataktürk and Katsaros, 1999; Harbeck, 1962; Heikinheimo et al., 1999; Kwan and Taylor, 1994; Schertzer et al., 2003; Strub and Powell, 1987; Venäläinen et al., 1998; Xiao et al., 2013).

Based on the curves with the highest correlation, in an attempt to minimise uncertainties regarding the adoption of parameter values suggested in the literature, the best-fitted linear regression was obtained for estimating the parameter values for BA and NA, the reservoirs without measured field data.

3.2.9 Hydrodynamic metrics

Hydrodynamic metrics were calculated based on the modelling results using the package rLakeAnalyzer (Winslow et al., 2018). In this study, mixing was assumed when the temperature difference (ΔT) between the surface and the bottom layers was smaller than 2.0 °C (Lewis, 2000), otherwise it was the stratification condition. The onset of stratification was the first day when $\Delta T > 2$ °C for a period longer than 96 h. Epilimnion and hypolimnion were defined, respectively, as the region above and below the thermocline, where the density gradient was lower than 0.1 kg m⁻³ per meter (Winslow et al., 2018).

The Schmidt's Stability Index (S_T ; J m⁻²) indicates the intensity of stratification, i.e., the dynamic stability of the system, by calculating the resistance to mechanical mixing due to the potential energy inherent in the stratification of the water column (Idso, 1973). S_T values represent the amount of work required to mix the entire water body to a uniform density. In this manner, the higher is S_T , the higher the strength of stratification is. Schmidt's Stability Index is calculated as:

$$S_T = \frac{g}{A_s} \int_0^{z_D} (z - z_v)(\rho_i - \rho_z) A_z dz \quad (3.5)$$

where g is the acceleration due to gravity (m s⁻²), A_s is the reservoir surface area (m²), A_z is the area of the reservoir at depth z (m²), z_D is the maximum depth of the reservoir (m), z_v is the depth of the volume center of the reservoir (m), ρ_i is the mean density value (kg m⁻³), and ρ_z is the water density at depth z (kg m⁻³).

The Wedderburn Number (W) describes the likelihood of water upwelling under stratified conditions. W was applied as an index of 1D suitability as it is a relative measure between the vertical stratification strength against the horizontal wind energy at surface. The 1D assumption is suitable for $W \gg 1$, when the mixed layer deepens slowly (Imberger and Patterson, 1990); otherwise ($W < 1$), there is a high potential for mixing events, predicting wind-induced internal waves. The Wedderburn number can be written as:

$$W = \frac{g' z_e^2}{u_*^2 L_s} \quad (3.6)$$

where $g' = g \times \Delta\rho/\rho_h$ is the reduced gravity (m s^{-2}) due to the difference $\Delta\rho$ between the hypolimnion density (ρ_h) and epilimnion density, z_e is the depth of the mixed layer (m), L_s is the reservoir fetch length (m) and u_* is the water friction velocity due to wind stress (m s^{-1}).

3.3 Results

3.3.1 Sensitivity analysis

The sensitivity analysis highlighted some variability across the ten parameters and three input data factors. As expected, the water level had the highest sensitivity to perturbations in inflow and outflow factors (Figure 3.3a). Additionally, there was a high level of sensitivity for the latent heat transfer coefficient (ce) and the wind factor. The sensitivity analysis regarding the water temperature revealed a consistent level of sensitivity for all reservoirs to the three coefficients related to surface heat exchange (latent heat transfer coefficient – ce , sensible heat transfer coefficient – ch , and momentum coefficient – cd), and to three input data factors (wind, inflow, and outflow factors, Figure 3.3b). For both water level and water temperature, there was little sensitivity to perturbations in mixing parameters.

Figure 3.3. Sensitivity Index for a) water level and b) water temperature.

Note: K_W : light extinction coefficient, ch : sensible heat transfer coefficient, ce : latent heat transfer coefficient, cd : momentum coefficient, C_K : efficiency of convective overturn, C_W : efficiency of wind stirring, C_S : efficiency of shear production, C_T : efficiency of unsteady turbulence, C_{KH} : efficiency of Kelvin-Helmholtz billowing, C_{HYP} : efficiency of hypolimnetic turbulence.

3.3.2 Model performance

The calibrated inflow and outflow factors that achieved the lowest discrepancies between simulated and measured water levels in the reservoirs ranged from 1.00 to 1.06 (Table 3.7). The optimisation of those factors enabled a fair estimate of the water balance, and the model succeeded in the prediction of the water level. The seasonal variations were simulated correctly, supporting the model's ability to compute the water balance. GLM tended to produce positive bias regarding the water level of BA and TI, overestimating the total volume. The RMSE varied from 0.12 m to 1.56 m ($n = 2922$) over the simulation period (see Figure A.4 in Appendix A), and r varied from 0.49 to 0.99 (see Figure A.5 and Table A.5 in Appendix A).

Table 3.7. Values of GLM parameters and input data factors for each reservoir.

Parameter/Factor	BB	BA	IB	PR	NA	TI
K_W	1.30	0.20	1.32	0.78	0.20	0.57
C_K	0.20	0.20	0.20	0.20	0.20	0.20
C_W	0.23	0.23	0.23	0.23	0.23	0.35
C_S	0.30	0.30	0.30	0.30	0.30	0.30
C_T	0.51	0.51	0.51	0.51	0.51	0.25
C_{KH}	0.30	0.30	0.30	0.30	0.30	0.30
C_{HYP}	0.50	0.50	0.50	0.50	0.50	0.50
ce	0.0007	0.0007	0.0007	0.0007	0.0011	0.0017
ch	0.0020	0.0013	0.0013	0.0020	0.0016	0.0020
cd	0.0013	0.0010	0.0011	0.0010	0.0011	0.0008
Inflow factor	1.01	1.00	1.00	1.00	1.00	1.06
Outflow factor	1.06	1.00	1.00	1.00	1.00	1.04
Wind speed factor	1.300	1.000	0.824	0.735	1.000	0.837

Note: Green cells were calculated from Secchi depth measurements; blue cells were calibrated ($SI > 0.01$); orange cells were estimated values through the parameterization strategy; and grey cells were assumed as initial values ($SI \leq 0.01$). K_W : light extinction coefficient, C_K : efficiency of convective overturn, C_W : efficiency of wind stirring, C_S : efficiency of shear production, C_T : efficiency of unsteady turbulence, C_{KH} : efficiency of Kelvin-Helmholtz billowing, C_{HYP} : efficiency of hypolimnetic turbulence, ce : latent heat transfer coefficient, ch : sensible heat transfer coefficient, cd : momentum coefficient.

For BB and PR reservoirs, three parameters (sensible heat transfer coefficient – ch , latent heat transfer coefficient – ce , and momentum coefficient – cd) and wind factor were calibrated instead of ten according to the sensitivity analysis; for IB reservoir, ce , cd , wind factor, and the light extinction coefficient (K_W) were calibrated; and for TI reservoir, mixing efficiency for wind stirring (C_W) and mixing efficiency for unsteady turbulence (C_T) were calibrated in addition to the aforementioned ones. Table 3.7 presents the optimised values that reached the best simulation results. Water temperatures were simulated accurately for the calibration period (mean RMSE of 1.49 °C) as well as for the validation period (mean RMSE of 1.65 °C; see Table A.6 in Appendix

A). Positive and negative deviations were observed for daily temperatures, but they were generally small (see Figure A.6 in Appendix A). Model efficiency for water temperature was similar across the four reservoirs, and correlations were quite high (Figure 3.4), indicating a robust fit for GLM.

Figure 3.4. Linear correlation between simulated and measured water temperature for a) Barra Bonita, b) Ibitinga, c) Promissão, and d) Três Irmãos reservoirs. The black line represents the identity line (1:1).

3.3.3 Parameterization strategy for non-monitored reservoirs applying regression curves

For BA and NA reservoirs, the lack of field data prevented the calibration procedure for the simulation of water temperature. Assuming that the parameters related to surface heat exchanges (latent heat transfer coefficient – ce , sensible heat transfer coefficient – ch , and momentum coefficient – cd) and the wind factor would present a high sensitivity index for these reservoirs as they presented for the other ones, their values were linear correlated to known morphometric and meteorological variables. Although the light extinction coefficient (K_w) showed a high SI for IB and TI reservoirs, it was not included in the parameterization strategy due to the unavailability of water quality data potentially related to K_w , such as suspended solids concentration, phytoplankton biovolume or chlorophyll-a concentration. Inflow and outflow factors were not included because water level data was available for their calibration in BA and NA reservoirs.

Linear correlation analysis revealed that surface heat exchange parameters were significantly correlated to mean wind speed, reservoir's mean depth, perimeter and fetch (Table 3.8). The correlation of the three parameters with the surface area was not significant. The latent heat transfer coefficient (ce) showed the highest linear correlation to the mean depth, the sensible heat transfer coefficient (ch) was mostly correlated to the reservoir's fetch, and the momentum

coefficient (cd) presented the highest linear correlation with wind speed. From the best-fitted relationships, the following regression equations were obtained:

$$ce \times 10^{-3} = 0.117055\bar{H} - 0.462997 \quad (3.7)$$

$$ch \times 10^{-3} = 0.075702F + 1.035025 \quad (3.8)$$

$$cd \times 10^{-3} = 0.181924U_{10} + 0.726093 \quad (3.9)$$

where $\bar{H}$ is the mean depth (m), F is the fetch (km) and U_{10} is the mean wind speed. The equations among the parameters and the other variables are presented in Table A.7 in Appendix A.

Table 3.8. Linear correlation between surface transfer coefficients and reservoir's variables.

Variables	ce	ch	cd	wind factor
Calibrated mean wind speed	-0.57*	0.19*	0.88*	0.92
Fetch	0.77*	0.81*	-0.78*	0.22*
Mean depth	0.92**	0.62**	-0.86**	0.28**
Surface area	0.69	0.79	-0.80	0.34
Perimeter	0.70*	0.75*	0.84*	0.39*

Note: ce : latent heat transfer coefficient, ch : sensible heat transfer coefficient, cd : momentum coefficient. * for p -value < 0.05, ** for p -value < 0.01.

The surface transfer coefficients calculated from the regression equations were adopted for the parameterization of BA and NA reservoirs (Figure 3.5). Linear regressions are valid for variable ranges that result in parameter values inside the pre-defined ranges according to literature. The value obtained for the latent heat transfer coefficient for BA Reservoir ($ce = 0.0005$) was slightly lower than the pre-defined range according to literature. In this case, ce coefficient was adopted as the minimum value in the range (0.0007).

Linear correlations of wind speed factor were significant for reservoir's mean depth, perimeter and fetch (Table 3.8). However, the correlation coefficients were small, revealing that the available data did not provide a sound basis enough for the parameterization procedure. In this manner, wind speed factors for BA and NA reservoirs were maintained at their initial values. The estimated parameter values for BA and NA reservoirs are presented in Table 3.7.

Figure 3.5. Best-fitted linear regression curves for estimation of surface transfer coefficients. Blue markers represent the calibrated parameter values for BB, IB, PR, and TI reservoirs, and red markers represent the estimated parameter values for BA and NA reservoirs.

3.3.4 Thermal regime

GLM simulated the thermal structure of the reservoirs over an 8-years period. Different thermal conditions in the water column were represented by the simulation: (a) BB and BA presented a polymictic behavior with full mixing events alternating with short periods (around 5 days) of thermal stratification throughout the year; and (b) IB, PR, NA, and TI showed a monomictic regime characterised by a periodic annual mixing event during the winter with a nearly uniform profile at 21.6 °C, mostly recorded from April to September, and the stratification was characterised by temperature gradients from 2.0 to 13.6 °C with a well-established thermocline between October and March (Figure 3.6).

Mean surface temperature varied from 22.3 to 26.3 °C, and mean bottom temperature varied from 19.7 to 22.9 °C (Table A.8 in Appendix A). The warmest mean temperature in surface (27.4 ± 2.1 °C) was recorded in February. During stratification events, the epilimnion depth varied from 1.3 to 18.3 m. The mean thermocline depth ranged from 2.0 to 19.3 m, and the metalimnion thickness varied between 0.7 and 4.2 m. Schmidt's Stability Index was calculated using simulated temperatures. The mean stratification intensity varied from $4 \pm 5 J m^{-2}$ (in BA) to $668 \pm 441 J m^{-2}$ (in TI) (Table A.8 in Appendix A) with peaks mostly in September and October, at the onset of the stratification period, and then gradually losing stability with lowest values from May to July. The Wedderburn Number reached the maximum values during the stratification period. Simulated mean values were much higher than one,

varying between 14 and 5143. W lower than one occurred in few occasions over the simulation period (from 0% to 4% of the time), except for PR reservoir, which experienced more mixing events (9% of the time) induced by wind.

Figure 3.6. Daily vertical temperature profiles of simulated data for a 1-year period (from July 2013 to June 2014) for a) Barra Bonita, b) Bariri, c) Ibitinga, d) Promissão, e) Nova Avanhandava, and f) Três Irmãos reservoirs.

3.4 Discussion

3.4.1 Sensitivity analysis

The 1D hydrodynamic model GLM was used for investigating time changes in thermal structure across six sub-tropical reservoirs with different physical characteristics. The sensitivity analysis revealed that water level simulation was highly sensitive to inflow and outflow factors, wind speed factor and to the bulk aerodynamic coefficient for latent heat transfer (ce). The expected high sensitivity to the inflow and outflow factors is due to their direct contribution to the reservoir's volume. The high sensitivity of both wind speed factor and ce on water level is

likely related to their influence on the calculation of evaporation rate. In the simulated reservoirs, evaporation rates varied from up to 2.6 mm day^{-1} in NA to up to 10.2 mm day^{-1} in TI, revealing the importance of evaporation as a component of water losses in subtropical lentic systems, where its rate is high in face of the high water temperatures (Ji, 2007, p. 70).

Regarding water temperature, the reservoir models were sensitive to surface energy exchanges parameters (ce , ch , cd), in addition to the factors related to input data (inflow, outflow, and wind speed), rather than by mixing efficiency. Inflow and outflow discharges are related not only to water level, surface area, and volume, but also to the heat budget as an input of kinetic energy. Wind is usually a major source of energy in lakes by supplying kinetic energy for the deepening of the surface mixed layer and for turbulent processes through internal waves. Its high sensitivity index is consistent with the literature. Indeed, several studies reported wind speed as a driver of the mixing behavior, as in Lake Iseo (Italy; Valerio et al., 2015), in Oneida Lake (United States; Hetherington et al., 2015) and in Rappbode Reservoir (Germany; Mi et al., 2018).

The latent heat transfer coefficient (ce) is related to heat loss due to evaporation. The sensible heat transfer coefficient (ch) accounts for heat gains and losses due to the heat flux between the surface water and the atmosphere when they have different temperatures. The momentum coefficient (cd) is related to heat losses through the action of the wind across the lake surface (Hipsey et al., 2019). The high sensitivity to surface energy exchange parameters was also reported for Lake Baratz (Italy) and Lake Ammersee (Germany; Bueche et al., 2020). Considering that all reservoirs have water temperature measured at surface, but not along the water column for two of them, it was expected a higher degree of sensitivity to changes in ce . Epilimnion temperatures are more sensitive to changes in ce while hypolimnion temperatures are more sensitive to changes in cd (Bruce et al., 2018). Indeed, IB Reservoir was the one with the deepest measured temperatures and the highest sensitivity to cd .

In particular, TI Reservoir was also sensitive to mixing efficiency for wind stirring (C_w) and for unsteady turbulence (C_T). These parameters are directly related to the transfer of wind energy to the mixing process; therefore, deep lakes with long residence time are generally sensitive to them since they require greater efficiency in transferring energy until the bottom of the water column. The lower sensitivity to the parameterization of the other mixing coefficients

indicates the dominance of surface boundary conditions in the thermal budget associated with the lack of measured temperatures in the hypolimnion for PR and TI reservoirs. The sensitivity analysis highlighted the importance of generating reliable hydrologic input data and the need for in-lake wind measurement. A further outcome of the sensitivity analysis was to identify the candidate parameters for the calibration exercise that future applications in tropical reservoirs can refer to.

3.4.2 *Model performance*

Since the model was sensitive to a set of parameters, the calibration process was recommended for the four reservoirs with available field data. Water level calibration resulted in good reproduction of the water balance. Differences between the simulated and observed water level were minimal through most of the reservoirs (RMSE between 0.12 m and 0.21 m), except for BB (RMSE of 0.90 m) and TI (RMSE of 1.56 m). However, considering their water level variation (5.8 m in BB and 9.4 m in TI), their normalised error (nRMSE) was in accordance with the others. RMSE values found in this study were in agreement with literature: RMSE from 0.15 to 0.20 m for Hsinshan Reservoir (Chang et al., 2015b), RMSE of 0.12 m for Grosse Dhuenn Reservoir (Weber et al., 2017) and RMSE from 0.36 to 0.73 m for Karaoun Reservoir (Fadel et al., 2017). Deviations between simulated and observed water levels could be attributed to non-measured withdrawals in the catchment basins, inaccurate knowledge of the reservoirs' geometry, and imprecise discharge measurements.

The simulation of the thermal structure performed well across the four reservoirs during the 8-years simulation period. Simulations of water temperature were satisfactory, with an average overall RMSE of 1.48 °C, in the range of previous studies applying GLM: 1.17 °C in Lake Ammersee and 1.30 °C in Lake Baratz (Bueche et al., 2020); 1.33–2.06 °C in Serra Azul Reservoir (Soares et al., 2019); 0.89 °C in Rappbode Reservoir (Mi et al., 2018); 1.34 °C in 32 lakes worldwide (Bruce et al., 2018); 0.19–1.18 °C in Lake Ammersee (Bueche et al., 2017); 1.23 °C in Grosse Dhuenn Reservoir (Weber et al., 2017); 0.87–1.49 °C in Lake Maggiore (Fenocchi et al., 2017); and 2.78 °C in 2368 lakes in the United States (Read et al., 2014). The results of the model validation confirmed the robustness of the calibrated model.

The discrepancies between measured and simulated temperature may be attributed to one or more of the following sources of uncertainty: 1) assumption of horizontal homogeneity. 1D models are not capable to fully account for three-dimensional processes, which can be important for vertical transport of heat below the epilimnion (Mi et al., 2018); 2) assumption of a single average light extinction coefficient (K_w) over eight annual seasonal cycles, particularly for lakes with high light extinction coefficient ($K_w > 0.5 \text{ m}^{-1}$), which were the case of four reservoirs (BB, IB, PR and TI). The lack of seasonal variation of K_w may exert a negative influence on the simulation accuracy (Bueche et al., 2017), and lakes with $K_w > 0.5 \text{ m}^{-1}$ recorded the greatest error in the prediction of temperatures in a previous study (Bruce et al., 2018). The incorporation of intra-annual effects of light extinction by providing K_w as forcing input to the model or coupling GLM to a water quality model with explicit light extinction feedback properties could help to improve model performance; 3) inaccuracies of measured field data. The meteorological data, especially wind speed, was not recorded *in-situ*, not being representative of actual meteorological conditions over the lake; and (4) the simple method for predicting daily inflow temperatures through linear regression with minimum and mean air temperature and solar radiation may provide inaccurate predictions (Arismendi et al., 2014), although previous studies have also applied this strategy with satisfactory results (*e.g.* Hornung, 2002; Bueche and Vetter, 2015). This uncertainty could be reduced in future studies by applying a more sophisticated method for estimating inflow temperatures, such as the tool *air2stream* which is based on daily air temperature and flow discharge and has obtained satisfactory results in a wide range of different rivers and conditions (Toffolon and Piccolroaz, 2015). Despite those uncertainties, the model was capable to meaningfully relate the hydro-meteorological forcing to the seasonal stratification dynamics, capturing the thermal behavior of each reservoir. In this sense, the model system was considered to be adequate for the purposes of the current study.

3.4.3 1D suitability

The fundamental assumption of 1D models is that the mixing within the lake can be constrained by processes acting in the vertical and that gradients in the horizontal plane, such as the degree of upwelling of the thermocline, are much lower having minimal impact on vertical transport. This assumption is usually valid for stratified lakes but can be disrupted by intense wind events inducing upwelling of cold water. Mean values of simulated Wedderburn number

were much higher than one ($W \gg 1$) for all reservoirs corroborating the suitability of the 1D approach. Upwelling occurred over short periods (up to 4% of the total simulation period), except for PR Reservoir (9% of the total simulation period). In this case, the model probably overmixed the water column and thus underestimated lake stability (Kerimoglu and Rinke, 2013).

3.4.4 *Thermal regime*

This work has advanced compared to previous studies by filling the gaps in the understanding of the reservoirs hydrodynamic processes. Overall, the hydrodynamics simulation successfully reproduced most aspects of the thermal structure and was able to replicate the intra-annual variability of the water temperature in all reservoirs. BB and BA presented a typical polymictic behavior of shallow lakes with intermittent mixing throughout the year halted by rapid stratification events. The thermal behavior of IB, PR, NA, and TI was comparable to what has been documented about tropical reservoirs, which are fundamentally warm monomictic with a mixing season during winter (Lewis, 2000). From October, stratification becomes stronger and the thermal structure remains stable until March. The variation of Schmidt's stability values throughout the year corroborated the simulated thermal behaviour.

3.4.5 *Parameterization strategy for non-monitored reservoirs applying regression curves*

Vertical transfer of heat and momentum between surface water and atmosphere is an important process for the energy budget of lentic systems, which is widely simulated in hydrodynamic models through empirical bulk aerodynamic formulae (see Strub and Powell, 1987 for further information on bulk formulae). In these formulae, surface transfer coefficients, *i.e.* coefficients of sensible heat, latent heat and momentum, represent the efficiency of turbulent transport between surface water and a reference level, usually 10 m above the surface (Heikinheimo et al., 1999).

Since bulk aerodynamic formulae are an empirical approach, estimation and calibration of surface transfer coefficient values in hydrodynamic models, such as GLM, is an important step for thermal processes simulation, especially for seasonal time-scales (Fischer et al., 1979; Brutsaert, 1982, p. 203). The surface transfer coefficient values in reservoirs and lakes may depend on the temporal scale of interest, atmospheric stability, wind speed, reservoir size, depth,

fetch and exposure to wind (Harbeck, 1962; Hicks, 1972; Strub and Powell, 1987; Ji, 2007, p. 31).

In this work, linear regression curves between calibrated surface transfer coefficients of monitored reservoirs and their morphometric features and wind speed were used in order to estimate parameters values for the non-monitored BA and NA reservoirs. The latent heat transfer coefficient (ce) showed a positive correlation with reservoir's mean depth, which is likely related to the greater capacity of deep lakes to store internal energy compared to shallow lakes (Venäläinen et al., 1998). As ce depends on the available energy in the lentic system to maintain evaporation, as well as on surface temperature, ce value tends to be higher in deep lakes than in shallow ones. The positive correlation between the sensible heat transfer coefficient (ch) and the reservoir's fetch is probably related to the increasing of wind speed with the fetch over the lake. Theoretically, a higher fetch enhances the mixing of the air and the local friction velocity, intensifying the efficiency of heat transport through turbulence. The momentum coefficient (cd) increases with the mean wind speed. Wind action over water generates waves, currents, and turbulence (MacIntyre, 1983), resulting in a rougher surface which enhances the vertical transfer of horizontal momentum from atmosphere to water (Ji, 2007, p. 169).

The wind speed factor should be estimated in face of its high sensitivity regarding both water level and temperature. However, the parameterization strategy could not be applied for this factor in face of the poor correlation coefficient with morphometric features of the reservoirs. Instead, for study sites where land use and cover are available both for the reservoir's surroundings and near the meteorological station, a correlation analysis could provide insights for its value estimation.

As an empirical method, the validity of the linear regressions is dependent on the morphometric features being within the range of this work and parameter values within the range recommended in the literature (see Table 3.4). The approach applied in this study could be extended to lakes and reservoirs with mean depth between 10 m and 18 m for ce estimation, fetch between 0 and 13 km for ch estimation, and mean wind speed between 0 and 14 m s⁻¹ for cd estimation. A wide spectrum of lakes and reservoirs in poorly monitored areas could benefit from this parameterization strategy, which is facilitated by the available and open-source module chain

of packages GLMr (Hipsey et al., 2014) – glmtools (Read et al., 2014) – glmGUI (Poschlod et al., 2018) – rLakeAnalyzer (Winslow et al., 2018).

The authors are aware of the limitations imposed by the few number of reservoirs used to construct the empirical relationships since the results presented here are based on measurements made on four reservoirs. However, the proposed approach represents an initial effort to estimate sensitive parameters for regional reservoirs which have different morphometric characteristics. It may be a conceptual strategy to enable modelling studies with better predictive capacity in the context of reservoirs with a lack of field data for calibration, which is quite frequent in tropical countries. Otherwise, the lack of field measurements would keep impairing modelling in regions with sparse data availability. This concept of “borrowing strength” from well-studied lakes to overcome problems of insufficient local data was introduced by Bruce et al. (2018). Remote sensing data may also contribute to improve knowledge about the thermal behaviour of non-monitored reservoirs (Calamita et al., 2019). For instance, Alcântara et al. (2010) applied satellite images to improve understanding of spatiotemporal variations in a Brazilian hydroelectric reservoir as a complement to the expensive and time consuming conventional water quality monitoring; Crosman and Horel (2009) proved the utility of using remote sensing data to monitor water temperature of lakes where in situ measurements are rarely available; and Nouchi et al. (2019) demonstrated the benefit of combining *in-situ* water analysis, hydrodynamic modelling and remote sensing for investigating biogeochemical processes.

To the knowledge of the authors, this is the first study aiming to optimise parameters for tropical lakes with no measurements of the temperature profile. Since the relationships are entirely empirical, further systematic investigations with other frequently monitored reservoirs are strongly recommended to increase the representativeness and the fit of curves for the non-monitored reservoirs that are exposed to the same regional climate.

3.5 Conclusions

This study presented the hydrodynamic simulation of a cascade system composed of six reservoirs in São Paulo (Brazil). Although the study sites have been the subject of numerous

investigations, as the authors are aware, the thermal behavior of these reservoirs was reproduced by a hydrodynamic model for the first time. Hindcast simulations applying GLM reconstituted the thermal structure over 2009–2016 and was able to provide the temperature profiles as well as stratification patterns. The model accurately predicted water levels and the thermal structure demonstrated good agreement based on the efficiency criteria RMSE between simulated and observed temperatures. The model revealed that the four reservoirs presented high sensitivity to surface energy exchange parameters, the coefficients for latent heat transfer, sensible heat transfer and momentum (ce , ch and cd , respectively), in addition to wind speed. This pattern could be used in future studies to identify the potential parameters for the calibration procedure. Besides, the sensitivity analysis further highlighted the importance of *in-situ* measurements of wind speed.

This modelling study enhanced the current knowledge of hydrodynamics for BB, IB, PR, and TI reservoirs, since the water temperature was recorded in a scarce frequency (every two months). A first representation of the thermal characteristics of BA and NA reservoirs, whose water temperature has never been monitored, was also provided through a parameterization strategy that benefited from the calibration of surface heat transfer parameters in the monitored reservoirs. Modelling results of the later reservoirs should be interpreted with care, since there is no available data for model performance assessment and errors may always arise. Indeed further work to test the parameterization curves for other reservoirs is strongly recommended to critically frame the obtained results. Nevertheless, it was considered that such simulations were useful for integrating the existing knowledge of thermal dynamics since, without this modelling approach, the thermal behavior of such reservoirs would remain unclear. It was provided a methodological insight for estimation of potential sensitive parameters that could be highly transferable to other reservoirs with hydrological and meteorological monitoring but with a lack of extended temperature records.

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Appendix A to Chapter 3

Figure A.1. Wind direction in each meteorological station: a) Barra Bonita, b) Bauru (for Bariri Reservoir), c) Ibitinga, d) José Bonifácio (for Promissão and Nova Avanhandava reservoirs), and e) Três Lagoas (for Três Irmãos Reservoir).

Figure A.2. Linear correlation between inflow temperature and meteorological variables (mean air temperature, maximum air temperature, minimum air temperature, delta air temperature, mean solar radiation and maximum solar radiation) for each reservoir.

Note: The black line represents the identity line (1:1). The graph corresponding to the highest correlation between inflow temperature and the meteorological variable is highlighted in red.

Figure A.3. Monthly input data across all reservoirs for shortwave radiation, relative humidity, wind speed, rainfall, air temperature, inflow temperature, inflow, and outflow. Horizontal lines represent the mean, 25th and 75th percentiles. Whiskers indicate the minimum and maximum values.

Figure A.4. Simulated (red line) and measured (blue line) water level ($n = 2922$) for each reservoir.

Figure A.5. Linear correlation ($n = 2922$) between simulated and measured water level for each reservoir. The black line represents the identity line (1:1).

Figure A.6. Simulated (blue line) and measured (red circle) water temperature at 0.3 m depth for a) Barra Bonita, b) Ibitinga, c) Promissão, and d) Três Irmãos reservoirs.

Table A.1. Multiple uses of the reservoirs Barra Bonita (BB), Bariri (BA), Ibitinga (IB), Promissão (PR), Nova Avanhandava (NA), and Três Irmãos (TI).

Uses	BB	BA	IB	PR	NA	TI
Hydroelectricity	x	x	x	x	x	x
Navigation	x	x	x	x	x	x
Tourism	x			x	x	
Irrigation	x				x	
Aquaculture	x			x	x	x
Water supply					x	
Flood control						x

Table A.2. Meteorological stations operated by the National Institute of Meteorology (INMET).

Name	Code	Latitude	Longitude	Altitude (m)	Distance from reservoir (km)
Barra Bonita	86867	22°28'16''S	48°33'27''W	534	7.7 from BB
Bauru	86865	22°21'28''S	49°01'44''W	636	40.3 from BA
Ibitinga	86843	21°51'20''S	48°47'59''W	497	23.3 from IB
José Bonifácio	86839	21°05'08''S	49°55'13''W	408	32.4 from PR; 30.2 from NA
Três Lagoas	86813	20°47'23''S	51°42'44''W	329	52.8 from TI

Table A.3. Missing values (%) of meteorological data.

	BB	BA	IB	PR/NA	TI
Air temperature	7%	11%	7%	2%	18%
Solar radiation	4%	7%	4%	2%	11%
Air relative humidity	8%	13%	10%	6%	18%
Wind speed	7%	11%	7%	2%	18%
Rainfall	8%	12%	8%	2%	18%

Table A.4. Pearson correlation coefficient (r) between meteorological stations for a) solar radiation, b) air temperature, and c) relative humidity.

	Barra Bonita	Bauru	Ibitinga	José Bonifácio	Três Lagoas
Barra Bonita	-	-	-	-	-
Bauru	0.83 ^a ; 0.95 ^b ; 0.90 ^c	-	-	-	-
Ibitinga	0.84 ^a ; 0.96 ^b ; 0.91 ^c	0.94 ^a ; 0.95 ^b ; 0.90 ^c	-	-	-
José Bonifácio	0.81 ^a ; 0.91 ^b ; 0.72 ^c	0.91 ^a ; 0.92 ^b ; 0.74 ^c	0.94 ^a ; 0.95 ^b ; 0.78 ^c	-	-
Três Lagoas	0.83 ^a ; 0.88 ^b ; 0.80 ^c	0.90 ^a ; 0.89 ^b ; 0.81 ^c	0.92 ^a ; 0.90 ^b ; 0.84 ^c	0.92 ^a ; 0.92 ^b ; 0.73 ^c	-

Table A.5. Model performance metrics for baseline simulation ($n = 2922$), calibration ($n = 1461$), validation ($n = 1461$), and complete period ($n = 2922$), regarding water level in each reservoir.

	Baseline			Calibration			Validation			Complete period		
	RMSE	nRMSE	r	RMSE	nRMSE	r	RMSE	nRMSE	r	RMSE	nRMSE	r
BB	0.97	0.16	0.86	0.93	0.19	0.88	0.89	0.15	0.86	0.90	0.15	0.86
BA	0.17	0.20	0.52	0.15	0.26	0.41	0.20	0.23	0.65	0.17	0.20	0.52
IB	0.12	0.20	0.46	0.11	0.21	0.06	0.13	0.26	0.51	0.12	0.20	0.49
PR	0.42	0.12	0.95	0.23	0.07	0.97	0.21	0.06	0.98	0.21	0.06	0.99
NA	0.40	0.34	0.78	0.12	0.27	0.30	0.16	0.14	0.88	0.14	0.12	0.91
TI	1.57	0.17	0.79	0.51	0.18	0.82	2.24	0.24	0.90	1.56	0.17	0.87

Note: Baseline and complete period refer to 2008–2016, calibration refers to 2009–2012, and validation refers to 2013–2016.

Table A.6. Model performance metrics for baseline simulation, calibration, validation, and complete period, regarding water temperature in each reservoir with available observed data.

	Baseline				Calibration				Validation				Complete period			
	n	RMSE	nRMSE	r	n	RMSE	nRMSE	r	n	RMSE	nRMSE	r	n	RMSE	nRMSE	r
BB	739	3.48	0.27	0.75	378	1.79	0.15	0.88	361	1.82	0.14	0.79	739	1.81	0.14	0.83
IB	651	1.89	0.19	0.98	651	0.89	0.09	0.97	-	-	-	-	-	-	-	-
PR	40	3.59	0.36	0.89	23	1.91	0.21	0.86	17	1.66	0.20	0.91	40	1.80	0.18	0.87
TI	48	1.49	0.12	0.88	24	1.37	0.12	0.89	24	1.46	0.14	0.86	48	1.42	0.11	0.88

Note: Baseline and complete period refer to 2008–2016, calibration refers to 2009–2012, and validation refers to 2013–2016.

Table A.7. Linear regressions between surface transfer coefficients and reservoir's morphometric and meteorologic variables.

Equation	<i>r</i>
<i>Coefficients for latent heat transfer (ce)</i>	
$ce = -0.273791U_{10} + 1.454060$	-0.57*
$ce = 0.073486F + 0.165103$	0.77*
$ce = 0.000786P + 0.338747$	0.70*
<i>Coefficient for sensible heat transfer (ch)</i>	
$ch = 0.068328U_{10} + 1.707125$	0.19*
$ch = 0.010126\bar{H} + 1.565384$	0.62**
$ch = 0.000631P + 1.350692$	0.75*
<i>Coefficients for transfer of momentum (cd)</i>	
$cd = -0.036818F + 1.455633$	-0.78*
$cd = -0.023866\bar{H} + 1.702003$	-0.86**
$cd = -0.000403P + 1.376064$	-0.84*
<i>Wind factor</i>	
$WF = -0.015869F + 1.091694$	-0.22*
$WF = -0.018862\bar{H} + 1.150348$	-0.28**
$WF = -0.000236P + 1.104739$	-0.39*

Note: U_{10} is the mean wind speed, F is the fetch, P is the perimeter, $\bar{H}$ is the mean depth. * for p -value < 0.05; ** for p -value < 0.01.

Table A.8. Simulated hydrodynamics metrics for each reservoir from 2009 to 2016.

Hydrodynamics metrics	BB	BA	IB	PR	NA	TI
Number of mixed days per year	355 (6)	365 (1)	185 (26)	151 (59)	142 (63)	32 (49)
Water column temperature (°C)	23.0 (2.4)	22.2 (2.2)	23.9 (2.8)	24.5 (3.6)	22.0 (3.0)	23.3 (2.9)
Surface temperature (°C)	23.3 (2.4)	22.3 (2.3)	25.1 (2.9)	25.9 (3.6)	23.5 (2.9)	26.3 (2.6)
Bottom temperature (°C)	22.9 (2.3)	22.1 (2.2)	22.8 (2.9)	22.9 (3.6)	19.7 (2.6)	20.0 (1.9)
Epilimnion depth (m)	5.0 (2.6)	1.3 (1.8)	7.1 (6.0)	8.7 (6.7)	18.3 (7.7)	15.2 (9.0)
Thermocline depth (m)	5.4 (2.6)	2.0 (1.6)	7.4 (6.0)	9.4 (6.6)	19.3 (7.8)	17.3 (8.6)
Metalimnion thickness (m)	0.8 (0.7)	1.4 (0.6)	0.7 (1.0)	1.6 (2.1)	1.9 (2.6)	4.2 (2.5)
Schmidt's Stability Index ($J m^{-2}$)	17 (19)	4 (5)	79 (51)	160 (151)	183 (186)	668 (441)
Wedderburn number	19 (87)	14 (39)	243 (2004)	383 (2483)	1537 (6557)	5143 (35768)
Percentage of time with Wedderburn number < 1	4%	0.03%	3%	9%	1%	0%

Note: Mean value (standard deviation). Surface is at depth 0 and bottom is at the deepest layer.

4

Climate change enhances deepwater warming of subtropical reservoirs: evidence from hydrodynamic modelling

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Lake surface warming and thermal responses to climate change have been widely reported, especially in temperate regions. Evidence of reservoirs' responses in low latitudes is still limited. In this study, the vertical profile of water temperature in the Barra Bonita Reservoir (Brazil) was simulated using the one-dimensional General Lake Model (GLM), calibrated and validated using in-situ data. Water temperature and reservoir hydrodynamics were simulated over 26 years (1993–2018) to investigate warming trends, seasonal patterns, Schmidt stability, and the number of stratified days per year. Results have indicated that the reservoir has experienced significant warming from surface to the bottom related to increasing air temperature and decreasing wind speed. Significant increasing trends were found for Schmidt stability and in the number of stratified days per year. Deepwater warming is directly related to increasing air temperature and frequent mixing episodes which transfer heat from surface to bottom waters. Our findings contribute to the understanding of subtropical reservoirs response to climate change and help to guide planning strategies for ensuring security of water storage and ecosystem services they provide.

Keywords: hydrodynamics, climate forcing, thermal structure, temporal trends, Sen's estimator of slope, General Lake Model (GLM).

4.1 Introduction

Several studies have assessed the impact of climate change on the thermal structure of lakes which are recognised as sentinels of such changes due to their sensitivity to atmospheric conditions and their ability to integrate the effects of climate-driven changes occurring within the catchment (Adrian et al., 2009). The increase in lake surface temperature, primarily driven by rises in air temperature, was the most frequent finding (Woolway and Merchant, 2019). In addition to warming, thermal dynamic responses have also been widely reported, such as the stronger (Sahoo et al., 2016) and longer (Magee et al., 2016) thermal stratification, and shallower thermocline depth (Bayer et al., 2013). Reservoirs also integrate atmospheric and catchment, thus ultimately capturing climate signals (Williamson et al., 2009). However, given their largely anthropogenically controlled hydrology, climate-related responses are influenced by specific features of individual systems.

Reservoirs play an important role in controlling and managing of water resources. They have been built over the past decades, reaching about 50,000 large reservoirs worldwide (Lehner et al., 2011). Their global expansion has increased access to drinking water, irrigation, navigation, flood control, and hydropower generation. Moreover, similar to lakes, reservoirs provide key ecosystem services of supporting, provisioning, regulating, and cultural services (Janssen et al., 2020). Although the lacustrine zone of reservoirs shares several similarities with natural lakes, they differ in attributes regarding their catchment, water body, management, and geographic distribution, leading to differences in ecosystem functioning (Hayes et al., 2017).

In Brazil, the National Dam Safety Information System registered more than 24,000 reservoirs until 2017, from which 69% have irrigation, livestock watering, or fish breeding as the main purpose (ANA, 2018a). In this context, understanding how reservoirs respond to climate change and their interactions with meteorological drivers are of paramount importance for ensuring security of water storage, ecological balance, goods, and ecosystem services they provide to society. Although recent studies investigated climate impacts on reservoirs (*e.g.* Zhang et al., 2015; Lewis Jr. et al., 2019), available information for lentic ecosystems in the tropics is still limited (Ramírez et al., 2020). As a result, while there is sufficient evidence on the effects of climate change over lakes under a temperate climate, a further understanding of how subtropical reservoirs respond is still required.

Accordingly, this study investigates the thermal changes of a subtropical reservoir over 26 years. Considering the low-frequency of field measurements, a one-dimensional hydrodynamic model was applied to simulate the reservoir's thermal structure aiming (1) to compute water column temperature trends, (2) to investigate trends in stratification strength and duration based on the Schmidt stability and the number of stratified days per year, (3) to describe the specific mechanisms of reservoir's internal response to climate forcing, and (4) to envisage potential driving factors explaining thermal changes. Considering a global boom in dam construction (Zarfl et al., 2014), understanding the mechanisms that govern reservoir response to climate change is becoming increasingly urgent.

4.2 Material and Methods

4.2.1 Study site

The subtropical Barra Bonita Reservoir is a medium-size water body situated in southeast Brazil (22°28'16''S, 48°33'27''W) at 451 m above sea level. The reservoir impounds the waters of the Tietê River, the Piracicaba River and several small creeks (Figure 4.1). The only reservoir outflow is the Tietê River with a mean annual discharge of $405 \text{ m}^3 \text{ s}^{-1}$. It was built in the 1960s to meet hydroelectric power demands and currently is also used for navigation, tourism, irrigation, and aquaculture. The reservoir has a maximum depth of 23.5 m and a mean depth of 10.2 m. Its mixing regime is typically polymictic with full mixing events alternating with short periods (around 5 days) of thermal stratification throughout the year (Soares et al., 2020).

Barra Bonita Reservoir differs from a typical lake in several ways that lead to differences in ecosystem functioning (Hayes et al., 2017): (1) long and narrow morphometry with a high degree of irregularity of the shoreline (see Figure 4.1); (2) storage of a large volume of water ($3.6 \times 10^9 \text{ m}^3$) and short hydraulic residence time (0.28 years); (3) an outlet structure controls the water level, resulting in a mean annual level fluctuation of about 5.0 m; (4) a large ratio of the catchment area (32,300 km^2) to reservoir surface area (310 km^2) and; (5) it is predominantly fed by surface water from higher order streams.

Figure 4.1. The Barra Bonita Reservoir, its bathymetry, and tributaries. The red circle indicates the monitoring station.

Barra Bonita Reservoir is located in a catchment area extensively occupied by agriculture (62%, mostly sugarcane), urban areas (12%), pasture (5%), vegetation (20%), and water bodies (1%) (IBGE, 2018). Its tributaries receive nutrient input from agricultural areas and domestic and industrial effluent discharges from large urban centres, including São Paulo Metropolitan Region. These are the key factors contributing to the degradation of the water quality causing its super-eutrophic status, shallow Secchi depth, frequent hypoxic events and Cyanobacteria blooms (CETESB, 2019).

The annual mean air temperature is 20.7 °C, the mean monthly air temperature varies from 17.1 °C in June to 23.1 °C in February. The mean total annual precipitation is 1,525 mm mostly occurring from October to March (mean values computed from 1993 to 2018, INMET, 2019).

4.2.2 Model description

The one-dimensional General Lake Model (GLM) version 2.2.0 (Hipsey et al., 2019) was used to simulate the hydrodynamics of the Barra Bonita Reservoir. GLM was developed in 2012 based on approaches from previous model platforms (Hamilton and Schladow, 1997; Imberger

and Patterson, 1990). A series of improvements were incorporated since then and so GLM has been applied to a variety of lentic environments (Bruce et al., 2018; Bueche et al., 2017; Read et al., 2014; Snortheim et al., 2017). It is an open-source code, which is available for free.

GLM simulates the vertical profiles of temperature, salinity, and density in lentic water bodies. The model adopts the fundamental assumption of 1D models, i.e. the mixing within the lake results from processes acting in the vertical and gradients in the horizontal plane are much smaller and have minimal impact on the vertical transport of energy and mass. The 1D assumption was validated for the Barra Bonita Reservoir in a previous study (Soares et al., 2020) through the computation of the Weddeburn number which was much higher than one. A flexible Lagrangian layer structure is used to discretise the water column into horizontal layers to simulate the vertical variation in water properties. This approach defines each layer as a “control volume” with homogeneous density computed from the simulated salinity and temperature. Each layer can change the thickness by contraction and expansion in response to inflows, outflows, mixing with adjacent layers, and surface mass fluxes.

Thermal mixing processes are simulated using the water balance and energy budget computed at every time step. Within the lake domain, the model solves the water balance regarding several water fluxes, including surface mass fluxes (evaporation and rainfall), inflows (surface and submerged inflows), and outflows (withdrawals, overflow, and seepage). GLM adopts a dynamic balance between kinetic and potential energy. On one hand, during stratification periods, as the water density gradient increases, potential energy is stored. Turbulent kinetic energy, on the other hand, is provided by wind stirring, convective overturn, shear production between layers, and Kelvin–Helmholtz billowing. When density instabilities occur between adjacent layers or when sufficient turbulent kinetic energy becomes available, the stable density gradients disrupt, and then layers merge, thereby accounting for the mixing process.

GLM requires the reservoir bathymetry, meteorological data (air temperature, wind speed, air relative humidity, rainfall, shortwave radiation, and longwave radiation or cloud cover), inflow (discharge, water temperature, and salinity) and outflow (discharge) data.

4.2.3 *Required data for hydrodynamic modelling*

Five monitoring stations provided meteorological, hydrological, and limnological data used in this work (Table B.1 in Appendix B). Reservoir's hypsographic curve was extracted from a 1-m resolution bathymetrical survey provided by Corrêa Filho et al. (2003). The model uses the information to internally compute the depth-area-volume relationship as the volume of the Lagrangian layers change.

Daily meteorological data on air temperature, wind speed, air relative humidity, rainfall, and cloud cover were provided by São Carlos station, and daily insolation data were provided by São Simão station. Both stations are operated by the National Institute of Meteorology (INMET, 2020) and they are located 80 km and 148 km, respectively, northeast of the reservoir. Occasional missing data (3%–14% of gaps for each variable) were replaced by linear interpolation. Although the insolation data were obtained from a different meteorological station, the location of both stations is subject to the same isocurve of daily insolation (Tiba, 2000). Solar radiation was estimated from insolation using the Angström-Prescott method (Angstrom, 1924; Prescott, 1940) and was subjected to a sine wave disaggregation by GLM to obtain a sub-daily light time-series. Cloud cover data were used for predicting longwave radiation.

Daily inflow and outflow discharges were provided by the National Water Agency (ANA, 2018b). A small number of missing values of inflow discharges (0.03% of gaps) was filled by linear interpolation. No missing values occurred in the outflow discharge time-series.

Inflow temperature and electrical conductivity were obtained from a fluviometric station (ANA, 2019) operated by the Environmental Company of São Paulo State (CETESB) at a bimonthly frequency in the Tietê River from 1999 to 2010. As the model requires daily inflow temperature, linear correlation analyses between inflow temperature and several meteorological variables were investigated. The highest linear correlation was found between inflow temperature and mean air temperature ($r = 0.78$, p -value < 0.001 ; Figure B.1 in Appendix B). Hence, bimonthly inflow temperature was converted into the daily frequency, following the same procedure found in previous studies (He et al., 2019; Hornung, 2002; Rolighed et al., 2016; Silva et al., 2019). Considering that direct tributaries contribute to a small fraction of the total annual inflow, variations in their water temperature were assumed to have a negligible impact on the

Barra Bonita Reservoir's thermal dynamics. The difference between water temperature in the Tietê River and Piracicaba River is not statistically significant (Mann-Whitney U test, p -value = 0.08). Therefore, the Tietê River water temperature was assumed to be representative of all inflows. Electrical conductivity data were used to estimate inflow salinity according to Hornung (2002). Due to the small salinity content in addition to its low influence in freshwater systems, salinity was assumed to be constant and equal to its average value (0.1 g kg^{-1}).

Additionally, GLM requires in-lake temperature, salinity, and water level for both model calibration and validation, as well as for setting its initial conditions. Surface water temperature and electrical conductivity in the Barra Bonita Reservoir has been reliably monitored since 2003, the Secchi depth since 2005, and water temperature measurements have been carried out at 1-m intervals from the surface to the bottom since 2008. All measurements are performed bi-monthly at a central location in the reservoir by CETESB (2019; see Figure 4.1). The reservoir's daily water level has been measured since 2003 by ANA (2018b). The abovementioned monitoring stations are presented in Figure B.2 and the methodological steps followed in this study (to be detailed in the following sections) are summarised in Figure B.3 in Appendix B.

4.2.4 Model setup and sensitivity analysis

GLM was set to simulate the Barra Bonita Reservoir water temperature at a daily step in response to the daily meteorological input data. A baseline simulation was run using the input data previously described and initial parameter values (Table B.2 in Appendix B) based on Hipsey et al. (2014). The simulation period was from 22nd January 2003, the first day with field measurements, to 31st December 2018. The light extinction coefficient ($K_w = 1.3 \text{ m}^{-1}$) was determined from the mean value of the Secchi depth (SD) measurements and assuming $K_w = 1.7/\text{SD}$ (Poole and Atkins, 1929). The initial conditions of water temperature in the reservoir came from *in-situ* water surface measurements on the first simulation day. The initial salinity was estimated from electrical conductivity measured at the water surface.

To identify the most sensitive of the eleven parameters frequently assessed in previous studies based on GLM (Table B.2 in Appendix B), a sensitivity analysis was carried out. The normalised sensitivity coefficient (SI) was computed from:

$$SI = \frac{\Delta Y/Y}{\Delta X/X} \quad (4.1)$$

where Y is the model performance for the reference value X of the parameter, which has a variation ΔX generating a model performance variation ΔY .

For sensitivity analysis, the model performance was assessed with Root Mean Square Error (RMSE). The one-at-a-time method was adopted by increasing and decreasing the parameter initial values by 10%. All parameters presented $SI < 0.05$ (Figure B.4 in Appendix B) indicating low to negligible individual influence in the model output (Bueche et al., 2019). Thus, all eleven parameters were included in the calibration procedure.

4.2.5 Model calibration and validation

For the calibration of water temperature and water level, a period of five years was simulated between 15th January 2008 and 31st December 2012, the first years with field monitoring of the vertical temperature profile. Calibration was manually implemented by an iterative trial-and-error process. Employing successive simulations, the parameters were adjusted up to reaching a minimum RMSE value computed from observed and simulated data. The range for the parameters' values (Table B.2 in Appendix B) was based on previous applications of 1D models (Tanentzap et al., 2007; Weinberger and Vetter, 2012; Kerimoglu and Rinke, 2013; Fadel et al., 2017; Huang et al., 2017; Snortheim et al., 2017).

In GLM model, hydrological and meteorological data may be adjusted through multiplicative factors which vary from 0 to 1 and will proportionally increase (or decrease) input data values. These multiplicative factors, such as wind factor or inflow factor, are commonly used in model calibration aiming at compensating uncertainties in field data, such as measurement errors, or differences between conditions around the monitoring station and conditions near the reservoir (Bueche et al., 2019; Huang et al., 2017; Soares et al., 2019). In this study, inflow and outflow factors were calibrated in the range of 0.9 to 1.1 to ensure a proper representation of the reservoir water balance. Multiplicative factors of shortwave, cloud cover, wind speed, air temperature, air relative humidity, and rainfall were also calibrated in the range of 0.7 to 1.3.

The validation of the best-fitted model used two independent datasets: the surface water temperature from 22nd January 2003 to 31st December 2007 and the vertical profile of temperature from 22nd January 2013 to 31st December 2018. The simulated water level was also validated for the same periods. RMSE was used as the objective function for assessing the model performance of water temperature and water level during calibration and validation periods.

4.2.6 Assessment of model performance

A continuous simulation was performed for 16 years, from January 2003 to December 2018 applying the calibrated parameters and multiplicative factors. The model performance was assessed through error measures calculated from simulated and observed water temperature. A warm-up period of nearly two months was adequate for model stabilisation, which is likely related to the homogeneous temperature along the water column on the first day of simulation. This warm-up period was left out from the performance assessment to avoid uncertainties of initial conditions. The model skill test was performed by applying the summary measures (Table B.3 in Appendix B) according to Willmott (1981): mean values of observed and simulated water temperature ($\bar{O}$ and $\bar{S}$), their standard deviation (s_o and s_s), the intercept (a) and slope (b) of the least-squares linear regression, mean absolute error (MAE), and root mean square error (RMSE). Additionally, a set of four commonly used measures of model fit was applied to identify deviations from observed data, highlighting different aspects of model performance (Bennett et al., 2013): mean absolute percentage error (MAPE), Pearson correlation coefficient (r), percent bias (PBIAS), and mean bias error (MBE).

4.2.7 Temporal trends in the reservoir and in forcing variables

Trends in the thermal regime of the Barra Bonita Reservoir were explored using GLM simulation for the complete period of available input data, from 1st January 1993 to 31st December 2018. Because field data is only available from 2003, the initial conditions of water temperature in the reservoir on 1st January 1993 were defined as the mean value of water temperature measured in January from 2008 to 2018 at every 1-m depth.

The assessment of the reservoir hydrodynamic behaviour used the mean water temperature at 2-m intervals over the water column, from the surface to 14 m depth, and the

thermal conditions were expressed by the Schmidt stability index (Idso, 1973) and the number of stratified days per year. The Schmidt stability index assesses the strength of the vertical temperature stratification and was implemented according to Read et al. (2011). The number of stratified days per year followed Lewis (2000) by computing the difference between surface and bottom temperatures higher than 2 °C.

As applied in previous studies (O' Reilly et al., 2015; Schmid and Koster, 2016; Winslow et al., 2017), the Theil-Sen's slope estimator (hereafter Sen's slope) was used in this study to estimate trends in the water temperature, Schmidt stability, and the number of stratified days per year, at the 0.05 significance level, considering their mean annual and monthly values. Sen's slope is a robust nonparametric method for estimating trends based on a simple linear regression where the fitted line is the median of the slopes of all lines that connect pairs of sample points (Sen, 1968). Hirsch et al. (1982) adapted Sen's slope to account for seasonality in data sets. Sen's slope and significance levels were computed using the MAKESENS software v. 1.0 (Salmi et al., 2002). The non-parametric Mann-Whitney *U* test and its significance level were computed using the PAST software v. 3.25 (Hammer, 2019) to compare the median of indicators between different time periods.

To explore the temporal trends in the forcing variables, Sen's slope was also computed for meteorological and hydrological input data (air temperature, solar radiation, cloud cover, air relative humidity, wind speed, rainfall, inflow discharge, and outflow discharge) considering the mean annual and monthly values. As the inflow temperature was obtained from the linear correlation with mean air temperature (see Section 4.2.3), its temporal trend was not computed to avoid duplicity with trends in air temperature.

To further explore the warming trends in water temperature, a detrended analysis of the wind speed was performed to verify whether the warming trends in the Barra Bonita Reservoir occurred regardless of the changes in wind speed. This variable was selected due to the distance between the meteorological station and the reservoir since among all variables, wind speed has the highest local-dependence. The simulation was performed for wind speed individually detrended by keeping the original series for the first simulation year and adopting the monthly means of 1993 for the following years. All other input variables remained unchanged.

4.3 Results

4.3.1 Model performance

During the calibration period (2008–2012), GLM showed an RMSE of 0.80 m between the simulated and measured water level. During the validation periods (2003–2007 and 2013–2018), RMSE for the water level was 0.64 m and 0.87 m, respectively (Figure B.5 in Appendix B). The water temperature was also well captured by the model. The mean RMSE along the vertical profile was 1.08 °C during the calibration period, 1.66 °C in the first validation period (2003–2007), and 1.07 °C in the second validation period (2013–2018). Minor positive and negative deviations between simulated and measured water temperatures were observed (Figure B.6 in Appendix B). Mean RMSE of water temperature at every depth from the surface to the bottom and at a monthly scale (Figures B.7a and B.7b, respectively, in Appendix B) was quite similar between calibration and validation periods. The RMSE values for water level and temperature were in agreement with the results of previous studies dealing with one-dimensional models (Bueche et al., 2019; Fadel et al., 2017; Fenocchi et al., 2017; Vinçon-Leite et al., 2014).

The metrics for model performance from January 2003 to December 2018 revealed similar results along the water column (Table B.4 in Appendix B), with values in the range of previous results reported in the literature (Bruce et al., 2018; Mi et al., 2019; Soares et al., 2019; Weber et al., 2017). The annual mean error during the 16-year simulation shows no systematic bias (Figure 4.2). Further details regarding the model performance for the 2003–2018 period, as well as the contour plot of simulated water temperature can be found in Figure B.8 and Figure B.9 in Appendix B.

Figure 4.2. The mean error between simulated and measured water temperature at different depths is represented by coloured circles during the 2003–2018 simulation period. Annual mean errors computed from all depths are represented by white circles with error bars referring to their standard deviation.

4.3.2 Trends in water temperature and thermal conditions

Trend analysis of the simulated annual water temperature showed a consistent significant increasing trend along the whole water column. Annual warming trends varied from 1.02 °C per decade to 0.33 °C per decade at the surface and 14 m depth, respectively (Figure 4.3). An intra-annual assessment indicated consistent warming throughout the year. Monthly warming trends were significantly above zero in the entire water column from March to August during the autumn and winter seasons. The highest increase rates were observed from May to July with values above 1.05 °C per decade even in the bottom layer. A decreasing trend was observed only at 12 m and 14 m depth in a few months, yet not significant.

A graphical analysis of the simulated Schmidt stability and the number of stratified days per year indicated that both indicators did not follow a linear trend, but rather they presented a jump in the annual mean series in 2009 (Figure 4.4). The mean values for both indicators from 1993 to 2008 and from 2009 to 2018 were significantly different (Mann-Whitney U test, p -value < 0.001), with mean values of Schmidt stability and number of stratified days per year increasing from 12.3 J m⁻² (1993–2008) to 58.0 J m⁻² (2009–2018) and from 2 days (1993–2008) to 89 days (2009–2018), respectively.

Figure 4.3. Warming trends in simulated water temperature at 2-m intervals from 1993 to 2018.

Note: *** for $p < 0.001$; ** for $p < 0.01$; * for $p < 0.05$.

Figure 4.4. Annual simulated indicators of hydrodynamic behaviour and thermal conditions (circles) for Barra Bonita Reservoir during 1993–2018, the shaded area representing their annual standard deviation, Sen’s slope (solid line), and its 95% confidence interval represented by the dotted lines.

4.3.3 Trends in forcing variables

Sen's slope at annual and monthly scales was computed for hydrological and meteorological data used as forcing variables in the model from 1993 to 2018. The trend analysis showed significant annual trends for air temperature (0.43 °C/decade), air relative humidity (−1.62 %/decade), and rainfall (−170.05 mm/decade) (Table 4.1). The graphical analysis of the wind speed revealed a jump in annual mean series from 2009 (Figure B.10 in Appendix B). The mean wind speed was significantly different (Mann-Whitney U test, p -value < 0.01) between 1993–2008 (mean value of 2.6 m s^{−1}) and 2009–2018 (mean value of 1.2 m s^{−1}). The remaining input variables displayed small temporal changes, in a range that might be attributed to the random interannual variability.

Table 4.1. Trends in measured meteorological and hydrological forcing variables from 1993 to 2018.

Forcing variable	Sen's slope
Solar radiation (W m ^{−2} /decade)	0.48
Cloudiness (%/decade)	−0.03
Air temperature (°C/decade)	0.43 ***
Air relative humidity (%/decade)	−1.62*
Wind speed (m s ^{−1} /decade)	−0.71***
Rainfall (mm/decade)	−170.05**
Inflow discharge (m ³ s ^{−1} /decade)	−26.24
Outflow discharge (m ³ s ^{−1} /decade)	−2.43

Note: *** for $p < 0.001$; ** for $p < 0.01$; * for $p < 0.05$.

Monthly significant warming in air temperature (Figure 4.5) was revealed mostly during the autumn and winter, with the highest increase rate in June (0.99 °C/decade). The air relative humidity significantly decreased in April, May, August, and December. The wind speed revealed a significant decrease throughout the year (p -value < 0.001). Although the annual rainfall trend was found to be significant, on a monthly basis, a significant trend was found only in February (−73.33 mm/decade). Finally, monthly trends in solar radiation and inflow discharge were significant only in a few months, while no significance was found for intra-annual variability in cloudiness and outflow discharge.

Figure 4.5. Monthly trends in the forcing variables for the 1993–2018 period (solid line). The shaded areas indicate 95% confidence intervals for Sen’s slopes, which means that the trend is greater (or smaller) than zero with 95% confidence if the shaded area is above (or below) the zero line for each month.

Indicators of hydrodynamic behaviour computed from the simulation with detrended wind speed showed positive annual warming trends of about 0.25 °C per decade, being significant during autumn and winter (Table B.5, Figure B.11 in Appendix B). The absence of a trend in wind speed resulted in a small increasing rate, although significant, for Schmidt stability at the annual scale, and not a single day during the 26 years was stratified. Then, the number of stratified days per year showed an absence of trend.

4.4 Discussion

4.4.1 Assessment of modelling performance

The modelling approach was able to quantify the trends in water temperature, which would not be possible to be computed from measured data considering the large time interval between the water sampling measurements (every two months). To assess potential biases between simulated and measured thermal conditions in the reservoir, efforts were made to closely assess the model performance through several goodness-of-fit measures at every 2-m depth intervals from the surface to the bottom. The GLM model successfully reproduced the mass balance, the vertical temperature profile, and the intra-annual thermal behaviour of the Barra Bonita Reservoir, achieving an acceptable degree of agreement with the measured data. Thus, the model was considered reliable to reproduce water temperature dynamics from 1993 to 2018.

Similar to other hydrodynamic models, GLM assumes some simplifications, such as the one-dimensional assumption inherent to the model configuration, which may introduce a level of uncertainty to simulation results. Additionally, the scarcity of field data could impair the model's ability to reproduce the thermal behaviour accordingly. For instance, a regression-based statistical approach was adopted to provide daily inflow temperature as input to the model. Despite the existence of uncertainties in inflow temperature prediction, the model could meaningfully relate the hydro-meteorological forcing to the seasonal stratification dynamics in Barra Bonita Reservoir.

We are aware that the collection of longer and more detailed input data could help refine the simulated magnitudes of trends. Nonetheless, the uncertainties of model results are not expected to change the key conclusion of the existence of a significant warming trend, which was found along the water column in the Barra Bonita Reservoir for the 1993–2018 period. The detrended analysis corroborated those trends regardless of changes in wind speed, which may be considered the most uncertain forcing variable, which is a good indication of the warming in the reservoir.

Finally, the simulation comprised the complete period of available input data; a total of 26 years. This period is not long enough when studying temporal changes of environmental variables. Continuous field campaigns will be necessary to encompass the long-term variability of hydrodynamic processes.

4.4.2 Thermal response of a subtropical reservoir under climate change

A consistent annual temperature increase was detected along the water column revealing the process of Barra Bonita Reservoir warming up with positive trends from the surface (1.02 °C per decade) to the bottom (0.33 °C per decade). In subtropical lentic systems, increase water temperature may bring greater impacts on thermal stratification when compared to lakes and reservoirs in higher latitudes because the nonlinear relationship between water temperature and density is characterised by stronger density response at higher temperatures. At around 24 °C, small temperature increases lead to relatively high stability increases (Lewis, 1996). The warm surface in Barra Bonita Reservoir (mean temperature of 23.4 ± 3.6 °C) resulted in a density gradient strong enough to hold stratification during several days, increasing the number of

stratified days at 19.4 days per decade, a rate greater than reported for lakes across the Northern hemisphere (4.13 days per decade, Woolway et al., 2019). This evidence corroborates that tropical water bodies tend to be more sensitive to climate change in terms of stability and resistance to mixing than lakes in temperate and arctic regions (Kraemer et al., 2015; Saulnier-Talbot et al., 2014).

In this study, results indicate that bottom waters are significantly warming, mainly during autumn and winter. Reported impacts of the warming climate on the temperature of deep waters reveal an inconsistent response among lentic systems, which were either cooling (Magee and Wu, 2017; Magee et al., 2016), showing no trends (Winslow et al., 2015), or in some cases, warming (Peeters et al., 2002). Conceptually, large and deep lakes experience increasing hypolimnic temperatures as they integrate the effects of meteorological forcing over longer periods of time, thus being able to carryover heat from one year to the next, while small and shallow lakes show only slight or no significant trends of rising hypolimnic temperatures due to the rapid loss of heat in autumn and winter (under ice-free condition) (Ficker et al., 2017). However, bottom waters may respond in more complex and variable ways (Butcher et al., 2015), thus divergent patterns from the theoretical background may occur due to the fact that hypolimnion temperatures are generally disconnected from atmospheric forcing and may respond to different drivers of the thermal structure (Richardson et al., 2017). For instance, deep waters in Lake Malawi (East Africa) are warming at 0.1 °C per decade due to reduced cold-water intrusions in warmer winters (Vollmer et al., 2005); deep waters in twelve lakes across Europe are warming at a similar rate of 0.1–0.2 °C per decade due to the mesoscale signal from the North Atlantic Oscillation (Dokulil et al., 2006); and SAMO Lake (Mexico) is profoundly warming (1.136 °C per decade) at about ten times larger than the mean global warming rate caused by thermal diffusion between surface and bottom water layers (Cardoso-Mohedano et al., 2019).

Barra Bonita Reservoir has a polymictic behaviour and surface waters are frequently mixed down to deeper layers efficiently transferring heat from surface to bottom layers (Figure B.9 in Appendix B). According to model results, on average, water temperature at 10 m depth increases by 0.31 °C in the first day of a mixing event succeeding a stratification period. Furthermore, the amount of heat input into deep waters is further enhanced in this reservoir by

the outlet structure and the high water level fluctuation, which are intrinsic characteristics of human-made and human-operated aquatic systems (Figure B.12 in Appendix B).

The outlet structure is a typical component of many reservoirs and may have a significant effect on the transfer and storage of heat in the water body primarily by determining the thermocline depth and hypolimnion volume (Casamitjana et al., 2003). In Barra Bonita Reservoir, water withdrawn occurs at 6.5 m from the bottom, which favours the storage of heat in the water body by retaining warmer surface water (23.4 °C on average) while withdrawing a volume with lower temperature (22.5 °C on average).

Additionally, reservoirs typically have more variable and complex hydrology than lakes due to anthropogenic operation of inflows and outflows, resulting in high water level fluctuations. In Barra Bonita Reservoir, mean annual water level variation is about 5.0 m. The reservoir filling up occurs during summer and autumn (wet season) and its drawdown over winter and spring (dry season). When the reservoir is shallower, its thermal stability is reduced and less energy is required to mix the water column (Soares et al., 2019). Mixing during winter following lower air temperatures, a typical behaviour of subtropical lakes (Lewis, 1996), is then amplified in subtropical reservoirs by the artificially imposed shallower depth in this season. Besides, as the reservoir's depth, surface area, and volume decrease with drawdown, the thermal inertia decreases in the shallower water body, ultimately reducing the time lag between air warming and water temperature variations (Toffolon et al., 2020).

4.4.3 Driving factors of trends in water temperature indicators

The significant trend in the observed air temperature, with an annual rate of 0.43 °C/decade, was in the range of those observed in different sites across the globe (Schmid and Koster, 2016; Winslow et al., 2017; Zhang et al., 2015). In general, air temperature is believed to be the main driver of lake surface temperature changes (Huang et al., 2017) due to its influence on both sensible and latent heat exchange, and in the net longwave radiation. Overall, the highest increase in water temperature from the surface to the bottom during winter (Figure 4.3) is consistent with and likely related to the higher air warming trend rate in this season (Figure 4.5). Increase trend in deepwater temperatures at Barra Bonita Reservoir are directly coupled to the increase in the air temperature. The peak in the increasing rate of air temperature

in June followed by a peak in the warming rate of water temperature in July exhibits how bottom layer temperatures are closely related to the near-surface temperature in this reservoir.

The significant warming of water temperature consistently exceeded the air temperature trends on annual and monthly scales, which may be explained by changes in other forcing variables influencing water warming. In the present study, the mechanism explaining a water warming trend stronger than the air temperature trend is an abrupt change in the wind speed time-series. Wind speed acts both on the exchange of latent and sensible heat and also forces the motion of water and thereby turbulent transport.

The lower wind speed was the main driver of the change in the thermal conditions of the Barra Bonita Reservoir by enhancing the duration of stratification events from 2009. The detrended simulation generated an artificial condition by removing the natural variability in wind speed, resulting in a permanently mixed water column. This analysis revealed that the annual trends in air temperature, air relative humidity and rainfall, although significant, were not enough to promote such hydrodynamic change. Therefore, air temperature and wind speed were the main driving factors of the warming trends in the reservoir. Each driver alone may not be strong enough to cause a major shift in the temperature indicators, but their combined effects interact synergistically by increasing gains (increasing air temperature) and decreasing losses (decreasing wind speed) from the energy budget.

Increased air temperature and decreased wind speed were also drivers of warmer temperatures and stronger stability in other lentic systems (Magee and Wu, 2017; Moras et al., 2019; Woolway et al., 2019; Zhang et al., 2015). The relative contribution of each forcing variable merits further investigation, but it is beyond the scope of the present study. Not only long-term temporal changes over the study period, but also antecedent conditions, large-scale meteorological forcing, and anomalies in atmospheric circulation may also be important drivers of water warming (Zhong et al., 2016).

4.4.4 Potential implications on water quality

Understanding water temperature trends and changes in the thermal structure of reservoirs are of great ecological significance because they can trigger a chemical reaction, cellular

temperature-dependent processes, and impact the habitat for macroinvertebrates and fishes, exerting a strong control on the ecosystem's biogeochemistry and ecology. Climate change will not result in a single change, but rather in a set of related consequences, and may pose further threats and complexity to freshwater ecosystems functioning (Sahoo et al., 2016) potentially impairing current multiple uses of water and its ecosystem services.

The Barra Bonita Reservoir receives high nutrient inputs from its catchment basin. Warming trends and stronger stability suggest that the current eutrophication related problems will probably become more drastic, adding further stress to the ecosystem, hampering the path to its sustainable use. One can foresee that mixing events could be severely reduced by the stronger stability if detected trends continue in the future. Greater water column stability and warmer temperatures, especially during winter, may favour algal blooms (Elliott, 2012) and extend its occurrence beyond summer season, as typically occurs, with further implications to the general reservoir ecology. Moreover, higher temperatures may exceed limits not only for the phytoplankton, but also for fishes, allowing some species to expand their range and forcing others to decline (Bachmann et al., 2020). In the tropics, the water temperature increase may strongly threaten species currently exposed to high temperatures, as the thermal optima and limits are close to current maximum ambient temperatures, leaving them with little scope for adapting to higher temperatures (Harrod, 2015).

The present results can be used as a proxy for future planning. Deeper insights could come from a robust and integrated climate–hydrologic–reservoir–ecological modelling framework (Sharma et al., 2018), moving towards a more resilient society and ecosystem to the reservoir warming up. While not in the scope of this study, management techniques at reservoir and catchment scales have the potential to buffer climate change signals (Yasarer and Sturm, 2016).

4.5 Conclusions

A simulation of hydrodynamics in the Barra Bonita Reservoir from 1993 to 2018 was conducted by applying a one-dimensional hydrodynamic model calibrated and validated using

field data from the study site. The mass balance and the vertical water temperature were reliably reproduced, revealing that the warming up process in the reservoir is already underway. A significant increasing temperature trend was detected along the whole water column, with annual trends varying from 0.33 °C/decade at the bottom to 1.02 °C/decade at the surface; stronger stability, at a rate of 12.83 J m⁻² per decade; and an increase of 19.40 stratified days per decade.

Surface water temperature in Barra Bonita Reservoir and the number of stratification events are increasing as a response of increase air temperature and decrease wind speed. Such changes in meteorological forcing also impact temperature of deep waters because frequent mixing events transfer heat from the surface to the bottom, mainly during the dry and cold season when water level is lower and colder water is withdrawn from a deep outlet structure. Furthermore, the greatest rates of air temperature increase were detected during the dry cold season and directly reflected in the deepwater warming in the reservoir.

Even though many studies have evaluated the impacts of climate change on lentic systems under temperate climate, literature is consensual that limited information is available for water bodies in lower latitudes. The present study identifies hydrodynamic changes in Barra Bonita Reservoir related to changes in meteorological forcing and discusses how the interaction between this latter and climatic, hydrological, hydrodynamic and operation characteristics reflects on the reservoir thermal response. The present findings are extendable to other polymictic reservoirs in the tropics and bring new contribution to understand how such water bodies may respond to climate changes.

Water temperature is a key variable controlling a large variety of physical, ecological, and biogeochemical processes, thus the current results might be of primary interest to water managers, as water warming will likely impact the associated ecosystems by the exacerbation of existing water quality problems. Expecting that climate is becoming more variable, resources need to be targeted at devising long-term monitoring programs and integrated modelling frameworks towards achieving a more accurate understanding of climate change effects on water resources that may help guide adaptation strategies.

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B

Appendix B to Chapter 4

Figure B.1. Linear correlation between inflow temperature and meteorological variables: maximum air temperature, minimum air temperature, mean air temperature, air temperature range, and insolation.

Figure B.2. Barra Bonita Reservoir location, tributaries, and monitoring stations: meteorological stations (a) São Carlos and (b) São Simão; fluviometric station (c) in the reservoir and (d) in Tietê River; and (e) water quality station in the middle of the central body of the reservoir.

Figure B.3. Flowchart of the methodological steps applied in this study.

Figure B.4. Normalised sensitivity coefficient (SI) for eleven GLM parameters. **Figure B.5.** Simulated (blue line) and measured (red line) water level for calibration and validation periods. **Figure B.6.** Simulated (blue line) and measured (red marker) water temperature for calibration and validation periods (a) at the surface, and (b) at 10 m depth.

Figure B.7. Model performance for water temperature for calibration (black line; 2008–2012) and validation (grey line; 2003–2007 and 2013–2018) periods (a) according to depth, (b) at a monthly scale (for those months with available data).

Figure B.8. Simulated versus observed water temperature along the vertical profile in Barra Bonita Reservoir from 2003 to 2018.

Figure B.9. Contour plot of simulated water temperature in Barra Bonita Reservoir for the 2003–2018 period.

Figure B.10. Annual measured meteorological and hydrological input variables (circles) during 1993–2018, the shaded area representing their annual standard deviation, Sen's slope (solid line), and its 95% confidence interval represented by the dotted lines.

Figure B.11. Monthly trends for the simulated indicators of hydrodynamics during the period 1993–2018 for the non-detrended analysis (a–d) and for the detrended analysis (e–h). The shaded areas indicate 95% confidence intervals for Sen’s slopes, which means that the trend is greater (or smaller) than zero with 95% confidence if the shaded area is above (or below) the zero line for each month.

Figure B.12. Mechanisms of the thermal response in Barra Bonita Reservoir that alter the amount of heat input into deep waters and enhances warming trends in bottom waters.

Table B.1. Monitoring stations.

Station	Code	Data type	Provided by	Latitude	Longitude
a	83726	Meteorologic	INMET	21°58'49''S	47°53'02''W
b	83669	Meteorologic	INMET	21°27'40''S	47°34'46''W
c	19040	Fluviometric	ANA	22°36'46''S	48°20'52''W
d	62541000	Fluviometric	CETESB	22°57'26''S	47°49'14''W
e	TIBB02700	Water quality	CETESB	22°32'30''S	48°26'42''W

Table B.2. Symbol, description, initial values (Hipsey et al., 2014), range for calibration, and calibrated values for GLM parameters and multiplicative factors.

Symbol	Description	Initial value	Range	Calibrated value
<i>Layer structure</i>				
$h_{\min}$	Minimum layer thickness (m)	0.5	0.1 – 0.5	0.1
$h_{\max}$	Maximum layer thickness (m)	1.5	0.6 – 3.0	2.3
<i>Mixing</i>				
C_K	Mixing efficiency of convective overturn	0.20	0.10 – 0.27	0.12
C_W	Mixing efficiency of wind stirring	0.23	0.20 – 0.90	0.60
C_S	Mixing efficiency of shear production	0.30	0.06 – 0.30	0.06
C_T	Mixing efficiency of unsteady turbulence	0.51	0.20 – 0.56	0.52
C_{KH}	Mixing efficiency of Kelvin-Helmholtz billows	0.30	0.25 – 0.35	0.35
C_{HYP}	Mixing efficiency of hypolimnetic turbulence	0.50	0.20 – 0.55	0.32
<i>Surface heat flux</i>				
ce	Bulk aerodynamic coefficient for latent heat transfer	0.0013	0.0011 – 0.0026	0.0015
ch	Bulk aerodynamic coefficient for sensible heat transfer	0.0013	0.0013 – 0.00132	0.0013
cd	Bulk aerodynamic coefficient for transfer of momentum	0.0013	0.0012 – 0.0019	0.0019
<i>Multiplicative factors</i>				
wind	Wind speed factor	1.00	0.70 – 1.30	1.20
sw	Shortwave radiation factor	1.00	0.70 – 1.30	1.08
lw	Longwave radiation factor	1.00	0.70 – 1.30	0.71
at	Air temperature factor	1.00	0.70 – 1.30	1.05
rh	Air relative humidity factor	1.00	0.70 – 1.30	1.20
rain	Rainfall factor	1.00	0.70 – 1.30	1.03
inflow	Inflow discharge factor	1.00	0.90 – 1.10	0.95
outflow	Outflow discharge factor	1.00	0.90 – 1.10	1.00

Table B.3. Formula, range, optimum value, and unit of model performance measures. N is the number of observations, O_i and S_i are the “ i^{th} ” observed and simulated data, respectively (Willmott, 1981; Bennett et al., 2013).

Measures of model performance	Formula	Range	Perfect match	Unit
Mean observed variable ($\bar{O}$)	$\bar{O} = \frac{\sum_{i=1}^N O_i}{N}$	$[-\infty, \infty]$	-	$^{\circ}\text{C}$
Mean simulated variable ($\bar{S}$)	$\bar{S} = \frac{\sum_{i=1}^N S_i}{N}$	$[-\infty, \infty]$	-	$^{\circ}\text{C}$
Standard deviation of the observed variable (s_O)	$s_O = \sqrt{\frac{\sum_{i=1}^N (O_i - \bar{O})^2}{N}}$	$[0, \infty]$	0	$^{\circ}\text{C}$
Standard deviation of the simulated variable (s_S)	$s_S = \sqrt{\frac{\sum_{i=1}^N (S_i - \bar{S})^2}{N}}$	$[0, \infty]$	0	$^{\circ}\text{C}$
Intercept (a) and slope (b) of the least-squares regression	$S_i = a + bO_i$	$[-\infty, \infty]$	0; 1	-
Mean Absolute Error (MAE)	$MAE = \frac{\sum_{i=1}^N S_i - O_i }{N}$	$[0, \infty]$	0	-
Root Mean Square Error (RMSE)	$RMSE = \sqrt{\frac{\sum_{i=1}^N (S_i - O_i)^2}{N}}$	$[0, \infty]$	0	$^{\circ}\text{C}$
Mean Absolute Percentage Error (MAPE)	$MAPE = \frac{\sum_{i=1}^N O_i - S_i /O_i}{N} \times 100$	$[0, 100]$	0	%
Pearson correlation coefficient (r)	$r = \frac{\sum_{i=1}^N (S_i - \bar{S})(O_i - \bar{O})}{[\sum_{i=1}^N (S_i - \bar{S})^2 \sum_{i=1}^N (O_i - \bar{O})^2]^{1/2}}$	$[-1, 1]$	1	-
Percent bias (PBIAS)	$PBIAS = \frac{\sum_{i=1}^N (S_i - O_i)}{\sum_{i=1}^N O_i} \times 100$	$[-\infty, \infty]$	0	%
Mean Bias Error (MBE)	$MBE = \frac{\sum_{i=1}^N (S_i - O_i)}{N}$	$[-\infty, \infty]$	0	$^{\circ}\text{C}$

Table B.4. Model performance measures from simulated and observed temperature at 2-m intervals over the water column of Barra Bonita Reservoir from 2003 to 2018.

Goodness-of-fit metrics	Depth (m)							
	0	2	4	6	8	10	12	14
N	92	63	63	63	63	61	59	49
$\bar{O}$ (°C)	24.34	24.18	23.99	23.86	23.72	23.61	23.36	23.03
$\bar{S}$ (°C)	23.99	24.30	24.04	23.82	23.63	23.39	23.07	22.48
s_o (°C)	2.91	2.70	2.66	2.61	2.62	2.67	2.67	2.73
s_s (°C)	3.47	3.29	3.20	3.16	3.04	2.94	2.83	2.84
A	-2.83	-3.79	-3.59	-3.86	-2.81	-1.32	-0.18	0.37
B	1.10	1.16	1.15	1.16	1.11	1.05	1.00	0.96
MAE	1.15	0.86	0.80	0.78	0.70	0.74	0.80	0.96
RMSE (°C)	1.40	1.09	1.01	1.00	0.91	0.94	1.02	1.19
MAPE (%)	4.79	3.63	3.44	3.38	3.06	3.21	3.50	4.18
r	0.92	0.95	0.96	0.96	0.96	0.95	0.94	0.93
PBIAS (%)	-1.46	0.50	0.18	-0.16	-0.35	-0.96	-1.25	-2.35
MBE (°C)	-0.35	0.12	0.04	-0.04	-0.08	-0.23	-0.29	-0.54

Table B.5. Annual and seasonal trends of the indicators of hydrodynamic behavior and thermal conditions computed from the simulation with detrended wind speed in Barra Bonita Reservoir from 1993 to 2018.

Indicator	Annual	Summer	Autumn	Winter	Spring
Water temperature at surface (°C/decade)	0.25*	-0.05	0.36**	0.61**	0.16
Water temperature at 2 m depth (°C/decade)	0.26*	-0.05	0.37**	0.58**	0.16
Water temperature at 10 m depth (°C/decade)	0.25*	-0.05	0.35**	0.60*	0.16
Mean temperature along the water column (°C/decade)	0.25*	-0.05	0.35**	0.59**	0.16
Schmidt stability (J m^{-2} /decade)	0.40*	-0.02	0.63*	1.05***	0.50
Number of stratified days (days/decade)	0	0	0	0	0

*** for $p < 0.001$; ** for $p < 0.01$; * for $p < 0.05$.

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5

Parameter sensitivity analysis for water quality modelling of subtropical reservoirs

Under review by Ecological Modelling

Sensitivity analysis is a standard practice in modelling applications to investigate the relative importance of model components that control the system's behaviour. In this study, a sensitivity analysis was implemented to identify the most influential parameters in a coupled hydrodynamic-biogeochemical model applied for three subtropical reservoirs. The one-dimensional General Lake Model coupled to the Aquatic EcoDynamics model (GLM-AED) was used to simulate the dynamics of dissolved oxygen, total phosphorus, nitrate, ammonium, and chlorophyll-a. Results reveal consistent sensitivity patterns between reservoirs, especially for a subset of thirteen temperature multipliers affecting dissolved oxygen and nutrients. In contrast, the sensitivity of chlorophyll-a is highly site-specific. Additionally, the majority of parameters are medium or high sensitive, which indicates the need for a calibration procedure to improve model accuracy. The analysis provides a detailed understanding of the governing ecosystem dynamics as a step forward to model identifiability and guidance for future model calibration.

Keywords: lakes, aquatic ecosystem, biogeochemistry, GLM-AED, one-at-a-time method, calibration.

5.1 Introduction

Modelling lake ecosystems plays an essential role in limnological studies for water quality assessment. In response to the increased demand for ecosystem services in conjunction with the degradation of freshwaters at a global scale, lake models experienced a rapid growth in the 1990s and 2000s decades, also triggered by technological progress, expansion and specialisation of the modelling community, and a new focus on the user interfaces and visualisation (Robson, 2014). The rapid advances came along with challenges, mostly regarding the most suitable approach and complexity, uncertainty and reliability, and the usage of complex models and integration approaches (Gal et al., 2014). In recent years, lake modelling move towards open source codes, further efforts supporting software environments, and rich sources of data, such as high-frequency sensors and satellite images (Frassl et al., 2019). Accordingly to the huge advances in lake modelling in the past decades, the sensitivity analysis (SA) has been widespread applied and regarded as a standard practice in modelling applications (Schmolke et al., 2010; Shimoda and Arhonditsis, 2016). Following the increased use of sensitivity analysis methods, recently reviews assessed its variety, motivation, and scope (Norton, 2015), compiled the software tools and techniques most used (Douglas-Smith et al., 2020), stated a practical best practice workflow (Pianosi et al., 2016), suggested guidelines for the proper use of the methods (Saltelli et al., 2019), and discussed its usage to evaluate uncertainty of deterministic models (Uusitalo et al., 2015).

The SA can be a helpful tool to investigate the role and importance of model components, such as parameters and forcing data, in producing model responses. For assessing the SA of model parameters, the basic idea is to alter their values on the basis of an acceptable range and evaluate the subsequent changes in model output. The model is sensitive to a parameter if the outputs change markedly when the parameter value is changed; otherwise, if the output values change only little, it is robust to changes in parameter values within the model, thereby implying in a small sensitivity. The insights provided by the SA concern both the magnitude of the variations and the direction of change (Borgonovo and Plischke, 2016), which can help to understand the model's intrinsic behaviour by identifying the governing processes in the system and enhancing model formulations. For instance, the SA can be conducted for several purposes in ecological modelling, including for elucidating which parameters require additional research or

are insignificant (Nelson et al., 2020), the consequences from changing the dominant controls of a system (Gal et al., 2009), and the correlation between input parameters and lake characteristics, such as residence time, meteorological conditions and trophic status (Bruce et al., 2018).

The SA is classified into local or global procedures (Saltelli et al., 2004, p. 44). A local sensitivity is performed by the one-at-a-time (OAT) method, which assesses the model output change against variations of a single parameter, while keeping all others fixed at their initial values (Hamby, 1994). The global sensitivity estimates the overall response of model outputs when all parameters vary simultaneously within their perturbation range, considering not only the direct influence of each parameter, but also the joint influence due to their interactions. Conceptually, the global approach provides a better characterisation of the ecosystem's governing processes in the expense of a higher demanding computational effort. Although the usage of the global SA is advised in the literature (*e.g.* Baroni and Tarantola, 2014), there are relatively few applications in ecological modelling of aquatic ecosystems, and the OAT method is still the most largely used technique (Ferretti et al., 2016).

In the context of lake models, sensitivity analysis is commonly used to compile a list of influential parameters that have a significant impact on the model response and should be the focus of the calibration procedure (*e.g.* Darko et al., 2019; Me et al., 2018; Snorheim et al., 2017; Tan et al., 2018). It is generally true that only a relatively small subset of model parameters dominate a particular output variable. However, these sensitive parameters are hardly to be predicted based on the sole intuition in face of the large number of model parameters and the interactions among them. The SA can largely reduce the complexity of model calibration by factor prioritisation (Saltelli et al., 2008) and keeping the insignificant parameters fixed in face of their low influence on model output (Cariboni et al., 2007).

The primary objective of this study was to characterise the sensitivity of several water quality outputs from a coupled hydrodynamic-biogeochemical model (General Lake Model coupled to Aquatic EcoDynamics, GLM-AED) applied to three subtropical reservoirs in Brazil (Barra Bonita Reservoir, Promissão Reservoir, and Três Irmãos Reservoir) using sensitivity analysis. For this purpose, the aims were (1) to quantify the sensitivity of model outputs to varying parameter values by applying the one-at-a-time method, (2) to identify the similarities

and disparities in the model's behaviour between the reservoirs, and (3) to determine a subset of the most sensitive parameters for calibration guidance. Despite the GLM-AED model has been widely applied, a comprehensive SA on the model's parameters remains limited. There are few SA for hydrodynamic parameters in previous GLM applications (Bruce et al., 2018; Bueche et al., 2019; Ladwig et al., 2018; Soares et al., 2020; Weber et al., 2017), and only one study performed the sensitivity analysis of AED model parameters (Ladwig et al., 2020). As the sensitivity analysis of the GLM-AED is, therefore, quite unexplored, especially for subtropical reservoirs, the motivation of this analysis was centered on gaining deeper knowledge about the most sensitive biogeochemical parameters and the properties of the actual ecosystems as a means to provide potential insights for model applications.

5.2 Material and methods

5.2.1 Sites description

Three reservoirs were selected for the current study: Barra Bonita Reservoir (BB), Promissão Reservoir (PR), and Três Irmãos Reservoir (TI), located southeast Brazil in the highest demographic density region in the country (Figure 5.1). The reservoirs were chosen for (i) their varied range of morphometric and water quality features (Table 5.1), (ii) their same climate condition (subtropical Cwa, according to Köppen, 1948), with an average air temperature of 22.6 °C and an annual rainfall of 1400 mm (INMET, 2019), and (iii) the availability of field data for model input. All three reservoirs were built in the Tietê River envisioning electricity generation and navigation to attend to the country demand. Nowadays, the reservoirs are intended for multiple uses. Between these reservoirs, there are other three reservoirs along the river, composing a cascade system. The other reservoirs were not selected for this study due to the lack of field data.

Barra Bonita (22°31'11'' S, 48°32'04'' W) is a meso-hypereutrophic reservoir located in an urbanised catchment, where is situated São Paulo Metropolitan Region and around of 24 million inhabitants (IBGE, 2019). It has been heavily loaded by sewage deriving from urban areas, resulting in a high-nutrient state (CETESB, 2019). It has a polymictic regime, with short

timescales of stratification. BB Reservoir is the shallowest and smallest of the three study sites, with a surface area of 226 km², maximum depth of 23.5 m, and residence time of 91 days. Promissão Reservoir (21°17'51'' S, 49°46'47'' W) is mesotrophic and monomictic. Summer stratification occurs from October to April, with surface temperatures of 25.9 °C and hypolimnetic temperatures of 22.9 °C. PR Reservoir has a surface area of 522 km², maximum depth of 24.5 m, and residence time of 141 days. Três Irmãos (20°40'10'' S, 51°17'57'' W) is the most downstream reservoir of the cascade system, and the largest one. It is an oligotrophic and monomictic water body. Summer stratification is also from October to April, with surface temperature of 26.3 °C. TI Reservoir has a surface area of 654 km², maximum depth of 45.6 m, and residence time of around 1.2 year.

Figure 5.1. Location of the study sites in southeast Brazil, monitoring stations, and their bathymetry. BB is Barra Bonita Reservoir, PR is Promissão Reservoir, and TI is Três Irmãos Reservoir.

Table 5.1. Morphometric features (AESTietê, 2019; CESP, 2013), mixing regime (Soares et al., 2020), and trophic status (Rotta et al., 2021; Watanabe et al., 2019) for all reservoirs.

	Barra Bonita	Promissão	Três Irmãos
Abbreviation	BB	PR	TI
Initial operation	1964	1975	1991
Elevation (m. a. s. l.)	451.5	384.0	328.0
Maximum volume (10^9 m ³)	3.16	8.11	11.46
Surface area at crest (km ²)	226	522	654
Maximum depth (m)	23.5	24.5	45.6
Hydraulic residence time (days)	91	141	442
Mixing regime	polymictic	monomictic	monomictic
Trophic status	meso-hypereutrophic	mesotrophic	oligotrophic

5.2.2 Model description

The process-based one-dimensional (1D) vertical General Lake Model (GLM; Hipsey et al., 2019) can be dynamically coupled to the Aquatic EcoDynamics library (AED; Hipsey et al., 2013) for modelling the hydrodynamics and biogeochemical processes in a variety of lentic water bodies, such as deep and shallow lakes, reservoirs, mining pit lakes, wastewater ponds, and urban wetlands. GLM-AED model was well-suited for this study because of its (1) freely and open source availability, which encourages future reproduction of the current study, (2) the 1D assumption that the vertical gradients are significantly larger than the horizontal ones is valid for the study sites, as previously assessed (Soares et al., 2020), and (3) recent applications in peer review studies (Bucak et al., 2018; Farrell et al., 2020; Fenocchi et al., 2019; Ladwig et al., 2018; Snorheim et al., 2017; Weng et al., 2020).

GLM simulates the vertical profiles of temperature, salinity and density by accounting for the effect of inflows and outflows on the water balance, in addition to surface heating and cooling, energy balance, and vertical mixing. The equations are based on assumptions that are common to previous model applications (Hamilton and Schladow, 1997; Imberger and Patterson, 1990). A flexible Lagrangian layer structure is used to discretise the water column into horizontal layers with homogeneous physical properties. The layer thickness can change by contraction and expansion in response to inflows, outflows, mixing with adjacent layers, and surface mass fluxes. The thermal processes of stratification and mixing are computed from the water balance and the energy budget at every time step. The water balance accounts for the effects of surface mass fluxes, inflows, and outflows. The energy budget is calculated based on the balance between

kinetic and potential energy: potential energy is stored during stratification periods, as the water density gradient increases; and turbulent kinetic energy is provided by wind stirring, convective overturn, shear production between layers, and Kelvin–Helmholtz billowing.

The vertical profile of temperature and the incident shortwave radiation are provided by GLM as input to AED at every time-step of the simulation. They are used for the computation of temperature-dependent chemical and biological processes, as well as to adjust the light extinction coefficient. Finally, the light extinction coefficient is provided from AED to GLM in the next time-step of simulation for calculations of the thermal processes.

AED comprises numerous modules that are designed as individual components allowing for different conceptualisations, either simple or complex. Model components are able to simulate dissolved oxygen (DO), carbon (C), nitrogen (N), phosphorus (P), and silica cycles, including organic matter, inorganic suspended solids and several functional groups of phytoplankton and zooplankton.

5.2.3 *Model configuration*

The General Lake Model v. 2.2.0 was coupled to the Aquatic EcoDynamics v. 4 for the simulation of hydrodynamics and biogeochemical processes in BB, PR, and TI reservoirs. A baseline simulation was run for each reservoir by applying the input data described below, GLM parameters previously calibrated and validated (Soares et al., 2020), and all AED parameters were set at their initial values (Table C.1 in Appendix C) based on Hipsey et al. (2013), being identical between reservoirs. The period of simulation was from the first day with field measurements in 2008 (15th January for BB and 12th February for PR and TI) to 31st December 2016, with a 1-h time-step. The statistical software R 3.2.5 was used to simulate and analyse modelling results through the packages GLMr (Hipsey et al., 2014) and GLMtools (Read et al., 2014).

The conceptual model included hydrodynamic processes computed by GLM and AED modules of sedimentation fluxes, dissolved oxygen, carbon, nitrogen, phosphorus, organic matter, phytoplankton, and suspended solids. The dominant geochemical processes in the water column were represented: fluxes between water-sediment interface (constant sediment flux),

mineralisation of dissolved organic matter, hydrolysis of particulate organic matter, nitrification, denitrification, and phytoplankton primary production, respiration, vertical movement, excretion, and mortality. The phytoplankton composition was limited to include only one group due to the absence of biomass data reported by groups. All chlorophyll-a concentration was simulated as cyanobacteria, the dominant functional group in all three reservoirs (CETESB, 2019; Santos, 2010). Fixed C:N and C:P ratios were assumed to model nutrient limitation with a half-saturation constant representing the effect of external nutrient concentrations on the phytoplankton growth rate. The conceptual diagram of the current application is illustrated in Figure 5.2.

Figure 5.2. Conceptual diagram of GLM-AED model for the current application.

Note: The white boxes are state variables: phytoplankton (Phyto), ammonium (NH₄), nitrate (NO₃), filterable reactive phosphorus (PO₄), dissolved inorganic carbon (DIC), dissolved organic nitrogen (DON), dissolved organic phosphorus (DOP), dissolved organic carbon (DOC), particulate organic nitrogen (PON), particulate organic phosphorus (POP), particulate organic carbon (POC), and dissolved oxygen (DO).

5.2.4 Required data

GLM requires the following input data: (i) reservoir's bathymetry, (ii) meteorological time-series, (iii) inflow and outflow discharges, and (iv) inflow temperature and salinity. In

addition, the following physical variables in the water body are required for setting initial conditions for the first day of the simulation and for model performance assessment: vertical profile of water temperature and salinity, water level, and light extinction coefficient. The hypsographic curve of each reservoir was extracted from the bathymetric survey performed by previous studies (BB Reservoir: Corrêa Filho et al., 2003; PR Reservoir: Maia, 2006; TI Reservoir: Albertin et al., 2010).

Terrestrial-based meteorological stations operated by the National Institute of Meteorology (INMET, 2020) provided hourly time-series of air temperature, wind speed, solar radiation, air relative humidity, and rainfall (green markers A–C in Figure 5.1). The missing values were filled by linear regression with data from a meteorological station with high correlation coefficient ($r > 0.72$, p -value < 0.05). Cloud cover data was not available and it was estimated by GLM through the Bird Clear Sky model. Daily hydrological data (inflow and outflow discharge, and water level) were provided by the National Water Agency (ANA, 2018). Gaps in daily inflow and outflow discharge were rare (less than 0.6% of total data), and they were filled by linear interpolation. Inflow temperature and electrical conductivity (which was used for the estimation of inflow salinity) were measured generally every two months by the Environmental Company of the State of São Paulo (CETESB) at their main tributaries (purple markers a–d in Figure 5.1; ANA, 2019). Due to the small salinity content and its low influence in freshwater systems, its mean value (below 0.2 pss) was assumed for the entire simulation period. Box plots are used to present monthly means and range of GLM input data across all three reservoirs from 2008 to 2016 (Figure 5.3). All the assumptions made, as well as all the processing of the physical variables required by the hydrodynamic model, were assumed exactly the same as a previous application of GLM for these reservoirs. Further detailed description is provided by Soares et al. (2020).

Figure 5.3. Monthly input data from 2008 to 2016 across Barra Bonita Reservoir, Promissão Reservoir, and Três Irmãos Reservoir: air temperature, wind speed, rainfall, relative humidity, solar radiation, inflow discharge, outflow discharge, and inflow temperature. Horizontal lines represent the median, 25th and 75th percentiles. Whiskers indicate the 5th and 95th percentiles.

AED requires the daily inflow nutrient concentrations as input data. In addition, the state variables measured in the water body are required for setting initial conditions for the first day of the simulation and for performance assessment. Input loads of DO, nitrate (NO₃), ammonium (NH₄), total phosphorus (TP), and chlorophyll-a were measured in the Tietê River (stations a, c, d in Figure 5.1) and the Piracicaba River (station b) every two months by CETESB (purple markers a–d in Figure 5.1; ANA, 2019). The mean seasonal input loads to the model were calculated each year for the wet period (from October to March) and the dry period (from April to September). Nutrient concentrations in minor tributaries were neglected due to the lack of field data. Box plots are used to present seasonal means and range of AED input data across all three reservoirs from 2008 to 2016 (Figure 5.4). Water temperature, salinity, Secchi depth, DO, NO₃, NH₄, TP, chlorophyll-a, and pH were collected from one monitoring station located at a central location in each reservoir (yellow markers 1–3 in Figure 5.1). Measurements were performed every two months by CETESB (2019) at water surface.

Figure 5.4. Seasonal input concentrations from 2008 to 2016 across Barra Bonita Reservoir (BB), Promissão Reservoir (PR), and Três Irmãos Reservoir (TI): dissolved oxygen (DO), nitrate (NO_3), ammonium (NH_4), total phosphorus (TP), and chlorophyll-a (chl-a). Horizontal lines represent the median, 25th and 75th percentiles. Whiskers indicate the 5th and 95th percentiles.

5.2.5 Sensitivity analysis

A local sensitivity analysis was applied for the baseline simulation of Barra Bonita Reservoir, Promissão Reservoir, and Três Irmãos Reservoir with reference to five state variables: DO, TP, NO_3 , NH_4 , and chlorophyll-a. A set of 64 AED parameters (Table C.1 in Appendix C) was selected for characterizing the entire system. The one-at-a-time (OAT) method was adopted by quantifying the effect of the variation of a given parameter on the model output while all other parameters were kept at their initial values. GLM parameters were not included because their sensitivity analysis was previously assessed for the current study sites (Soares et al., 2020).

The conventional variation by a fixed percentage of the initial parameter value, *e.g.* $\pm 10\%$ (Bucak et al., 2018), $\pm 20\%$ (Bruce et al., 2018), and $\pm 50\%$ (Rangel-Peraza et al., 2016), is problematic. First, because the model response to parameter variations is nonlinear, then small

initial values lead to a small variation while high initial values lead to a large variation; second, if the initial parameter value is located nearby the upper or lower bound of the range, the variation can lead to inadmissible values beyond the valid boundaries of the range (Lenhart et al., 2002). As the sensitivity of the model output can be significantly different according to the selected perturbation range (Yi et al., 2016), instead of increase and decrease parameter values by a defined percentage, each parameter's entire range of possible values was defined by the minimum and maximum values found in previous applications of one-dimensional lake models in order to assess true parameter sensitivities (Table C.1 in Appendix C).

The sensitivity of the model output to parameters values changing was quantified using a normalised sensitivity indicator (SI), equal to the ratio between the change in a model output variable compared to the baseline model output for the respective variable and the change in model parameter compared to its initial value, calculated as:

$$SI = \frac{\Delta Y/Y}{\Delta X/X} \quad (5.1)$$

where Y is the model performance for the reference value X of the parameter, which has a variation ΔX from its maximum value to its minimum value in a single step, i.e. $\Delta X = X_{\text{maximum}} - X_{\text{minimum}}$, generating a model performance variation ΔY .

A value of SI equal to 1 or -1 indicates a proportional change of the model output for the respective change of a model parameter value. The sensitivity index was classified according to Lenhart et al. (2002) into four classes: $0 \leq |SI| < 0.05$ is small to negligible, $0.05 \leq |SI| < 0.20$ is medium, $0.20 \leq |SI| < 1.00$ is high, and $|SI| \geq 1.00$ is very high. The objective function applied for model performance assessment was the root mean square error (RMSE), calculated as:

$$RMSE = \sqrt{\frac{\sum_{i=1}^N (S_i - O_i)^2}{N}} \quad (5.2)$$

where N is the number of observations, O_i and S_i are the “ith” observed and simulated data, respectively. The first year of simulation (2008) was considered as a warm-up period, and thus it was not included for performance assessment to ensure the independence of the simulation results from the initial conditions.

5.3 Results

The sensitivity analysis for five output variables (DO, TP, NH_4 , NO_3 , and chlorophyll-a) was applied to 64 parameters (Figure 5.5). In total, the sensitivity analysis resulted in 960 values of SI, which ranged from -2.35 to 1.68 , revealing the most critical parameters that govern the simulated water quality outputs in each site. A minority of 19 parameter changes resulted in SI values within the negligible range (i.e. $|SI| < 0.05$) in all three reservoirs, while the other 45 parameter changes resulted in some sensitivity in model output for at least one of the five state variables.

The analysis indicates the importance of the temperature multipliers, as all of them presented at least medium sensitivity for some variable. Additionally, it also demonstrates the influence of nitrogen-related parameters (Fsed_nit, theta_nitrif, and theta_sed_nit) and phytoplankton growth (R_growth, theta_growth), respiration (theta_resp), and temperature limitation (theta_opt, theta_max), which were consistently sensitive across reservoirs.

Common sensitivity features could be quantified between reservoirs: (1) DO concentration is clearly affected by temperature multipliers. However, there was some effect of varying other parameters on DO concentration, particularly Fsed_oxy, Fsed_nit, Fsed_doc, R_growth, and R_resp; (2) the nitrogen-related output variables, NH_4 and NO_3 , were sensitive mainly to parameters associated with the specific output, i.e. parameters that are part of the equations used to calculate the output variable in question. For instance, NH_4 was most sensitive to Fsed_amm, R_nitrif, K_nitrif, theta_nitrif, and theta_sed_amm. Similarly, nitrate was found to be sensitive to Fsed_nit and theta_sed_nit, whereas all other parameters had a little effect on this modeled variable; (3) in contrast, TP was sensitive to parameters that are not directly related to it, such as theta_sed_amm, theta_sed_nit, and theta_doc_miner, thereby demonstrating the usefulness of the method for exploring the ecosystem governing processes.

Figure 5.5. Sensitivity indices for 64 parameters in Barra Bonita (BB), Promissão (PR), and Três Irmãos (TI) reservoirs based on a 8-year period relative to a) dissolved oxygen, b) total phosphorus, c) ammonium, d) nitrate, and e) chlorophyll-a concentration.

The sensitive factors for the five constituents share some similarity, although clear disparities existed. The most notable difference between reservoirs is related to the sensitivities of chlorophyll-a. While none parameter was medium or high sensitive in Promissão Reservoir regarding chlorophyll-a at water surface, there were twelve sensitive parameters in Barra Bonita Reservoir, all of them from the phytoplankton sub-model (except for θ_{doc_miner}). In Três Irmãos Reservoir, chlorophyll-a was sensitive to 35 out of 64 parameters (55%), relative to all the sub-models components.

5.4 Discussion

5.4.1 Similarities between reservoirs

The results successfully distinguished the influential parameters for each state variable. The temperature multipliers were found as an important factor for the ecosystem in Barra Bonita, Promissão, and Três Irmãos reservoirs, being more influential than their corresponding parameters. Indeed, the temperature coefficients were higher than their related rates for sediment fluxes ($\theta_{sed_oxy} > F_{sed_oxy}$, $\theta_{sed_amm} > F_{sed_amm}$, $\theta_{sed_nit} > F_{sed_nit}$, and $\theta_{sed_frp} > F_{sed_frp}$), nitrification ($\theta_{nitrif} > R_{nitrif}$), denitrification ($\theta_{denit} > R_{denit}$), hydrolysis ($\theta_{pon_miner} > R_{pon_miner}$, $\theta_{pop_miner} > R_{pop_miner}$, and $\theta_{poc_miner} > R_{poc_miner}$), and mineralisation ($\theta_{don_miner} > R_{don_miner}$ and $\theta_{dop_miner} > R_{dop_miner}$). The same features were observed for phytoplankton growth ($\theta_{growth} > R_{growth}$) and respiration ($\theta_{resp} > R_{resp}$ for most variables). Ecologically, this means that a dominant system driver is the water temperature, which highly influences temperature-dependent processes as a core mechanism used to balance the nutrient budget in the reservoirs.

The importance of temperature multipliers influencing state variables as indicated in this analysis might be attributed to the regional subtropical climate resulting in quite warm surface waters in the study sites, which varied in a range of 16.7–30.9 °C in BB Reservoir, 18.5–33.4 °C in PR Reservoir, and 20.6–32.0 °C in TI Reservoir (Soares et al., 2020). In line with the high sensitivities found for temperature multipliers in simulated biogeochemical dynamics, the

importance of suitable water temperature is corroborated by the fact that the optimum and maximum temperature were consistently sensitive for the three reservoirs. As the temperature multipliers directly affects the response of biogeochemical rates to water temperature, potential implications can be foreseen in respect to climate change and water warming globally (O' Reilly et al., 2015).

The observed sensitivities for dissolved oxygen at water surface are consistent with qualitative expectations on the basis of the conceptual model. DO was most sensitive to parameters that directly affect oxygen utilisation in the water column (θ_{nitrif} , $\theta_{\text{doc_miner}}$) and in the sediments ($F_{\text{sed_oxy}}$, $F_{\text{sed_nit}}$, $F_{\text{sed_doc}}$, $\theta_{\text{sed_oxy}}$). Another informative trend is the high sensitivities to parameters that indirectly control photosynthetic oxygen production by changing the growth of phytoplankton (R_{growth} , θ_{growth} , θ_{opt} , θ_{max} , R_{resp} , and θ_{resp}).

Changing phytoplankton growth (R_{growth} and θ_{growth}), respiration (R_{resp} and θ_{resp}), and temperature limitation (θ_{opt} and θ_{max}) parameters affected dissolved oxygen and nutrient concentrations; whereas parameters related to phytoplankton nutrient uptake had a minimal effect on them. The processes of hydrolysis of particulate organic matter into dissolved organic matter and its mineralisation into dissolved inorganic matter appeared highly robust against the parameterization as perturbations of their initial values ($R_{\text{pon_miner}}$, $K_{\text{pon_miner}}$, $R_{\text{don_miner}}$, $K_{\text{don_miner}}$, $R_{\text{pop_miner}}$, $K_{\text{pop_miner}}$, $R_{\text{dop_miner}}$, $K_{\text{dop_miner}}$, $R_{\text{poc_miner}}$, $K_{\text{poc_miner}}$, $R_{\text{doc_miner}}$, and $K_{\text{doc_miner}}$) rarely produced considerable changes in state variables. In face of the consistency of the abovementioned similarities between reservoirs, it is expected that the sensitive parameters found in this study could be quite transferable to other reservoirs with the same climate condition.

5.4.2 Disparities between reservoirs

The sensitivity analysis reveals that although all reservoirs are subjected to the same kinetic processes and functional group of phytoplankton, the dynamic behavior is controlled by different sensitive parameters. Most noticeably, remarkable differences appeared regarding chlorophyll-a sensitivities in each reservoir. In BB and PR reservoirs, chlorophyll-a was not considerably sensitive to any parameter out of the phytoplankton sub-model (except for

theta_doc_miner in BB Reservoir). The minimum influence of parameters changes on chlorophyll-a output may be attributed to the trophic condition in the water bodies. As both of them are nutrient-rich, parameter changes in the assigned range were not enough to provoke considerable changes in chlorophyll-a in face of the high availability of TP, NH_4 , and NO_3 in water surface. In contrast, in the oligotrophic TI Reservoir, chlorophyll-a was sensitive to 24 parameters out of 44 (55%) from the DO, C, N, and P sub-models. Additionally, the importance of nutrient-related processes for chlorophyll-a concentration in TI Reservoir was confirmed by the high sensitivity of parameters such as theta_denit, theta_sed_amm, theta_sed_nit, theta_sed_frp, and theta_pop_miner that are related to key mechanisms for regulating nutrient recycling rates, such as denitrification, nutrient sedimentation fluxes, and mineralisation of particulate organic phosphorus. The differences in model behavior, particularly the sensitivity of chlorophyll-a to several parameters in TI Reservoir, demonstrate that oligotrophic ecosystems are more susceptible to parameterization than meso- and eutrophic reservoirs are.

Chlorophyll-a sensitivity to parameters related to the phytoplankton sub-model were surprisingly insensitive to the assumed variations in model parameters for Promissão Reservoir; however, quite similar sensitivities were found between BB and TI reservoirs. The dynamics of the chlorophyll-a at water surface is sensitive to the parameters that are related to phytoplankton growth (R_{growth} and θ_{growth}), water temperature (θ_{std} , θ_{opt} , and θ_{max}), uptake of phosphorus (X_{pcon}), and more pronounced to autotrophic respiration (R_{resp} and θ_{resp}). The sensitivity of chlorophyll-a to parameters that directly alter growth rates and the uptake of phosphorus is a common found in the literature (Darko et al., 2019; Jones et al., 2018; Schladow and Hamilton, 1997). The few exceptions to their similarities are the saturating light intensity (I_{S}), the metabolic loss by excretion to the dissolved organic pool (k_{fdom}), and the nutrients concentration below which uptake is zero (N_{o} and P_{o}). The sensitivity to light penetration in the water column observed only in BB Reservoir can be explained by its polymictic regime. In waters with strong vertical mixing, a higher turbidity along the water column reduces transparency resulting in a shallower euphotic zone, ultimately affecting the sufficient sunlight for photosynthesis. The sensitivity to nutrients concentration below which uptake is zero was found only in TI Reservoir and can also be explained by the different trophic

status between BB and TI reservoirs, as discussed above. On the basis of the variabilities found for chlorophyll-a sensitivity, it becomes clear that a SA is required to determine the most influential parameters for a particular water body.

5.4.3 *Implications for model calibration*

The outcomes of the sensitivity analysis provided a quantitative measure of the sensitivity of the output variables to the parameters changes. The majority of parameters being medium or high sensitive, as found in this study, clearly indicates that there is a potential uncertainty in their values that should be determined by a calibration procedure to improve model accuracy. All the remaining insensitive parameters could be fixed constant at their initial values and be removed from the calibration process. Based on the sensitivity indices, a posteriori calibration can concentrate on medium and/or high sensitive parameters given their large influence on the governing processes of the ecosystem. For instance, the number of model parameters to be included in a calibration could be reduced from 64 to 21 in BB Reservoir, 15 in PR Reservoir, and 39 in TI Reservoir (Table 5.2). In view of the still high number of sensitive parameters, particularly for TI Reservoir, the efficiency of calibration could benefit by selecting parameters from a descending order of sensitivity, i.e. firstly, prioritizing high sensitive parameters and, if needed, include other parameters following their sensitivity index. This guidance is valid for a calibration procedure that applies parameter ranges assigned in this study, as well as the same assumptions made regarding the model forcing functions.

The sensitivity of model outcomes to dissolved oxygen and nutrients have a more generalizable nature, as some of the medium, high, and very high sensitive parameters, such as *Fsed_nit*, *theta_nitrif*, *theta_sed_amm*, *theta_sed_nit*, *theta_sed_frp*, and *theta_pop_miner* to cite some, are often recognised as sensitive and used as tuning parameters for calibration in different lakes and reservoirs worldwide (*e.g.* Fenocchi et al., 2019; Gal et al., 2009; Me et al., 2018; Snorheim et al., 2017). In the case of chlorophyll-a in PR Reservoir, given the low sensitivity of the model output to changes in all parameter values, it is claimed that the calibration of DO and nutrients will be enough to achieve a good performance of chlorophyll-a simulation.

Table 5.2. Summary of biogeochemical parameters with medium and high sensitivity for Barra Bonita (BB), Promissão (PR), and Três Irmãos (TI) reservoirs.

Symbol	BB	PR	TI	Symbol	BB	PR	TI	Symbol	BB	PR	TI
Fsed_oxy	○	■	▲	theta_sed_amm	○	■	▲▲	theta_doc_miner	■	■	▲▲
Fsed_amm	○	○	■	theta_sed_nit	▲▲	■	▲▲	Ycc	■	○	▲
Fsed_nit	▲	▲	■	Ksed_frp	○	○	■	R_growth	■	■	■
Fsed_frp	○	○	■	theta_sed_frp	○	■	▲▲	theta_growth	▲	▲	▲
Fsed_pop	○	○	■	w_pon	○	○	■	theta_std	■	○	■
Fsed_poc	○	○	■	theta_pon_miner	○	○	▲	theta_opt	▲	▲	▲
Fsed_doc	○	▲	▲	theta_don_miner	○	○	▲	theta_max	■	■	▲
Ksed_oxy	○	○	■	w_pop	○	○	■	I_S	■	○	○
theta_sed_oxy	○	■	▲	Rdop_miner	○	○	■	R_resp	■	■	▲▲
Rnitrif	■	○	○	Kdop_miner	○	○	■	theta_resp	▲	▲	▲
Knitrif	■	○	■	theta_pop_miner	○	○	▲▲	k_fres	○	○	■
Kdenit	■	○	○	theta_dop_miner	○	○	■	k_fdom	■	○	○
Ksed_nit	■	○	○	w_poc	▲	○	○	N_0	○	○	■
theta_nitrif	▲▲	▲	▲	Kdoc_miner	○	○	■	P_0	○	○	■
theta_denit	▲	○	▲▲	theta_poc_miner	○	○	■	X_pcon	■	○	▲

Note: Sensitivity: ▲▲ very high; ▲ high; ■ medium; ○ low.

5.4.4 Limitations of the sensitivity analysis

For the purpose of this study, a local sensitivity analysis was conducted on selected model parameters using a one-at-a-time method. This approach is computationally very efficient compared to more demanding techniques and chosen in most practical cases. The sensitivity analysis was able to provide the sub-set of most influential parameters, revealing consistent similarities between reservoirs regarding nutrients parameters, as well as the particular sensitivities directly influenced by both the thermal regime and the trophic state, which should be assessed individually. Additionally, the method is a comprehensive guidance supporting a posteriori calibration procedure.

The one-at-a-time method, however, comprises a relatively simplistic process representation as it is unable to capture the interactions between parameters in such a complex ecological model. Hence, the method only explores a fraction of the input space of variations in parameter values. To overcome the inability of the local approach to account for interactions between parameters, a multiparameter or a global analysis is required for a complete understanding on how a complex and nonlinear model behaves (Saltelli et al., 2008). In global sensitivity analysis, such as the Monte-Carlo approach, all model parameters are iteratively adjusted within value ranges, resulting in several, even thousands, of simulations. Alternatively, the Morris method is based on the one-at-a-time approach but is classified as a global sensitivity

analysis because it samples partial derivatives at multiple locations in the input space. While the local approach does not capture some aspects of nonlinearity that can be captured by the global approach, we suggest that it is advantageous to consider the local analysis in model evaluation, possibly as a preliminary step to provide insights, which can be used to improve the design of more demanding methods.

5.5 Conclusions

The one-at-a-time method was implemented to conduct a local sensitivity analysis for a coupled hydrodynamic-biogeochemical model (GLM-AED) in three subtropical reservoirs. The analysis focused on the response of five water quality constituents, including DO, TP, NH_4 , NO_3 , and chlorophyll-a, to 64 parameters. The study shows the capability of the sensitivity analysis to explicitly identify the input parameters that exert the most influence on model outputs according to a defined perturbation range.

Three important insights were gained through the sensitivity analysis. First, the model behavior could be explained largely based on water temperature, as a subset of thirteen temperature multipliers were consistently higher sensitive than their corresponding rates between reservoirs. Although these results are specific to BB, PR, and TI reservoirs, this outcome is likely to be an indicator that those dominant parameters are generally important and their sensitivity would be also valid to other similar systems. Second, the patterns of parametric control on chlorophyll-a were somewhat unique for each reservoir. The differences were attributed to their thermal regime, either polymictic or monomictic, and their trophic status, either oligo-, meso-, or eutrophic, which suggests the importance of conducting systematic sensitivity analysis for a specific water body to acquire additional insights into the dynamics of the particular system. Finally, the high number of sensitive parameters confirms the need of the calibration procedure aiming at reducing parameter uncertainties and increasing model accuracy for a proper representation of the real ecosystems.

This study supplies an investigation of the governing ecosystem dynamics as a means to overcome the limited information from the subtropics. Additionally, the analysis further provides

a potential guidance for prioritizing research efforts by reducing the number of parameters that require calibration. In our future work, we will calibrate the model for each reservoir based on the sensitivity analysis results for better supporting future management decisions in the cascade reservoirs of the Tietê River.

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C

Appendix C to Chapter 5

Table C.1. Description of AED parameters, their units, initial values (Hipsey et al., 2013), and range for the sensitivity analysis.

Symbol	Description	Unit	Initial value	Range
<i>Sedimentation flux</i>				
Fsed_oxy	Sedimentation flux for dissolved oxygen	mmol m ⁻² d ⁻¹	6.00	-20.00 ^a – 87.50 ^b
Fsed_amm	Sedimentation flux for ammonium	mmol m ⁻² d ⁻¹	3.00	0.01 ^a – 22.16 ^c
Fsed_nit	Sedimentation flux for nitrate	mmol m ⁻² d ⁻¹	-14.00	-14.00 – -1.87 ^d
Fsed_frp	Sedimentation flux for filterable reactive phosphorus	mmol m ⁻² d ⁻¹	0.12	0.001 ^a – 0.84 ^b
Fsed_pop	Sedimentation flux for particulate organic phosphorus	mmol m ⁻² d ⁻¹	-0.01	-0.01 – 0 ^a
Fsed_dop	Sedimentation flux for dissolved organic phosphorus	mmol m ⁻² d ⁻¹	0.03	0.001 ^a – 0.10 ^a
Fsed_poc	Sedimentation flux for particulate organic carbon	mmol m ⁻² d ⁻¹	-0.01	-0.009 [*] – -0.011 [*]
Fsed_doc	Sedimentation flux for dissolved organic carbon	mmol m ⁻² d ⁻¹	30.00	0.01 ^c – 30.00
Fsed_ch4	Sedimentation flux for methane	mmol m ⁻² d ⁻¹	0.00	0 – 10.00 ^a
<i>Dissolved oxygen</i>				
Ksed_oxy	Half saturation constant of sediment oxygen flux	mmol m ⁻³	15.6	6.8 ^a – 51.6 ^c
theta_sed_oxy	Temperature multiplier for sediment oxygen flux	-	1.08	1.02 ^d – 1.14 ^d
<i>Nitrogen</i>				
Rnitrif	Maximum reaction rate of nitrification at 20 °C	d ⁻¹	0.03	0.01 ^b – 0.34 ^e
Rdenit	Maximum reaction rate of denitrification at 20 °C	d ⁻¹	0.01	0.0005 ^e – 0.50 ^f
Knitrif	Half saturation constant for oxygen dependence of nitrification	mmol m ⁻³	62.5	12.5 ^d – 93.7 ^e
Kdenit	Half saturation constant for oxygen dependence of denitrification	mmol m ⁻³	15.6	12.5 ^e – 18.0 ^a
Ksed_amm	Half saturation constant of ammonium flux	mmol m ⁻³	15.6	15.0 ^a – 65.7 ^c
Ksed_nit	Half saturation constant of nitrate flux	mmol m ⁻³	15.6	15.0 ^a – 23.4 ^d
theta_nitrif	Temperature multiplier for temperature dependence of nitrification	-	1.08	1.02 ^e – 1.14 ^e
theta_denit	Temperature multiplier for temperature dependence of denitrification	-	1.05	1.045 ^e – 1.08 ^e
theta_sed_amm	Temperature multiplier for sediment ammonium flux	-	1.08	1.07 ^a – 1.14 ^c
theta_sed_nit	Temperature multiplier for sediment nitrate flux	-	1.08	1.055 ^c – 1.08
<i>Phosphorus</i>				
Ksed_frp	Half saturation constant of filterable reactive phosphorus flux	mmol m ⁻³	15.6	15.6 – 69.5 ^c
theta_sed_frp	Temperature multiplier for sediment phosphate flux	-	1.08	1.032 ^c – 1.08

Cont. **Table C.1.** Description of AED parameters, their units, initial values (Hipsey et al., 2013), and range for the sensitivity analysis.

Symbol	Description	Unit	Initial value	Range
<i>Organic matter: nitrogen</i>				
w_pon	Settling rate of detrital nitrogen pool	m d ⁻¹	-1.0	-1.0 – -0.015 ^a
Rpon_miner	Maximum rate of hydrolysis of particulate organic nitrogen	d ⁻¹	0.01	0.003 ^g – 0.80 ^h
Rdon_miner	Maximum rate of mineralisation of dissolved organic nitrogen	d ⁻¹	0.01	0.003 ^e – 0.05 ^e
Kpon_miner	Half saturation constant for particulate organic nitrogen breakdown	mmol m ⁻³	78.0	31.25 ⁱ – 156.25 ^g
Kdon_miner	Half saturation constant for dissolved organic nitrogen mineralisation	mmol m ⁻³	78.0	31.25 ⁱ – 156.25 ^g
theta_pon_miner	Temperature multiplier for particulate organic nitrogen breakdown	-	1.08	1.02 ^e – 1.14 ^e
theta_don_miner	Temperature multiplier for dissolved organic nitrogen mineralisation	-	1.08	1.02 ^e – 1.14 ^e
<i>Organic matter: phosphorus</i>				
w_pop	Settling rate of detrital phosphorus pool	m d ⁻¹	-1.0	-1.0 – -0.03 ^a
Rpop_miner	Maximum rate of hydrolysis of particulate organic phosphorus	d ⁻¹	0.03	0.001 ^j – 0.50 ⁱ
Rdop_miner	Maximum rate of mineralisation of dissolved organic phosphorus	d ⁻¹	0.05	0.005 ^e – 0.05
Kpop_miner	Half saturation constant for particulate organic phosphorus breakdown	mmol m ⁻³	78.0	31.25 ⁱ – 156.25 ^g
Kdop_miner	Half saturation constant for dissolved organic phosphorus mineralisation	mmol m ⁻³	78.0	31.25 ⁱ – 78.1 ^e
theta_pop_miner	Temperature multiplier for particulate organic phosphorus breakdown	-	1.08	1.02 ^e – 1.14 ^e
theta_dop_miner	Temperature multiplier for dissolved organic phosphorus mineralisation	-	1.08	1.02 ^e – 1.14 ^e
<i>Organic matter: carbon</i>				
w_poc	Settling rate of detrital carbon pool	m d ⁻¹	-1.0	-1.0 – -0.05 ^a
Rpoc_miner	Maximum rate of hydrolysis of particulate organic carbon	d ⁻¹	0.01	0.001 ^a – 0.50 ⁱ
Rdoc_miner	Maximum rate of mineralisation of dissolved organic carbon	d ⁻¹	0.01	0.001 ^a – 0.50 ⁱ
Kpoc_miner	Half saturation constant for particulate organic carbon breakdown	mmol m ⁻³	78.0	31.25 ⁱ – 156.2 ^e
Kdoc_miner	Half saturation constant for dissolved organic carbon mineralisation	mmol m ⁻³	78.0	31.25 ⁱ – 156.2 ^e
theta_poc_miner	Temperature multiplier for particulate organic carbon breakdown	-	1.08	1.02 ^e – 1.14 ^e
theta_doc_miner	Temperature multiplier for dissolved organic carbon mineralisation	-	1.08	1.02 ^e – 1.14 ^e
<i>Phytoplankton</i>				
w_p	Phytoplankton sedimentation rate	m d ⁻¹	-0.02	-0.10 ^k – 4.32 ^b
Ycc	Carbon to chlorophyll-a ratio	mg C (mg chl-a) ⁻¹	50	45 [*] – 55 [*]
R_growth	Phytoplankton growth rate at 20 °C	d ⁻¹	1.9	0.6 ^d – 2.9 ^e
theta_growth	Arrhenius temperature scaling for growth	-	1.06	1.05 ^j – 1.11 ^l

Cont. **Table C.1.** Description of AED parameters, their units, initial values (Hipsey et al., 2013), and range for the sensitivity analysis.

Symbol	Description	Unit	Initial value	Range
theta_std	Standard temperature	°C	20.0	19.0 ^c – 23.0 ^l
theta_opt	Optimum temperature	°C	28.0	24.0 ^c – 30.0 ^d
theta_max	Maximum temperature	°C	35.0	32.0 ^k – 40.0 ^d
I_S	Saturating light intensity	$\mu\text{E m}^{-2} \text{s}^{-1}$	150	150 – 250 ^d
KePHY	Specific attenuation coefficient for phytoplankton	m^{-1}	0.005	0.002 ^a – 0.198 ^d
f_pr	Fraction of primary production lost to exudation	d^{-1}	0.005	0.005 – 0.070 ^c
R_resp	Phytoplankton respiration rate at 20 °C	d^{-1}	0.05	0.01 ^d – 0.09 ^m
theta_resp	Arrhenius temperature scaling for respiration	-	1.05	1.05 – 1.12 ^k
k_fres	Fraction of metabolic loss that is respiration	-	0.25	0.25 – 0.75 ^a
k_fdom	Fraction of metabolic loss that is dissolved organic matter	-	0.20	0.20 – 0.25 ^a
N_o	Nitrogen concentration below which uptake is zero	mmol N m^{-3}	0.25	0 ^a – 0.25
K_N	Half saturation concentration of nitrogen	mmol N m^{-3}	1.00	0.02 ^d – 3.50 ^k
X_ncon	Constant internal nitrogen concentration	$\text{mmol N (mmol C)}^{-1}$	0.035	0.035 – 0.380 ^c
P_o	Phosphorus concentration below which uptake is zero	mmol P m^{-3}	0.03	0 ^a – 0.03
K_P	Half saturation concentration of phosphorus	mmol P m^{-3}	0.05	0.002 ^d – 0.26 ^c
X_pcon	Constant internal phosphorus concentration	$\text{mmol P (mmol C)}^{-1}$	0.0015	0.0015 – 0.0020 ^a

Note: * As a range of values was not found in the literature, the $\pm 10\%$ range was adopted.

^a Farrell et al., 2020; ^b Burger et al., 2008; ^c Snorheim et al., 2017; ^d Kara et al., 2012; ^e Fenocchi et al., 2019; ^f Me et al., 2018;

^g Romero et al., 2004; ^h Schladow and Hamilton, 1997; ⁱ AED Science Manual (Hipsey et al., 2013); ^j Özkundakci et al., 2011;

^k Ladwig et al., 2018; ^l Bucak et al., 2018; ^m Cui et al., 2016.

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6

A sequential approach for modelling aquatic ecosystems in interconnected reservoirs along a cascade system

Submitted to Environmental Modelling & Software

Cascading systems of interconnected reservoirs have been constructed along large rivers worldwide, establishing a network of aquatic environments. To better understand the water quality along a cascade system, the General Lake Model coupled to the Aquatic EcoDynamics (GLM-AED) was applied to simulate biogeochemical processes in six reservoirs situated in the Tietê River (Brazil). The model was calibrated and validated against measured field data. The present study implements a novel approach that fully links reservoir processes along the cascade system, taking into account the feedback from one water body to the next. Different scenarios were simulated to explore whether the water quality and trophic state in connected aquatic ecosystems can be affected by a common restoration measure of reducing external nutrient loads. Modelling results demonstrated a synergistic interaction among reservoirs, revealing that management strategies could be amplified according to the location of the direct input load reduction.

Keywords: lakes, water quality, trophic state, GLM-AED model, scenarios, Tietê River.

6.1 Introduction

Cascade reservoirs consist of a chain of reservoirs constructed along a single river, which are hydrologically connected and whose operation is interrelated toward fulfilling a common goal (Straškraba and Tundisi, 1999). This configuration is usually adopted to improve the efficiency of hydroelectric energy production as numerous consecutive dams can better regulate the flow regime. Thus, a percentage of the generated energy in each reservoir is due to the regulated flow in the upstream ones. Additional benefits are that the excess water release from a reservoir with lower storage capacity can be saved in the storage of a downstream one and the downstream reservoirs within the system require a smaller storage volume. Many cascading systems of interconnected reservoirs have been constructed in sequence along large rivers worldwide, establishing a network of aquatic environments, for instance, in the Lancang River (China), the Tennessee River (USA), the Volga River (Russia), and the Zambezi River (southeastern Africa).

In cascade reservoir systems, the upstream ones affect the dynamics of those further downstream, and abiotic and biotic factors in the water accumulate until the last reservoir receives contributions from all the previous water bodies (Barbosa et al., 1999). Overall, water quality is highly affected by the cascade system as a result of the retention of the nutrients and pollutants in preceding reservoirs (Straškraba and Tundisi, 1999), leading to a trophic gradient from up to downstream. Additionally, cascade systems strongly influence the composition of phytoplankton (Hu et al., 2017), macroinvertebrates (Callisto et al., 2005), and fishes (Santos et al., 2018).

Globally, lakes and reservoirs are subject to intensive human pressure, especially to eutrophication, the major cause of the degradation of the ecological state in inland waters (Downing, 2014). The general causal factors of the systematic water quality degradation are high levels of nutrient inputs from the basin catchment (Vinçon-Leite and Casenave, 2019). In the Southern hemisphere, allochthonous nutrient loads from point sources are still the main stressor despite the fact that it was recognised more than 60 years ago that nutrients are critical for eutrophication in aquatic ecosystems (Jenny et al., 2020). For instance, in Brazil, the removal of nutrients from domestic sewage is far from satisfactory because the urbanisation process over the last decades was not accompanied by a proportional increase in sewage collection and treatment services, which has dramatically reduced the ecological quality of many lakes and reservoirs

(ANA, 2012). The most notable effect of eutrophication is the excessive proliferation of phytoplankton (Le Moal et al., 2019), which found a widespread increase since the 1980s (Ho et al., 2019).

Limnological research in a specific reservoir of such cascade systems is quite common, but studies in which the whole chain is considered step-like continuous systems are rare (Miranda and Dembkowski, 2016). Lakes and reservoirs interconnected in chains can be simulated as an isolated water body to represent internal processes individually. However, the use of an interconnected approach provides important insights into mechanisms acting among them, which brings relevant information for management purposes (Gerven et al., 2017; Hilt et al., 2011).

Coupled hydrodynamic-ecological models are often used to capture biogeochemical cycles and can provide an opportunity to evaluate an in-lake response to external forcing in the ecosystem. Despite the widespread application of models to lakes and reservoirs since the 1970s, previous modelling studies still do not consider the effects of connectivity along a cascade system. To better understand the role of reservoir connectivity on water quality along a cascade system, this study proposed a novel approach by coupling the General Lake Model to the Aquatic EcoDynamics (GLM-AED) to simulate biogeochemical dynamics in six reservoirs situated in the Tietê River (in southeast Brazil), taking into account the hydrological connection between reservoirs along the cascade. The sensitivity of each reservoir to reduce external nutrient loads, a common restoration measure, was assessed by the simulation of different scenarios to investigate the reservoirs' response in terms of water quality and trophic state improvements along the chain.

6.2 Methods

6.2.1 Site description

The Tietê River is situated in southeastern Brazil (Figure 6.1) in the region with the highest population density in the country. It has been subjected to successive damming since the 1960s aiming at power generation and navigation. Six reservoirs were built in the middle and lower stretches of the river, forming a cascade system of hydrologically and operationally

interconnected reservoirs, from upstream to downstream: Barra Bonita (BB), Bariri (BA), Ibitinga (IB), Promissão (PR), Nova Avanhandava (NA), and Três Irmãos (TI). Currently, these reservoirs have their navigation and hydroelectric potential highly exploited and they also serve multiple water uses, including drinking water supply, irrigation, fishery, flood regulation and tourism.

Figure 6.1. Six reservoirs along the cascade system, their location, bathymetry and monitoring stations.

Note: Each reservoir is associated with a two-letter code: Barra Bonita (BB), Bariri (BA), Ibitinga (IB), Promissão (PR), Nova Avanhandava (NA), and Três Irmãos (TI).

There are no important tributaries between the reservoirs neither in terms of discharge nor external loads, and the river stretch between them is short, varying from 22 km between BB and BA reservoirs to less than 7 km between the other reservoirs. The reservoirs have a varied range of morphometric features and water quality conditions (Table 6.1). They are situated in a sub-tropical climate (Cwa; Köppen, 1948) with an average air temperature of 22.6 °C and an annual rainfall of 1400 mm (INMET, 2019). The rainy season occurs from October to March, which accounts for more than 80% of the annual rainfall, and the dry season occurs from April to September.

Table 6.1. Morphometric features and water quality conditions for the six reservoirs along the cascade system (AESTietê, 2020; CESP, 2013; CETESB, 2019; Soares et al., 2020).

	BB	BA	IB	PR	NA	TI
Initial operation	1964	1969	1969	1975	1985	1991
Elevation (m. a. s. l.)	451.5	427.5	404.0	384.0	358.0	328.0
Maximum volume (10 ⁹ m ³)	3.16	0.61	1.10	8.11	2.83	11.46
Surface area at crest (km ²)	226	46	85	522	195	654
Maximum depth (m)	23.5	22.5	19.2	24.5	29.8	45.6
Hydraulic residence time (days)	91	15	23	141	46	442
Drainage area (km ²)	32,330	35,430	43,500	57,610	62,300	69,900
Mixing regime	polymictic	polymictic	monomictic	monomictic	monomictic	monomictic
Chlorophyll-a (µg L ⁻¹)	33.5 (35.1)	-	-	22.3 (53.9)	-	3.8 (2.6)
Total phosphorus (mg L ⁻¹)	0.17 (0.21)	-	-	0.03 (0.05)	-	0.02 (0.01)
Ammonium (mg L ⁻¹)	0.32 (0.36)	-	-	0.13 (0.08)	-	0.10 (0.02)
Nitrate (mg L ⁻¹)	3.14 (1.16)	-	-	0.95 (0.27)	-	0.65 (0.31)
Trophic status	meso-hyper	meso-hyper	meso-hyper	meso	meso	oligo

Water quality values: average value (standard deviation) for the study period (2008–2016).

Land uses in the drainage basin consist of agriculture (71%), native vegetation (10%), urban areas (7%), pasture (7%), water bodies (3%), and forestry (2%) (IBGE, 2018). Detailed land cover is presented in Figure D.1 in Appendix D. Most urban areas are in the upstream region, where the São Paulo Metropolitan Region is situated with around 24 million inhabitants. Since the 1970s, the uppermost reservoirs have been receiving high sewage volume from urban areas, resulting in high in-lake nutrient concentrations. As a result, BB, BA and IB reservoirs are classified as meso-hypereutrophic (Watanabe et al., 2019). In the middle reach, the intensive agricultural activities are the major nitrogen and phosphorus sources for PR and NA reservoirs, which have a mesotrophic status (Rotta et al., 2021). In contrast, nutrient inputs to the downstream reservoir (TI) are low.

6.2.2 Model description

The General Lake Model (GLM; Hipsey et al., 2019) is a deterministic one-dimensional hydrodynamic model that simulates physical dynamics in lentic water bodies. GLM can be dynamically coupled with the Aquatic EcoDynamics (AED; Hipsey et al., 2013) modules for representing the major biogeochemical processes influencing water quality. GLM-AED is suitable for deep and shallow lakes, reservoirs, mining pit lakes, wastewater ponds and urban wetlands. The choice of an 1D model in this study is supported by previous calculations based on the Wedderburn number (Soares et al., 2020). Furthermore, the GLM-AED model was well-suited because of (1) the flexibility of AED module configuration, (2) freely and open-source

availability, which encourages future reproduction of the current study, and (3) recent applications in peer review studies. GLM-AED was successfully applied to assess management strategies that address nutrient pollution (Weng et al., 2020), to explore the effects of changes in climate drivers on lake hypolimnetic anoxia (Snorheim et al., 2017), to estimate changes in concentrations of dissolved oxygen and phosphate under climate change (Ladwig et al., 2018), to reproduce future projections of deep-water chemistry and phytoplankton biomass (Fenocchi et al., 2019), and to model the effects of climate and land use changes on phytoplankton and water quality (Bucak et al., 2018).

GLM computes vertical profiles of temperature, salinity and density in lentic water bodies. The model employs a Lagrangian approach to represent horizontal layers, assuming each one as a control volume with homogeneous properties. Layers can contract, expand, merge and split in order to sufficiently resolve the vertical density gradient with fine resolution occurring in the thermocline and thicker cells where mixing occurs. GLM solves the water balance from surface mass fluxes, inflows and outflows. The model adopts an energy balance approach whereby mixing events occur when sufficient kinetic energy becomes available to overcome the potential energy stored by stable density gradients during stratification events (Hipsey et al., 2019).

The vertical profile of temperature is provided by GLM as an input to AED at every time-step of simulation for the computation of temperature-dependent chemical and biological processes. Incident shortwave radiation is also supplied by GLM to AED, where it is converted to photosynthetically active radiation for primary production, and the light extinction coefficient is dynamically adjusted to account for variability in the concentrations of algal, inorganic particulates, and dissolved organic carbon. Finally, the light extinction coefficient is provided from AED to GLM in the next time-step of simulation for calculations of shortwave penetration into the water column (Hipsey et al., 2013).

AED comprises numerous modules that are designed as individual components allowing for different conceptualisations, either simple or complex. Model components are able to simulate dissolved oxygen (DO), carbon (C), nitrogen (N), phosphorus (P), and silica (Si) cycles, including organic matter, inorganic suspended solids, and several functional groups of phytoplankton and zooplankton. DO equations account for atmospheric exchange, sediment

oxygen demand, organic matter mineralisation and nitrification, photosynthetic oxygen production and respiratory oxygen consumption. Both inorganic and organic, dissolved and particulate forms of C, N and P are modelled explicitly along the degradation pathway of particulate organic matter to dissolved organic matter and then to dissolved inorganic matter. The nitrogen cycle includes the additional processes of denitrification, nitrification, and nitrogen fixation. The phosphorus cycle also accounts for adsorption/desorption of filterable reactive phosphorus onto suspended solids. The silica cycle is simpler and is suitable for the simulation of diatoms. Phytoplankton biomass in the water column is determined by primary production, respiration, mortality, excretion, settling or resuspension, and grazing processes. Photosynthesis is parameterised as the uptake of carbon and limitation functions are implemented at non-optimal conditions of temperature, light and nutrient availability.

6.2.3 Required data

GLM requires the reservoir's bathymetry, meteorological time-series, inflow and outflow discharges, and inflow temperature and salinity. In addition, the following physical variables in the water body are required for setting initial conditions for the first day of the simulation, and for calibration and validation procedures: vertical profile of water temperature and salinity, water level, and light extinction coefficient. All the processing of the physical variables required by the hydrodynamic model, as well as all the assumptions made, were assumed exactly the same as a previous application of GLM in the current study sites. Its detailed description is provided by Soares et al. (2020).

AED requires daily inflow nutrient concentrations as input data. In addition, chemical and biological variables in the water body are required for setting initial conditions for the first day of the simulation, and for calibration and validation procedures. Concentrations of DO, nitrate (NO_3), ammonium (NH_4), total phosphorus (TP), and chlorophyll-a (chl-a) in the inflows were measured in the major tributaries of Barra Bonita Reservoir (station a in the Tietê River and station b in the Piracicaba River, which contribute with 63% and 28%, respectively, of the annual discharge into the reservoir, see Figure 6.1). Additionally, the filterable reactive phosphorus (PO_4) was measured only in the Piracicaba River (station b).

Water quality measurements in the reservoir's body were available only for BB, PR and TI reservoirs (stations 1, 2 and 3 in Figure 6.1), where concentrations of DO, TP, NO₃, NH₄, chl-a, and pH were measured on the surface. For the BB Reservoir, the vertical profile measurements of DO were also available. All required data were measured every two months by the Environmental Company of the State of São Paulo (CETESB; ANA, 2019) and were available for the 2008–2016 period.

6.2.4 Model configuration

The General Lake Model v. 2.2.0 was coupled to the Aquatic EcoDynamics v. 4 for the simulation of biogeochemical processes in each reservoir. AED modules of sedimentation fluxes, dissolved oxygen, carbon, nitrogen, phosphorus, organic matter, phytoplankton, and suspended solids were included to represent the dominant fluxes in the water column: sedimentation, mineralisation of dissolved organic matter, hydrolysis of particulate organic matter, nitrification, denitrification, adsorption, desorption, and the consumption and release by phytoplankton. A constant sediment flux model was assumed, which acted as a sink/source for dissolved oxygen, nitrate and phosphate in the sediment-water interface. Nutrient release from sediments was considered regarding the occurrence of hypoxic conditions in the uppermost reservoir. In view of the absence of vertical profile measurements of DO in the other reservoirs, the same assumption was adopted for them.

Phytoplankton was simulated as cyanobacteria, the dominant functional group in both BB, PR and TI reservoirs (CETESB, 2019; Santos, 2010). Other groups could not be included because field data was unavailable. As diatoms were not explicitly simulated, silica uptake was not included. Mortality of phytoplankton due to grazing by zooplankton was represented through a constant algal loss term, which also accounts for the effects of respiration and mortality. The vertical movements of the algal cells were modelled through a constant settling and migration velocity. The following assumptions were adopted: (i) photoinhibition; (ii) undertaking of atmospheric nitrogen; and (iii) fixed C:N and C:P ratios were assumed to model nutrient limitation with a half-saturation constant representing the effect of external nutrient concentrations on the growth rate. As AED computes phytoplankton biomass in units of carbon, field chlorophyll-a measurements were converted into carbon concentrations by the application of

a ratio 50:1 by weight according to Reynolds (2006). The conceptual diagram of the current application is illustrated in Figure 6.2.

Figure 6.2. Conceptual diagram of AED model for the current application.

Note: Cyano: cyanobacteria; DIC: dissolved inorganic carbon; DO: dissolved oxygen; DON, DOP, DOC: dissolved organic nitrogen, phosphorus and carbon, respectively; N_2 : atmospheric nitrogen; NH_4 : ammonium; NO_3 : nitrate; PON, POP, POC: particulate organic nitrogen, phosphorus and carbon, respectively; PO_4 : filterable reactive phosphorus; and $PO_{4,ads}$: adsorbed filterable reactive phosphorus.

6.2.5 Model calibration and validation

GLM-AED was run at an hourly time-step, aligning with the time-resolution of the hydrodynamic model's input data. Model calibration for simulation of DO, TP, NH_4 , NO_3 , and chl-a was performed for BB, PR and TI reservoirs from the first day with measured field data in 2008 (15th January for BB and 12th February for PR and TI) to 31st December 2012 (Table 6.2). Firstly, GLM parameters previously calibrated and validated (Soares et al., 2020) were applied. Then, the AED parameters to be calibrated were selected considering their medium or high influence in model outputs according to a previous sensitivity analysis over 64 parameters (Soares and Calijuri, 2021). They were simultaneously adjusted using a manual trial and error approach, within a range of values set according to the literature. Calibration was performed until the fit to observations could no longer be appreciably improved. The final set of calibrated parameters were then used for model validation over the four-year period from the first day with

measured field data in 2013 (29th January for BB, 28th January for PR, and 26th February for TI) to 31st December 2016.

Table 6.2. Monitoring station, calibration period, and validation period for DO, TP, NO₃, NH₄, and chl-a in each reservoir.

	Monitoring station	Calibration period	Validation period
BB	(1) TIBB02700	From 15 th Jan 2008 to 31 st Dec 2012	From 29 th Jan 2013 to 31 st Dec 2016
BA	Absent	Absent	Absent
IB	Absent	Absent	Absent
PR	(2) TIPR02990	From 12 th Feb 2008 to 31 st Dec 2012	From 28 th Jan 2013 to 31 st Dec 2016
NA	Absent	Absent	Absent
TI	(3) TITR02800	From 12 th Feb 2008 to 31 st Dec 2012	From 26 th Feb 2013 to 31 st Dec 2016

Note: measurements were taken on the surface every two months by CETESB (2019).

The model skill test was performed by computing a set of summary measures and goodness-of-fit metrics from simulated and observed data, highlighting different aspects of model performance (Willmott, 1981; Bennett et al., 2013; see Table D.1 in Appendix D): mean values of observed and simulated variables ($\bar{O}$ and $\bar{S}$), their standard deviation (s_o and s_s), mean absolute error (MAE), normalised mean absolute error (NMAE), root mean square error (RMSE), Pearson correlation coefficient (r), percent bias (PBIAS), and mean bias error (MBE). These metrics were compared with previous modelling studies to state their acceptability. The first year of simulation (2008) was not used for the performance assessment as it was assumed as a warm-up period to address uncertainties in model initial conditions, following the same period adopted for the previous hydrodynamic modelling of the study sites (Soares et al., 2020).

As BA, IB and NA reservoirs lack field data, the calibration and validation procedures could not be performed for them. Then, the AED parameters were maintained at their initial values based on AED manual (Hipsey et al., 2013) and the literature, and the initial concentrations of the state variables were set as the same as the upstream reservoir (Table 6.2).

6.2.6 Sequential modelling approach

For the BB Reservoir, the input loads from the Tietê River and the Piracicaba River were assumed as the average seasonal value for the wet period (from October to March) and the dry period (from April to September) for each year of simulation. Both inflows to the BB Reservoir were merged into one inflow for the simulation purposes of this study. Nutrient and chlorophyll-a concentration for the single inflow were computed from discharge-weighted averages of Tietê

and Piracicaba rivers. As PO_4 was measured only at the Piracicaba gauge station, its concentration in the Tietê River was estimated as 30.0% of the measured TP, based on the median proportion of PO_4 measured at the Piracicaba gauge. Figure D.2 in Appendix D displays the annual input load of PO_4 , NO_3 , and NH_4 into the BB Reservoir.

The DO, nutrients and chl-a simulated in the outflow of each reservoir were counted separately for the single withdrawal outlet and for the overflow, which occurred when the water volume exceeded the maximum storage volume. In order to take into account the hydrological connection between reservoirs along the cascade, the simulated daily concentrations of PO_4 , NO_3 and NH_4 in both the outlet and the overflow were summed and weighted by each discharge, then they were used as nutrients input in the inflow of the next reservoir along the cascade.

As the phytoplankton was found to survive for more than 1 h in a 40-km channel between two reservoirs (Xiao et al., 2016), its transportation in the connected waters were considered from one water body to another downstream. The simulated chl-a concentration only in the overflow was used as input for the next reservoir. Similarly, the DO was adopted as the overflow concentration because its concentration in the outlet water is excessively high due to the aeration promoted by the turbines, which was not representative of the conditions in the Tietê River. Hence, simulated BB outflow was used as input into BA Reservoir; simulated BA outflow was used as input into IB reservoir, and thus successively until TI, the last reservoir along the cascade system. The description of applied input data for all reservoirs is provided in Table 6.3.

Table 6.3. Summary of AED input data applied for all reservoirs for the 2008–2016 period.

Reservoir	Source of input data	DO	PO_4	NO_3	NH_4	chl-a
BB	(a) TIET02450; (b) PCAB02800	discharge-weighted averages for wet and dry seasons each year				
BA	Simulated from BB output	Overflow	Overflow + outlet		Overflow	
IB	Simulated from BA output	Overflow	Overflow + outlet		Overflow	
PR	Simulated from IB output	Overflow	Overflow + outlet		Overflow	
NA	Simulated from PR output	Overflow	Overflow + outlet		Overflow	
TI	Simulated from NA output	Overflow	Overflow + outlet		Overflow	

6.2.7 Assessment of trophic state and nutrient retention within the reservoirs

The water quality in each reservoir was assessed by calculating the trophic state index adapted for subtropical water bodies (TSI_{tsr} ; Cunha et al., 2013) based on the simulated annual geometric mean concentrations of TP and chl-a at surface for the 2009–2016 period:

$$TSI_{tsr} = \frac{TSI(TP)_{tsr} + TSI(chla)_{tsr}}{2} \quad (6.1)$$

$$TSI(TP)_{tsr} = 10 \left[6 - \left(\frac{-0.27637 \ln TP + 1.329766}{\ln 2} \right) \right] \quad (6.2)$$

$$TSI(chla)_{tsr} = 10 \left[6 - \left(\frac{-0.2512 \ln chla + 0.842257}{\ln 2} \right) \right] \quad (6.3)$$

The reservoirs were classified within six categories: ultraoligotrophic ($TSI_{tsr} \leq 51.1$), oligotrophic ($51.2 < TSI_{tsr} \leq 53.1$), mesotrophic ($53.2 < TSI_{tsr} \leq 55.7$), eutrophic ($55.8 < TSI_{tsr} \leq 58.1$), supereutrophic ($58.2 < TSI_{tsr} \leq 59.0$), and hypereutrophic ($TSI_{tsr} \geq 59.1$).

Nutrient retention (R , %) within the reservoirs was estimated as the difference between the input and output loads:

$$R = \frac{\overline{IN}_{load} - \overline{OUT}_{load}}{\overline{IN}_{load}} \times 100 \quad (6.4)$$

where $\overline{IN}_{load}$ and $\overline{OUT}_{load}$ are the simulated loads at the inflow and outflow of the system, respectively, in units of tons per year. The outflow load was computed as the sum of loads at the outlet and the overflow.

6.2.8 Design of scenarios

Nutrients load scenarios were simulated to carry out a first evaluation of the impacts of nutrient loads reduction along the cascading reservoirs. A reference scenario (S0) was assumed as the current condition for the 2009–2016 period. The external nutrient load was reduced from the inflow of the reference scenario in each reservoir by 30% for PO_4 , NH_4 , and NO_3 , separately, resulting in eighteen scenarios (Table 6.4). The model was run from 2009 to 2016 using the calibrated parameter set. The reduction in each nutrient input was propagated along the cascade to assess any synergistic or antagonistic interaction among reservoirs that could maximise or

minimise management efforts, in an attempt to identify where management strategies should be devoted. Reservoirs' response to each scenario was assessed in terms of concentrations of NH_4 , NO_3 , and TP, rather than PO_4 , because (i) TP is widely used as a strong predictor of numerous indicators of water quality, and (ii) PO_4 was not calibrated in face of the lack of field data. The impacts of nutrient load reduction on downstream reservoirs were assessed through the difference between the daily concentrations relative to the reference scenario. The surface concentrations, i.e. at depth 0.3 m, for the period 2009–2016 were adopted, as used for the TSI assessment. The daily differences were averaged to calculate the percentage change in comparison to the reference scenario.

Table 6.4. Scenarios of reduction in external input loads into the reservoirs.

Current conditions	30% reduction in inflow load			Reservoir with reduction in inflow load	Reduction propagation downstream
	PO_4	NH_4	NO_3		
S0	-	-	-	-	-
	S1	S7	S13	BB	BA, IB, PR, NA, and TI
	S2	S8	S14	BA	IB, PR, NA, and TI
	S3	S9	S15	IB	PR, NA, and TI
	S4	S10	S16	PR	NA and TI
	S5	S11	S17	NA	TI
	S6	S12	S18	TI	-

6.3 Results

6.3.1 Model performance

The GLM-AED model was able to reasonably reproduce TP, NO_3 , NH_4 , DO, and chl-a in BB, PR and TI reservoirs from 2009 to 2016. An overview of all calibrated parameters and final assigned values for each reservoir is given in Table D.2 in Appendix D. The goodness-of-fit metrics revealed a similar performance among reservoirs (Table 6.5). The model generally followed the magnitude of the observed data, especially for TP, DO, and chl-a (Figure 6.3). For NH_4 and NO_3 , a high proportion of field data measurements (between 8% and 92%) were below analytical detection limits, which may compromise the ability of performance metrics to define model error, especially for the correlation coefficient.

Table 6.5. Summary measures and goodness-of-fit metrics for the simulated state variables (TP, NH₄, NO₃, DO, and chl-a) in Barra Bonita (BB), Promissão (PR), and Três Irmãos (TI) reservoirs.

Metric Unit	$\bar{O}$ mg L ⁻¹	$\bar{S}$ mg L ⁻¹	s _o mg L ⁻¹	s _s mg L ⁻¹	MAE mg L ⁻¹	NMAE -	RMSE mg L ⁻¹	r -	PBIAS %	MBE mg L ⁻¹
<i>TP</i>										
BB	0.15	0.12	0.12	0.03	0.09	0.05	0.13	0.01	-18.88	-0.03
PR	0.03	0.03	0.05	0.04	0.03	0.06	0.06	0.21	7.40	0.002
TI	0.02	0.01	0.01	0.01	0.01	0.02	0.01	0.10	-19.53	-0.003
<i>NH₄</i>										
BB	0.32	0.25	0.36	0.14	0.23	0.02	0.38	0.09	-20.35	-0.07
PR	0.13	0.11	0.08	0.10	0.10	0.01	0.14	-0.15	-14.13	-0.02
TI	0.10	0.06	0.02	0.04	0.06	0.01	0.06	0.14	-49.27	-0.05
<i>NO₃</i>										
BB	3.14	2.63	1.16	3.57	3.20	0.06	3.79	-0.04	-16.06	-0.50
PR	0.95	0.59	0.28	1.26	1.04	0.07	1.25	0.28	-38.21	-0.36
TI	0.65	0.58	0.31	0.54	0.38	0.04	0.54	0.27	-11.68	-0.08
<i>DO</i>										
BB	6.73	6.14	3.15	1.60	2.65	0.02	3.34	0.15	-8.77	-0.59
PR	7.34	7.26	1.59	2.77	2.22	0.01	2.78	0.26	-1.04	-0.08
TI	7.20	7.24	0.76	1.64	1.20	0.01	1.59	0.27	0.53	0.04
<i>Chl-a</i>										
BB	33.53	22.76	35.12	6.92	21.52	1.76	36.13	0.12	-32.12	-10.77
PR	22.78	23.86	53.89	27.33	27.28	24.71	50.82	0.33	4.75	1.08
TI	3.82	1.44	2.61	1.44	2.89	0.62	3.92	-0.16	-62.37	-2.38

Note: For chl-a, the unit is µg L⁻¹.

6.3.2 Trophic state and nutrient retention within the reservoirs

Simulated concentrations of the calibrated state variables at the surface water in the reservoirs during an 8-year period (2009–2016) revealed a decreasing tendency in nutrients and chlorophyll-a concentrations from up-to-downstream. Figure 6.4 illustrates the decreasing concentrations among reservoirs for a representative year (2013) during the simulation period. As a consequence, the TSI adapted for subtropical reservoirs demonstrated a longitudinal gradient in terms of water quality along the cascade. In the uppermost reservoirs, BB, BA and IB, where intensive agriculture and urban areas are nearby, TSI ranged from eutrophic to hypereutrophic; in the PR Reservoir, its category ranged from ultraoligotrophic to eutrophic; in the NA Reservoir, its status ranged from ultraoligotrophic to mesotrophic; and in the TI Reservoir, the lowermost one, its status was ultraoligotrophic (Figure 6.5).

Figure 6.3. Simulated and measured state variables at surface in Barra Bonita (BB), Promissão (PR), and Três Irmãos (TI) reservoirs for 2009–2016 period.

Note: The horizontal line inside the box plot indicates the median, and the boundaries of the box plot indicate the 25th and 75th percentiles. Whiskers indicate the 10th and 90th percentiles. The white marker represents the mean.

The mean nutrient retention by the reservoirs computed from annual nutrient retention values from 2009 to 2016 showed a tendency to retain nutrients within the water bodies (Table 6.6). The only exception was TI reservoir, where nutrient loads were higher in the outflow than in the inflow. Nutrient retention differed from one element to another and also presented great discrepancy among reservoirs. The BB Reservoir was able to retain PO₄ and NH₄, but not NO₃. BA and IB reservoirs presented similar behavior, with low retention values. The PR Reservoir showed very high nutrient retention values, all above 73%, while the NA Reservoir showed moderate retention.

Figure 6.4. Simulated state variables in Barra Bonita (BB), Promissão (PR), and Três Irmãos (TI) reservoirs for a 1-year period (2013).

Figure 6.5. TSI adapted for subtropical reservoirs for the 2009–2016 period based on a) simulated and b) measured data.

Note: The horizontal line inside the box plot indicates the median, and the boundaries of the box plot indicate the 25th and 75th percentiles. Whiskers indicate the 10th and 90th percentiles. The white marker represents the mean.

Table 6.6. Mean nutrient retention by the reservoirs computed from annual values of the 2009–2016 period.

Reservoir	BB	BA	IB	PR	NA	TI
PO ₄	13%	9%	1%	96%	28%	–154%
NH ₄	95%	13%	25%	73%	35%	–19%
NO ₃	–118%	15%	14%	80%	61%	–104%

Note: Annual nutrient retention was computed according to Equation 4.

6.3.3 Reductions in external nutrient loads along the cascade system

Eighteen scenarios of a 30% reduction in the external nutrient load (PO₄, NH₄, and NO₃, separately) in the inflow of each reservoir were simulated to assess the impact on the reservoir water quality. Results showed that the reduction in input loads was transferred to all downstream reservoirs, corroborating the interconnection along the cascade system (Figure 6.6). Indeed, compared to the reference input loads (scenario S0), a 30% reduction of the PO₄ load in the inflow of an upstream reservoir resulted in higher reduction rates in downstream reservoirs, revealing their capacity to act as a sink of PO₄. The reduction of the NH₄ load resulted in downstream load reductions at the same order of magnitude (around 30%) along the cascade system (S7–S12). In contrast, the reduction of NO₃ load showed different reductions downstream (S13–S18).

Figure 6.6. Propagation of the reduction in external input loads into the reservoir inflows along the cascade system.

Reduction in PO ₄ load (%)							Reduction in NH ₄ load (%)							Reduction in NO ₃ load (%)						
	BB	BA	IB	PR	NA	TI		BB	BA	IB	PR	NA	TI		BB	BA	IB	PR	NA	TI
S1	30	32	36	36	65	23	S7	30	32	32	32	32	24	S13	30	13	10	23	29	17
S2		30	33	33	69	22	S8		30	30	29	28	21	S14		30	25	36	60	34
S3			30	30	64	21	S9			30	29	28	21	S15			30	34	38	37
S4				30	62	21	S10				30	28	21	S16				30	29	33
S5					30	12	S11					30	24	S17					30	32
S6						30	S12						30	S18						30

70

Reduction (%)

0

0
70
Reduction (%)

6.3.4 Reservoirs' response to reducing external nutrient loads

Nutrient concentrations within the water bodies were sensitive to the reductions in inflow loads in all upstream reservoirs, revealing a synergistic interaction among them. For instance, a 30% reduction in PO₄ and NO₃ loads led to reductions as high as 54% and 52% in TP and NO₃ concentrations in a downstream reservoir (S3, S14; Figure 6.7). In general, the further

downstream the PO₄ and NH₄ load reductions were implemented, the lower the downstream reservoir response was. Therefore, reducing the nutrient load into the uppermost reservoir (BB) led to the optimised system-wide improvement in water quality, with the highest effect in all reservoirs along the cascade, when considering TP and NH₄ concentrations. The PR Reservoir was the most sensitive one as both TP and NO₃ concentrations experienced the highest decreases in this reservoir than in the others. Indeed, TP and NO₃ reductions in PR Reservoir were amplified, achieving percentage reductions higher than the 30% applied for inflow load reductions. In contrast, the TI Reservoir was the lowest sensitive to reductions in nutrient loads.

Figure 6.7. Reduction in nutrients and chlorophyll-a concentration within the reservoirs.

Reductions in TP concentration within BB, BA, and IB reservoirs were not enough to affect chl-a concentration, whose decrease was below 2% (S1–S3). In contrast, chl-a concentration in PR, NA, and TI reservoirs considerably decreased in response to the TP reduction (S1–S6). The chl-a concentration in all reservoirs was negligibly sensitive to NH₄ and NO₃ load reductions (S7–S18).

6.4 Discussion

6.4.1 *Modelling interconnected reservoirs*

GLM-AED was applied for a sequential modelling approach in a network of unidirectional water flow transporting energy, substances and biota among interconnected reservoirs. As far as the authors are aware, this study represents the first work applying a coupled hydrodynamic-biogeochemical model following an interconnected approach to represent a cascade system. Treating the interconnection between reservoirs along the cascade, instead of simulating each reservoir alone, enabled the simulation of a reduction in nutrient external load and the assessment of its impact from one water body to the next in terms of TP, NH_4 , NO_3 , and chl-a concentrations at the surface water. The methodological steps followed in this study revealed how dams impacted nutrients export from up-to-downstream reservoirs along the cascade system.

The reference scenario represented the current condition, which was characterised by a downstream decrease of nutrient concentrations at surface, revealing an improvement of the ecosystem state along the cascade system. High nutrient loads into the uppermost reservoir (BB) led to a severe degradation of water quality resulting in a hypereutrophic condition in this lentic system. The trophic state gradually improved, reaching the ultraoligotrophic status in the lowermost reservoir (TI). In the 1990s, Barbosa et al. (1999) proposed the Cascading Reservoir Continuum Concept as a theoretical basis to explain the water quality gradient along the reservoirs in the Tietê River's cascade system. They argued that biological processes within any of the reservoirs are consequent upon the changes in the upstream one. The present study corroborates with the Cascading Reservoir Continuum Concept in the connected reservoirs of the Tietê River.

The decreasing nutrient concentrations from up-to-downstream can be explained by their retention within the water bodies as a result of physico-chemical and biological processes. Both NH_4 , NO_3 , and PO_4 retention within the reservoir encompasses two processes: first, the uptake by the phytoplankton, which converts them into particulate form (PON and POP); and second, the sedimentation of the particulate form. Additionally, NO_3 is released into the atmosphere via denitrification, which is considered to be the dominant pathway for N vanishing (David et al.,

2006). Given the slow velocities in lentic systems, which provide enhanced opportunities for settling, lakes and reservoirs are considered hotspots for N and P retention, acting as biogeochemical sinks in the landscape (Cheng and Basu, 2017). Several lakes and reservoirs were estimated to retain 47%–58% of N and 58%–65% of PO₄ inflow loads (Cheng and Basu, 2017; David et al., 2006; Harrison et al., 2009; Salvia-Castellvi et al., 2001).

It is worth noting that the studied reservoirs presented different levels of sensitivity to the direct reduction of inflow loads. Nutrient fate within water bodies are most commonly explained as a function of the hydraulic residence time rather than be correlated to other morphometric characteristics (Brett and Benjamin, 2008; Schmadel et al., 2018). Short residence times are associated with a short time for reactions to occur, thus corresponding to low nutrient retention within the reservoir (Soranno et al., 1999). According to the model simulation, nutrients retention in BA, IB and NA reservoirs were found to be from low to moderate, ranging from 1% to 61% (Table 6.6), which may be attributed to the shorter hydraulic residence time of these systems (15 days, 23 days, and 46 days, respectively) as they are run-of-river systems. High retention rates were found in the PR Reservoir in response to its higher hydraulic residence time (around five months), favoring sedimentation and biogeochemical processing. In addition, the stable hydrodynamic of the reservoir, which has a monomictic behavior (Soares et al., 2020), and the progressive eutrophication may enhance those processes.

BB Reservoir retained only 13% of the PO₄ load (Table 6.6). The polymictic behavior of the reservoir with frequent mixing events (Soares et al., 2020) may prevent the sedimentation of PO₄, resulting in low retention efficiency. Frequent hypoxic events at the bottom of the BB Reservoir (CETESB, 2019) may explain the reservoir acting as a source, instead of as a sink, of NO₃. The high NH₄ retention in the reservoir merits further investigation. High nutrient retention in the TI Reservoir was expected due to a longer hydraulic residence time (1.2 year). However, the opposite was found: TI Reservoir acted as a source of nutrients, rather than a sink, suggesting that the mechanism of nutrients processing was not affected by the hydraulic residence time in this aquatic system. The release of nutrients from the sediments possibly occurred during seasonal full mixing events. However, the absence of measured field data at the bottom layers prevented the verification of this hypothesis.

As expected, the phosphorus was the major factor determining phytoplankton biomass in the reservoirs with meso to ultraoligotrophic state (PR, NA, and TI), since 30% of PO_4 load reductions promoted the reduction of 4%–52% of chl-a concentration in these water bodies. In contrast, neither the reduction of NH_4 , nor NO_3 , was enough to promote considerable reductions on the chl-a concentration. From an ecological perspective, PO_4 is potentially available for biological assimilation and was in short supply relative to NH_4 and NO_3 , demonstrating to be the limiting nutrient in this cascade system. Historically, phosphorus has been identified as the key factor controlling eutrophication of inland waters (Lee et al., 1980) and is usually found as the limiting nutrient for many ecological systems (Brett and Benjamin, 2008; Maavara et al., 2015; Xu et al., 2020).

6.4.2 Implications for management and restoration strategies

Reducing external nutrient loads from the current condition in the reservoirs was propagated through one reservoir to the next, triggering a domino effect along the cascade system. A synergistic interaction caused by the retention capacity of nutrients in the upstream reservoir enhanced responses further downstream. Our results corroborate that the modelling of connected systems is worthwhile given that feedback from one system to the next is an important driver of the resulting state of the next system (Teurlincx et al., 2019).

In addition, the reservoirs tended to be more sensitive to nutrient reductions into BB Reservoir than its reduction in any other water body of the cascade system, revealing that the reservoir's response could be amplified according to the location of the inflow load reduction. Rather than site-specific, the magnitude of nutrient response to the reduction of inflow loads had a cascade-scale, revealing that water managers should see the problem on the scale of a whole system instead of the scale of a single water body. In view of the domino effect, devoting efforts to the uppermost reservoir is the optimised way to maximise the retention capacity along the water network and to achieve water quality standards. Similarly, Hilt et al. (2011) found that any local efforts should start in the first lakes in a chain of connected systems, which would propagate in the downstream direction due to a domino effect. Hence, the authors recommend that a priori management strategies should be focused on the BB Reservoir for successful restoration of aquatic ecosystems along the cascade system.

The reduction of allochthonous PO_4 loads is imperative for recovering the trophic state and ecosystem management of the reservoirs. However, in the case of the badly degraded systems (BB, BA, and IB), where the 30% of PO_4 load reductions were not enough to affect chl-a concentration, higher reductions would necessarily be demanded. Predicting phosphorus release from the sediments in the BB Reservoir suggests that internal recycling of legacy phosphorus in sediment can support TP enrichment of the water column, resulting in a hysteresis effect that slows down the response to external load reductions (Reddy et al., 2007). For instance, internal load recovery may be delayed for 10–15 years after a reduction in the external nutrient load, and heavily impacted lakes may experience even longer periods (Rolighed et al., 2016). Therefore, in-lake treatments are required for the removal of the current TP concentrations in the water column of BB, BA, and IB reservoirs. The degraded trophic state found in BB, BA, and IB reservoirs raised concerns about the current ecosystem conditions and services they can provide, demanding urgent restoration efforts.

6.4.3 Model limitations and validity

Overall, the model was able to capture the magnitude of nutrients and chl-a concentrations in the calibrated reservoirs (BB, PR and TI) and was able to represent the state variables at the water surface to a credible and acceptable extent for the purposes of this study. Despite the low-temporal resolution of field data necessary to calibrate and validate the model, the goodness-of-fit metrics attested that model accuracy was largely similar to that of the literature and was within the range of previous 1D model applications (Table D.3 in Appendix D). Differences between simulated state variables and measured field data may be attributed to several causes. (1) Firstly, given the fact that the study sites are poorly monitored, simplifications were required for input data treatment. For instance, nutrient and chlorophyll-a inflow concentrations into the BB Reservoir consisted of seasonal average values and thus the model was not able to fully reproduce intra-annual variation. Another constraint of the model was (2) field measurements taken on the water surface, hence it is not known how well the model represents the nutrients at the bottom. (3) Besides, particularly for NH_4 , field data were often close to or below analytical detection limits, considerably impairing statistics of model performance. (4) Finally, the model configuration adopts constant parameters over the entire

simulation period, which was recognised in previous studies (*e.g.* Ladwig et al., 2020) as a source of uncertainty.

The magnitude of nutrient and chlorophyll-a concentration could not be attested in BA, IB, and NA reservoirs in face of the absence of field measurements, thus it should be critically viewed. However, the 8-year period of scenarios simulation provided indications on where management strategies for controlling nutrient loads are more efficiently internalised by the reservoirs. It is expected that the decrease of nutrients in connected systems and the domino effect along the cascade apply to other connected lakes and reservoirs because the mechanisms of nutrient retention is valid to any water body.

6.5 Conclusions

GLM-AED model was applied to simulate biogeochemical processes along a cascade system following an original interconnected modelling approach. The present case study provided an understanding of the nutrient load propagation along six interconnected reservoirs. The model was calibrated and validated against measured field data, and the goodness-of-fit metrics proved its valuable contribution as a tool to overcome the low frequency of monitoring data. Modelling results corroborated the water quality gradient along the cascade from up-to-downstream and presented a preliminary estimation of water quality conditions in non-monitored reservoirs (BA, IB, and NA).

Based on eighteen nutrient load reduction scenarios, the model contributed to a deeper understanding of the response of ecosystems and provided guidance for restoration and management strategies. The primary finding was that all six reservoirs were sensitive to nutrient load reductions, which triggered a domino effect along the cascade, revealing a synergistic interaction among reservoirs. Any local efforts to support reductions in nutrient loads should start in the uppermost reservoir of the chain, propagating improvements in water quality in the downstream direction, acting on a basin scale. Thus, rather than the simulation of the reservoirs as isolated water bodies, the reservoirs' ecosystems should be treated as a whole system at the

whole catchment spatial scale. Besides, the reduction of PO_4 loads is mandatory for ecosystem management and restoration efforts.

The modelling approach here applied is particularly useful to identify the most strategic reservoir to devote management actions, especially in developing countries where resources, infrastructure, and preparedness are frequently scarce. The authors expect that the main messages of the present study also apply to other interconnected lakes and reservoirs worldwide, providing relevant information for increasing water resources sustainability and aquatic biodiversity, in face of cumulative stressors such as population growth, agricultural development, deforestation, urbanisation, and climate change.

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D

Appendix D to Chapter 6

Figure D.1. Major land uses in the basin catchment of the Tietê River.

Figure D.2. Inflow loads from the Tietê River (blue bars) and the Piracicaba River (orange bars) of filterable reactive phosphorus (PO_4), nitrate (NO_3), and ammonium (NH_4) into the Barra Bonita Reservoir from 2008 to 2016.

Table D.1. Formula, range, optimum value, and unit of summary measures and goodness-of-fit metrics. N is the number of observations, O_i and S_i are the “ith” observed and simulated data, and $\bar{O}$ and $\bar{S}$ are the mean observed and simulated data, respectively.

Measures of model performance	Formula	Range	Optimum value	Unit
Mean observed variable ($\bar{O}$)	$\frac{\sum_{i=1}^N O_i}{N}$	$[-\infty, \infty]$	-	same as the variable
Mean simulated variable ($\bar{S}$)	$\frac{\sum_{i=1}^N S_i}{N}$	$[-\infty, \infty]$	-	same as the variable
Standard deviation of the observed variable (s_O)	$\sqrt{\frac{\sum_{i=1}^N (O_i - \bar{O})^2}{N}}$	$[0, \infty]$	0	same as the variable
Standard deviation of the simulated variable (s_S)	$\sqrt{\frac{\sum_{i=1}^N (S_i - \bar{S})^2}{N}}$	$[0, \infty]$	0	same as the variable
Mean Absolute Error (MAE)	$\frac{\sum_{i=1}^N S_i - O_i }{N}$	$[0, \infty]$	0	same as the variable
Normalised Mean Absolute Error (NMAE)	$\frac{\sum_{i=1}^N (S_i - O_i)/O_i }{N}$	$[0, \infty]$	0	-
Root Mean Square Error (RMSE)	$\sqrt{\frac{\sum_{i=1}^N (S_i - O_i)^2}{N}}$	$[0, \infty]$	0	same as the variable
Pearson correlation coefficient (r)	$\frac{\sum_{i=1}^N (S_i - \bar{S})(O_i - \bar{O})}{[\sum_{i=1}^N (S_i - \bar{S})^2 \sum_{i=1}^N (O_i - \bar{O})^2]^{1/2}}$	$[-1, 1]$	1	-
Percent bias (PBIAS)	$\frac{\sum_{i=1}^N (S_i - O_i)}{\sum_{i=1}^N O_i} \times 100$	$[-\infty, \infty]$	0	%
Mean Bias Error (MBE)	$\frac{\sum_{i=1}^N (S_i - O_i)}{N}$	$[-\infty, \infty]$	0	same as the variable

Table D.2. Description of calibrated AED parameters, their initial values from the AED science manual (Hipsey et al., 2013), range, and final assigned values for each reservoir.

Symbol	Description	Initial value	Range	Calibrated value		
				BB	PR	TI
<i>Oxygen</i>						
Fsed_oxy	Sedimentation flux for dissolved oxygen ($\text{mmol m}^{-2} \text{d}^{-1}$)	6.00	$-20.00^{\text{a}} - 87.50^{\text{b}}$	-	-11.00	1.00
theta_sed_oxy	Temperature multiplier for oxygen sediment flux	1.08	$1.02^{\text{c}} - 1.14^{\text{c}}$	-	1.08	1.08
<i>Nitrogen</i>						
Fsed_nit	Sedimentation flux for nitrate ($\text{mmol m}^{-2} \text{d}^{-1}$)	-14.00	$-14.00 - -1.87^{\text{c}}$	-40.00	-18	-0.40
Rnitrif	Maximum reaction rate of nitrification at 20 °C (d^{-1})	0.03	$0.01^{\text{b}} - 0.34^{\text{d}}$	0.28	-	-
Knitrif	Half saturation constant for oxygen dependence of nitrification (mmol m^{-3})	62.5	$12.5^{\text{c}} - 93.7^{\text{d}}$	25.00	-	-
Kdenit	Half saturation constant for oxygen dependence of denitrification (mmol m^{-3})	15.6	$12.5^{\text{d}} - 18.0^{\text{a}}$	17.5	-	-
Ksed_nit	Half saturation constant of nitrate flux (mmol m^{-3})	15.6	$15.0^{\text{a}} - 23.4^{\text{c}}$	15.2	-	-
theta_nitrif	Temperature multiplier for temperature dependence of nitrification	1.08	$1.02^{\text{d}} - 1.14^{\text{d}}$	1.02	1.14	1.02
theta_denit	Temperature multiplier for temperature dependence of denitrification	1.05	$1.045^{\text{d}} - 1.08^{\text{d}}$	1.06	-	1.08
theta_sed_amm	Temperature multiplier for sediment ammonium flux	1.08	$1.07^{\text{a}} - 1.14^{\text{c}}$	-	1.09	1.14
theta_sed_nit	Temperature multiplier for sediment nitrate flux	1.08	$1.055^{\text{c}} - 1.08$	1.08	1.06	1.08
<i>Phosphorus</i>						
Fsed_frp	Sedimentation flux for phosphate ($\text{mmol m}^{-2} \text{d}^{-1}$)	0.12	$0.001^{\text{a}} - 0.84^{\text{b}}$	-	-18.00	-
theta_sed_frp	Temperature multiplier for sediment phosphate flux	1.08	$1.032^{\text{c}} - 1.08$	-	1.06	1.08
<i>Organic matter: nitrogen</i>						
theta_pon_miner	Temperature multiplier for particulate organic nitrogen breakdown	1.08	$1.02^{\text{d}} - 1.14^{\text{d}}$	-	-	1.05
theta_don_miner	Temperature multiplier for dissolved organic nitrogen mineralisation	1.08	$1.02^{\text{d}} - 1.14^{\text{d}}$	-	-	1.09
<i>Organic matter: phosphorus</i>						
theta_pop_miner	Temperature multiplier for particulate organic phosphorus breakdown	1.08	$1.02^{\text{d}} - 1.14^{\text{d}}$	-	-	1.09

Cont. **Table D.2.** Description of calibrated AED parameters, their initial values from the AED science manual (Hipsey et al., 2013), range, and final assigned values for each reservoir.

				Calibrated value		
Symbol	Description	Initial value	Range	BB	PR	TI
<i>Organic matter: carbon</i>						
w_poc	Settling rate of detrital carbon pool (m d^{-1})	-1.0	-1.0 – -0.05 ^a	-0.05	-	-
Fsed_doc	Sedimentation flux for dissolved organic carbon ($\text{mmol m}^{-2} \text{d}^{-1}$)	30.0	0.01 ^e – 30.00	-	30.0	30.0
Rdoc_miner	Maximum rate of mineralisation of dissolved organic carbon (d^{-1})	0.01	0.001 ^a – 0.50 ^f	-	0.003	-
theta_doc_miner	Temperature multiplier for dissolved organic carbon mineralisation	1.08	1.02 ^d – 1.14 ^d	1.08	1.08	1.08
Rpoc_miner	Maximum rate of hydrolysis/breakdown of particulate organic carbon (d^{-1})	0.01	0.001 ^a – 0.50 ^f	-	0.20	-
<i>Phytoplankton</i>						
R_growth	Phytoplankton growth rate at 20 °C (d^{-1})	1.9	0.6 ^c – 2.9 ^d	2.8	2.3	-
theta_growth	Arrhenius temperature scaling for growth	1.06	1.05 ^g – 1.11 ^h	1.06	1.09	1.05
theta_std	Standard temperature (°C)	20.0	19.0 ^e – 23.0 ^h	20.0	-	-
theta_opt	Optimum temperature (°C)	28.0	24.0 ^e – 30.0 ^c	28.0	29.0	24.0
theta_max	Maximum temperature (°C)	35.0	32.0 ⁱ – 40.0 ^c	38.0	38.0	32.0
I_S	Saturating light intensity ($\mu\text{E m}^{-2} \text{s}^{-1}$)	150	150 – 250 ^c	190	-	-
R_resp	Phytoplankton respiration rate at 20 °C (d^{-1})	0.05	0.01 ^c – 0.09 ^j	0.03	0.01	0.09
theta_resp	Arrhenius temperature scaling for respiration	1.05	1.05 – 1.12 ⁱ	1.05	1.05	1.12
k_fdom	Fraction of metabolic loss that is dissolved organic matter	0.20	0.20 – 0.25 ^a	0.20	-	-
X_pcon	Constant internal phosphorus concentration ($\text{mmol P (mmol C)}^{-1}$)	0.0015	0.0015 – 0.0020 ^a	0.0015	-	0.0020

Note: The parameters that were not calibrated for a given reservoir were maintained at their initial values and are represented as “-”. ^aFarrell et al., 2020; ^bBurger et al., 2008; ^cKara et al., 2012; ^dFenocchi et al., 2019; ^eSnorheim et al., 2017; ^fAED Science Manual (Hipsey et al., 2013); ^gÖzkundakci et al., 2011; ^hBucak et al., 2018; ⁱLadwig et al., 2018; ^jCui et al., 2016.

Table D.3. Range of goodness-of-fit metrics from previous studies applying one-dimensional models.

State variable	RMSE	<i>r</i>	NMAE	PBIAS
TP	0.006 ^a –0.118 ^a	0.10 ^a –0.85 ^b	0.15 ^c –1.50 ^a	12.1 ^d –16.5 ^d
NH ₄	0.012 ^d –2.91 ^e	-0.19 ^f –0.85 ^g	0.43 ^g –1.8 ^h	-38.1 ^d –13.8 ^d
NO ₃	0.005 ^b –1.2 ⁱ	-0.29 ^b –0.93 ^g	0.28 ^h –0.82 ^c	-72.3 ^d –40.1 ^d
DO	0.96 ^a –3.60 ^j	0.00 ⁱ –0.89 ^b	0.06 ^a –0.37 ^g	-
Chl-a	2.66 ^c –13.12 ^k	0.09 ^d –0.75 ^c	1.00 ^h	10.8 ^d –24.1 ^d

^aFarrell et al., 2020; ^bBurger et al., 2008; ^cCui et al., 2016; ^dMe et al., 2018; ^eBucak et al., 2018; ^fFenocchi et al., 2019; ^gSnorheim et al., 2017; ^hKara et al., 2012; ⁱLadwig et al., 2018; ^jWeng et al., 2020; ^kMueller et al., 2019.

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7

Restoration from eutrophication in interconnected reservoirs: using a model approach to assess the propagation of water quality improvements downstream along a cascade system

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A coupled hydrodynamic-biogeochemical model was applied to simulate scenarios of classic restoration practices to address eutrophication in a cascade system comprised of six reservoirs along the Tietê River (Brazil) from 2008 to 2016. Each restoration scenario was propagated along the cascade system by using a sequential modelling approach. The simulated scenarios revealed which on-land and in-lake restoration techniques are capable of promoting water quality improvements that are propagated to all downstream reservoirs along the cascade system. The present findings may provide a useful management strategy to develop better restoration practices at a basin catchment scale for other lakes and reservoirs along cascade systems worldwide, especially in highly anthropogenic impacted areas, taking advantage of the propagation of water quality improvements in a downstream direction due to a domino effect triggered by the feedback from one water body to the next in a chain.

Keywords: lake degradation, GLM-AED model, phosphorus, chlorophyll-a, Trophic State Index, water management.

7.1 Introduction

Cultural eutrophication is widespread globally and across lake types, regardless of latitude or morphometry (Ho et al., 2019) and is the major problem facing inland waters (Downing, 2014). Eutrophication impacts can seriously impair the delivery of ecosystem services (Janssen et al., 2020) and also promote negative economic consequences, such as increased costs for public health and losses in commercially important fisheries (McCrackin et al., 2017). According to the period of exposure and degradation intensity, eutrophication in water bodies can move from reversible when restoration follows the reduction of nutrient inputs, to hysteretic when eutrophication can be reversed by combining nutrient input controls with temporary interventions, then to irreversible when eutrophication cannot be reversed even by severe reductions in nutrient input (Carpenter et al., 1999). Therefore, during the past several decades, much effort has been made to restore degraded lakes and reservoirs.

As nutrient input is the primary cause of eutrophication in aquatic ecosystems worldwide, great efforts and vast amounts of financial resources have been used to reduce the external nutrient loadings (Chou et al., 2021) by managing both point and nonpoint sources in the basin catchment (Dolph et al., 2019). In addition, to accelerate recovery, a suite of physical-chemical and biological methods are applied after external loading reduction (Jeppesen et al., 2017) to reactively combat both causes and consequences of eutrophication. These methods are based on (i) reducing internal nutrient loads, such as using an inactivation agent to permanently bind phosphorus in the sediments (Gibbs et al., 2011; Huser et al., 2016b; Lucena-Silva et al., 2019), (ii) biomanipulation (Burns et al., 2014; Jeppesen et al., 2007), (iii) phytoplankton control by application of algicides (Matthijs et al., 2016) or natural polymers as flocculants (Yuan et al., 2016; Zou et al., 2006), and (iv) hydrologic manipulation (Niemistö et al., 2016).

While these methods have been discussed for decades, eutrophication problems persist and recovery remains a global challenge (Wurtsbaugh et al., 2019), either because external loading has not been reduced sufficiently or because internal lake mechanisms prevent or delay recovery (Søndergaard et al., 2007). Fortunately, an increasing number of water bodies are reversing towards re-oligotrophication in Western Europe and North America (Anneville et al., 2019). Indeed, many of Europe's largest lakes have been recovered from eutrophication

(Schindler, 2012) following tertiary wastewater treatment and the removal of phosphorus from sewage effluent (Jeppesen et al., 2005).

In developing countries, in contrast, point sources are now progressively increasing to affect the quality of the environment for various systems (Jenny et al., 2020). Despite successes in North America and Europe in reducing eutrophication, the number of case studies on the recovery from eutrophication in tropical climates is far less advanced than in temperate lakes (Coveney et al., 2005; Liu et al., 2018). In the case of Brazilian lakes and reservoirs, the effects of rapid population growth not accompanied by a proportionate increase in sanitation infrastructure have resulted in eutrophication in 57% of the lentic environments (ANA, 2012). However, this number is potentially quite underestimated considering that there are not many monitored water bodies. In addition, the country faces sociopolitical challenges due to conflicts because of overarching goals for economic development in detriment of adequate attention to environmental protection by the state (Thomaz et al., 2020), which poses further stress in highly degraded aquatic ecosystems.

A large body of literature reports the response of aquatic ecosystems to restoration methods for individual study sites. However, the effects of restoration methods on lakes and reservoirs situated along a cascade system are understudied. The feedback from one water body to the next in a chain is of crucial importance due to a domino effect in water quality along the network (Teurlinx et al., 2019). In this study, we recognise the need of incorporating the connectivity through reservoirs to potentialise restoration efforts in water bodies connected by a cascade system. A cascade system comprised of six reservoirs located in southeast Brazil was selected as the case study. The main goals were: (1) to apply the hydrodynamic General Lake Model coupled to the biogeochemical Aquatic EcoDynamics library (GLM-AED), previously calibrated and validated, to simulate scenarios of classic restoration methods and investigate the reservoirs' response in terms of the trophic state index; (2) to investigate how the restoration scenarios are propagated along the cascade system by using a sequential modelling approach to transport the feedback from one reservoir to the next one in the chain; and (3) to elaborate a scenario consisting of a combination of the most efficient restoration methods to promote an overall improvement in water quality not only in one reservoir, but in all water bodies along the cascade system. We intend to provide subsidies for water managers to develop better restoration

methods at a basin catchment scale to recover aquatic ecosystems considering the synergistic propagation in a downstream direction.

7.2 Methods

7.2.1 Site description

From the 1960s to the 1990s, a cascade system comprised of six reservoirs was built along the Tietê River, southeast Brazil. The reservoirs are from up- to downstream: Barra Bonita (BB), Bariri (BA), Ibitinga (IB), Promissão (PR), Nova Avanhandava (NA), and Três Irmãos (TI). They are hydrologically connected through the Tietê River for operational optimisation through flow regulation to attend the common purpose of hydropower generation. As a result, reservoirs affect water quantity and quality from up- to downstream along the cascade system. Besides, they attend multiple uses, including navigation, drinking water supply, irrigation, fishery, flood regulation, and tourism.

The reservoirs have a varied range of physical characteristics, with maximum depth from 19.2 to 45.6 m, surface area from 46 to 654 km², and hydraulic residence time from 15 days to 1.2 years. The thermal regime in the first two reservoirs is polymictic and in the other four reservoirs it is warm monomictic. More detailed morphometric and hydrodynamic features of the reservoirs are described in Soares et al. (2020).

The reservoirs are located in a sub-tropical climate (Cwa; Köppen, 1948). The annual mean air temperature is 22.6 °C and the mean rainfall is 1400 mm of which about 80% falls from October to March (INMET, 2019).

7.2.2 Land use within the catchment and sources of external nutrient loads

The total catchment basin of the cascade system covers 69,900 km². The land within the catchment is mostly used for agriculture, urban, and pasture purposes, while fragments of forestry and native vegetation cover small areas (Table 7.1; IBGE, 2018). Barra Bonita's catchment is the highest density region in the country, where the São Paulo Metropolitan Region is located. There are large urban areas with more than 25 million inhabitants and several industries. In addition,

there are agricultural lands, mostly for sugarcane crops. The sub-catchments of BA, IB, PR, and NA reservoirs are quite similar in terms of land use and occupation. Agriculture lands, mostly for the cultivation of oranges to attend the food industry and sugarcane to attend the sugar and alcohol industry are dominant in the sub-catchments. There are a total of 2 million inhabitants, of which 94% live in urban areas. In the TI reservoir's sub-catchment, the land is used also for sugarcane crops and for cattle pasture. There are 500,000 inhabitants, 91% of whom live in urban areas.

Table 7.1. Land uses in the sub-catchment of each reservoir (IBGE, 2018).

Land uses	BB	BA	IB	PR	NA	TI
Sub-catchment area (km ²)	32,330	3,100	8,070	14,110	4,690	7,600
Agriculture	62%	83%	83%	83%	87%	60%
Urban	12%	7%	3%	2%	1%	2%
Pasture	5%	4%	5%	6%	4%	27%
Forestry	3%	5%	4%	2%	-	-
Native vegetation	17%	-	4%	4%	3%	4%
Water bodies	1%	1%	1%	3%	5%	7%

Note: Each reservoir is associated with a two-letter code: Barra Bonita (BB), Bariri (BA), Ibitinga (IB), Promissão (PR), Nova Avanhandava (NA), and Três Irmãos (TI).

7.2.3 *Water quality within the reservoirs*

The water quality along the cascade system is characterised by a remarked trophic state gradient from up- to downstream in response to the capacity of nutrient removal in each sub-catchment basin (Figure 7.1). Historically, the uppermost reservoir (Barra Bonita) receives high amounts of nutrient loads from the high population density in its sub-catchment. The water quality has been severely compromised in this reservoir since the 1980s when cyanobacteria blooms became established (Calijuri, 1988). External nutrient loads to the reservoir are dominated by point-sources from domestic raw sewage, effluents from several industrial plants, and discharges from wastewater plants with primary and secondary treatments, which have low efficiency of nutrient removal (CETESB, 2019). In addition, the inappropriate disposal of solid waste and improper discharge of sewage into the rainfall drainage system are other common sources of external nutrient loads (ANA, 2012). In the BA and IB sub-catchments, nutrient loads come from the discharge of domestic raw sewage in freshwaters. Fertilisers applied in the intensive agriculture, which reach the surroundings of the reservoirs in some stretches, are other important contributors to the total nutrient load. The PR Reservoir is currently in the process of

eutrophication due to external nutrient loads mostly from urban and agricultural non-point sources. In NA and TI sub-catchments, external nutrient loads come mostly from non-point sources, such as agriculture, pasture, and runoff from urban areas.

Figure 7.1. Reservoirs' cascade system along the Tietê River and the capacity of nutrient removal in each city within the catchment (ANA, 2017).

Note: Each reservoir is associated with a two-letter code: Barra Bonita (BB), Bariri (BA), Ibitinga (IB), Promissão (PR), Nova Avanhandava (NA), and Três Irmãos (TI).

7.2.4 Coupled hydrodynamic and biogeochemical modelling

The one-dimensional vertical General Lake Model (GLM) coupled to the Aquatic EcoDynamics (AED) library simulates the hydrodynamics and biogeochemistry processes in lentic water bodies (Hipsey et al., 2019, 2013). Both GLM and AED are open-source and freely available. GLM-AED has been found to successfully reproduce observed water temperatures and quality of lakes with varying conditions around the world (Bucak et al., 2018; Fenocchi et al., 2019; Ladwig et al., 2018; Snorheim et al., 2017; Weng et al., 2020).

GLM dynamically simulates vertical temperature profiles, density and salinity at a single point in the water body by using a Lagrangian approach to the layer structure where layers can split and combine based on changing vertical gradients. Both the mass balance and the energy budget are computed every time step of the simulation. AED simulates the interactions between nutrients, organic matter, phytoplankton and zooplankton. The model accounts for the processes of atmospheric exchange, sediment oxygen demand, organic matter hydrolysis and mineralisation, nitrification, denitrification, nitrogen fixation, and adsorption/desorption of filterable reactive phosphorus (PO_4). The biological process of primary production, respiration, mortality, excretion, settling or resuspension, and grazing processes are also included in the model components. Further information regarding the model process equations, state variables and parameters can be found in the science manuals for GLM (Hipsey et al., 2019) and AED (Hipsey et al., 2013).

7.2.5 Modelling procedure

GLM-AED version 2.2.0 was previously applied to the study sites following a sequential approach for modelling the reservoirs in an interconnected way, accounting for the feedback from one water body to the next (Soares et al., 2021a). The model 1D assumption was proved to be valid for the study sites, a sensitivity analysis was performed, the model was calibrated and validated against measured field data, and goodness-of-fit metrics attested the accuracy of model outputs. All required data, input processing, modelling good practices, and performance assessment are detailed described in Soares et al. (2020), Soares et al. (2021a), and Soares and Calijuri (2021).

In the present study, GLM-AED was assumed exactly the same as its previous application in the current study sites (Soares et al., 2021a). The major processes in the water column were represented to simulate water temperature, dissolved oxygen (DO), total phosphorus (TP), nitrate (NO_3), ammonium (NH_4), and phytoplankton in the lacustrine zone of each reservoir. Within the phytoplankton module, all chlorophyll-a was assumed to be cyanobacteria. The model was run at an hourly time step over a 9-year period, from 2008 to 2016.

7.2.6 *Assessment of the trophic state index*

The trophic state index (TSI) adapted for subtropical reservoirs (Cunha et al., 2013) was computed for the six reservoirs based on the simulated geometrical mean of TP and chlorophyll-a (chl-a) concentrations on the surface. The index classifies the trophic state into six categories: ultraoligotrophic ($TSI \leq 51.1$), oligotrophic ($51.2 < TSI \leq 53.1$), mesotrophic ($53.2 < TSI \leq 55.7$), eutrophic ($55.8 < TSI \leq 58.1$), supereutrophic ($58.2 < TSI \leq 59.0$), and hypereutrophic ($TSI \geq 59.1$).

The simulated current trophic state in each reservoir is (Soares et al., 2021a): BB and BA are hypereutrophic ($TSI = 59.3$ and $TSI = 60.9$, respectively), IB is eutrophic ($TSI = 57.9$), PR is mesotrophic ($TSI = 53.9$), NA is oligotrophic ($TSI = 52.2$), and TI is ultraoligotrophic ($TSI = 50.1$).

7.2.7 *Design of scenarios*

Two major findings of a previous modelling application in the study sites were the basis for the present study (Soares et al., 2021a): (i) management strategies should be devoted in the uppermost reservoir in the chain as their impacts are propagated through one reservoir to the next, triggering a domino restoration effect of aquatic ecosystems along the cascade system; and (ii) phosphorus reduction within the water bodies is mandatory for recovering the trophic state in the reservoirs. Based on the abovementioned recommendations, six scenarios (S1–S6) were simulated to represent classical restoration practices encompassing both external and internal techniques that are usually used to address eutrophication in lakes and reservoirs worldwide (Abell et al., 2020; ILEC, 2005; Jilbert et al., 2020; Lüring et al., 2016; Stroom and Kardinaal, 2016).

The scenarios were simulated by the model by changing specific forcing variables and parameter values that would be directly affected by the restoration method (Table 7.2):

(S1) Reduction of external PO_4 load. The reduction of PO_4 loads from point and non-point sources within the basin catchment was represented by the reduction of the current daily inflow loads into the BB Reservoir;

(S2) Reduction of internal PO_4 load by inactivation. The usage of chemical agents to adsorb PO_4 , enhancing its precipitation from the water column and immobilisation on the sediment, was simulated by increasing the PO_4 sedimentation constant ($F_{sed}^{PO_4}$);

(S3) Reduction of phytoplankton biomass by algicides. The usage of compounds to increase cyanobacteria mortality was represented by increasing the phytoplankton metabolic loss (R_{resp});

(S4) Reduction of phytoplankton biomass by sedimentation. The usage of flocculants to enhance phytoplankton settling was represented by increasing the phytoplankton sedimentation rate (ω_{phy});

(S5) Hypolimnetic withdrawal. The discharge of nutrient-rich hypolimnetic water, reducing the nutrient availability for epilimnetic primary producers, was simulated by changing the withdrawal elevation (outl_elvs) to be closer to the bottom;

(S6) Hypolimnetic aeration and oxygenation. The increase of DO concentration at the bottom to suppress sediment release and entrainment of nutrient-rich bottom waters into the epilimnion was simulated by decreasing the sediment oxygen demand ($F_{sed}^{O_2}$). The parameter's value was decreased until the mean DO concentration at the bottom reached 10 mg L^{-1} .

Table 7.2. Scenarios of restoration practices and the associated simulation strategy.

Restoration practice	Simulation strategy	Symbol description
S1 – Reduction of external PO_4 load	Decrease PO_4 load	-
S2 – Reduction of internal PO_4 load by inactivation	Increase $F_{sed}^{PO_4}$	Sedimentation flux for PO_4
S3 – Reduction of phytoplankton biomass by algicides	Increase R_{resp}	Phytoplankton metabolic loss
S4 – Reduction of phytoplankton biomass by sedimentation	Increase ω_{phy}	Phytoplankton sedimentation rate
S5 – Hypolimnetic withdrawal	Deeper outl_elvs	Outlet elevation
S6 – Hypolimnetic aeration and oxygenation	Decrease $F_{sed}^{O_2}$	Sedimentation flux for DO

The daily PO_4 load into the BB reservoir is directly related to the TP concentration within the water body (Equation 7.1), thus decreasing the external PO_4 load will reduce the reservoir's TP concentration; the parameter $F_{sed}^{PO_4}$ is directly related to the PO_4 sedimentation to the bottom

($f_{sed}^{PO_4}$; Equation 7.2), thus its increase will increase PO_4 concentration at the bottom and decrease its availability for primary production on the surface; parameter R_{resp} is directly related to phytoplankton mortality (f_{mort} ; Equation 7.3), thus its increase will reduce phytoplankton biomass in the water column; the parameter ω_{phy} is directly related to phytoplankton settling to the bottom (f_{sett} ; Equation 7.4), thus its increase will reduce phytoplankton biomass at the euphotic zone; the user-defined outlet elevation ($outl_elvs$) determines if the withdrawal is shallow or deep within the water column, thus a deeper outlet elevation will promote the withdrawal of hypolimnetic waters; and the parameter $F_{sed}^{O_2}$ is inversely related to the sediment DO demand at the bottom ($f_{sed}^{O_2}$; Equation 7.5), thus its decrease will increase the hypolimnetic oxygenation.

$$TP = PO_4 + PO_4^{ads} + DOP + POP + PHY_P \quad (7.1)$$

$$f_{sed}^{PO_4} = F_{sed}^{PO_4} \frac{K_{sed}^{PO_4}}{K_{sed}^{PO_4} + [O_2]} (\theta_{sed}^{PO_4})^{T-20} \quad (7.2)$$

$$f_{mort} = (1 - k_{fdom}) \times R_{resp} \times [PHY_{N,P}] \quad (7.3)$$

$$f_{sett} = \frac{\omega_{phy}}{dz} [PHY_{N,P}] \quad (7.4)$$

$$f_{sed}^{O_2} = -F_{sed}^{O_2} \frac{[O_2]}{K_{sed}^{O_2} + [O_2]} (\theta_{sed}^{O_2})^{T-20} \quad (7.5)$$

where PO_4 is the concentration of filterable reactive phosphorus, PO_4^{ads} is the concentration of adsorbed filterable reactive phosphorus, DOP is the concentration of dissolved organic phosphorus, POP is the concentration of particulate organic phosphorus, $PHY_{N,P}$ is the internal nitrogen and phosphorus concentration, respectively, within the phytoplankton, $K_{sed}^{PO_4}$ is the half saturation constant for oxygen dependence of sediment PO_4 flux, $[O_2]$ is the DO concentration in the water, $\theta_{sed}^{PO_4}$ is the Arrhenius temperature multiplier for sediment PO_4 flux, T is the water temperature, k_{fdom} is the fraction of metabolic loss that is dissolved organic matter, dz is the thickness of the z^{th} layer in the water column, $K_{sed}^{O_2}$ is the half saturation constant for oxygen

dependence of sediment oxygen flux, and $\theta_{sed}^{O_2}$ is the Arrhenius temperature multiplier for sediment oxygen flux.

7.2.8 *Simulation of scenarios*

Each scenario was simulated for the uppermost reservoir and then it was propagated along the cascade system by applying a sequential modelling approach to take into account the feedback from one reservoir to the next. The forcing variable and parameter values were increased or decreased until the mean trophic state index in the BB Reservoir was changed from the hypereutrophic to the mesotrophic category. Each scenario was simulated separately, changing the corresponding forcing variable or parameter, while all other conditions were kept at their initial values.

The trophic state index in each reservoir was compared with the current condition (S0) to assess the most efficient strategies for restoration and management of the cascade system. From the simulated S1–S6 scenarios, the most efficient ones were selected to comprise an additional scenario (S7) in which the restoration methods were simulated simultaneously. The scenarios were simulated for the 2008–2016 period, but the first year of simulation (2008) was not considered for comparison purposes to eliminate the uncertainties of the model initial conditions.

7.3 **Results**

7.3.1 *Scenarios of individual restoration methods*

In the Tietê River's cascade system, PO₄ mainly originates from allochthonous inflow loads from the catchment, reaching 2,290 tons per year into the BB Reservoir. Hence, the restoration method intended to reduce external PO₄ load was expected to be successful. Indeed, the simulation results show that the reduction of external PO₄ load (S1) considerably decreased both the TP and chl-a concentrations in the BB Reservoir, with mean values of 0.022 mg L⁻¹ and 14.62 µg L⁻¹, respectively (Table 7.3), fulfilling the water quality threshold for avoiding mean TSI at the eutrophic categories. Similarly, a substantial effect on both TP and chl-a concentrations was also found for the reduction of internal PO₄ load by inactivation (S2),

revealing that the autochthonous PO_4 content that is released from the sediments is also an important source of phosphorus in the BB Reservoir. The decrease in chl-a concentration following the reduction of PO_4 loads indicates that the phytoplankton is under direct bottom-up control of phosphorus.

Table 7.3. Simulated mean total phosphorus (TP) and chlorophyll-a (chl-a) concentration at water surface over 2009–2016 period within the reservoirs for each simulated scenario.

	Scenarios							
	S0	S1	S2	S3	S4	S5	S6	S7
<i>TP ($\mu\text{g L}^{-1}$)</i>								
BB	114.05	22.14	26.06	97.98	96.79	113.82	112.23	24.34
BA	147.96	10.17	24.60	158.06	156.93	152.32	144.65	18.73
IB	127.07	6.61	17.73	141.26	139.86	131.75	123.08	11.81
PR	17.48	2.36	2.61	19.59	19.79	11.71	21.46	2.38
NA	12.27	3.39	4.00	14.60	14.31	10.62	13.59	3.60
TI	10.98	8.18	8.29	12.21	12.09	11.45	11.01	8.05
<i>Chl-a ($\mu\text{g L}^{-1}$)</i>								
BB	21.75	14.62	12.56	2.74	2.85	21.93	22.15	13.76
BA	39.27	6.10	12.71	37.85	37.96	39.79	39.18	11.06
IB	8.99	2.55	4.65	8.66	8.77	9.28	9.07	4.17
PR	11.99	1.81	1.99	13.15	13.30	8.22	14.51	1.83
NA	6.77	1.80	2.11	8.02	7.83	5.83	7.50	1.91
TI	1.85	1.48	1.50	1.92	1.93	1.91	1.89	1.45

The BB Reservoir's response to S1 and S2 scenarios was propagated along the cascade system, promoting a domino effect of restoration and improving conditions in the five downstream reservoirs. The decrease in TP and chl-a concentrations were substantial in all reservoirs resulting in the suppression of eutrophy not only in the BB Reservoir, but along the cascade system (Figure 7.2). Hence, the reduction of PO_4 loads was proved to be an efficient method for restoration at the basin catchment scale. However, the requirements for achieving the mesotrophic threshold are as enormously high as the 95% reduction of external PO_4 load relative to the current condition, and a sedimentation flux for phosphate of $-3.000 \text{ mmol m}^{-2} \text{ d}^{-1}$, which was out of the range of values found in the literature (Table 7.4).

Figure 7.2. Simulated Trophic State Index in the reservoirs along the cascade system for each scenario (S1–S6).

Note: Each colour area corresponds to a trophic state category: blue is ultraoligotrophic, green is oligotrophic, yellow is mesotrophic, brown is eutrophic, red is supereutrophic, and purple is hypereutrophic.

Table 7.4. The altered parameters and forcing variable in each scenario, their unit, initial values, literature range, and final values.

Scenario	Parameters and forcing variable				
	Symbol	Unit	Initial value	Literature range	Final value
S1	PO ₄ external load	mmol m ⁻³	-	-	-95%
S2	$F_{sed}^{PO_4}$	mmol m ⁻² d ⁻¹	0.125	0.001 ^a – 0.840 ^b	-3.000
S3	R_{resp}	d ⁻¹	0.03	0.01 ^c – 0.09 ^d	0.09
S4	ω_{phy}	m d ⁻¹	-0.02	-4.32 ^b – -0.01 ^c	-0.60
S5	outl _{elvs}	m	439.5	-	433.5
S6	$F_{sed}^{O_2}$	mmol m ⁻² d ⁻¹	6.00	-20.00 ^a – 87.50 ^b	180.00
S7	PO ₄ external load + $F_{sed}^{PO_4}$	-	-	-	-60%; -0.84

Note: References: ^a Farrell et al., 2020; ^b Burger et al., 2008; ^c Kara et al., 2012; ^d Cui et al., 2016; ^e Romero et al., 2004.

Restoration methods devoted to decreasing the phytoplankton biomass by its mortality using algicides (S3) or by its sedimentation using flocculants (S4) resulted in a markedly reduction on chl-a concentration in the BB Reservoir. TP concentration also declined, and thus the TSI was changed from hypereutrophic to mesotrophic in both scenarios. These methods were proved to be successful at a local scale, however improvements in the TSI of the BB Reservoir

were not propagated throughout the reservoirs' cascade system, thus the TSI was unchanged in the other five downstream reservoirs. Both parameter alterations, $R_{resp} = 0.09$ and $\omega_{phy} = -0.60$, were in the range of values founded in previous studies, indicating the viability of these methods to reduce phytoplankton biomass.

Simulations of hypolimnetic withdrawal (S5) showed that even if the outlet elevation was at 433.5 m, only 0.5 m from the bottom, the effects on TP and chl-a concentrations would be small and not sufficient to improve the trophic condition in the BB Reservoir. Similarly, the increase of the sedimentation flux for DO from 6.00 to 180.00 mmol m⁻² d⁻¹ to promote hypolimnetic aeration and oxygenation (S6) was not sufficient to improve the TSI in the BB Reservoir, despite a high DO concentration on the bottom layers. For both scenarios, the TSI remained above 59.1 sustaining the hypertrophy within the reservoir. No significant effects of these restoration methods were observed in the downstream reservoirs as well.

The low efficiency of both hydrological methods is attributed to the polymictic behaviour of the BB Reservoir, where the outlet elevation is of lower importance as nutrient concentrations are frequently uniform along the water column. The current DO depletion and hypoxic conditions developed in the bottom waters were not suppressed even by a high increase in the sedimentation flux for DO, which was out of the literature range.

7.3.2 *Scenarios of restoration methods acting simultaneously*

Based on the simulated TSI for S1–S6 scenarios, scenario S7 was comprised of the two methods intended to treat the excessive PO₄ load within the BB Reservoir (S1 and S2), i.e., the root-cause of its severely degraded condition. Firstly, the PO₄ sedimentation constant ($F_{sed}^{PO_4}$) in the BB Reservoir was adopted as -0.84 mmol m⁻² d⁻¹ to be within the literature range, which was assumed as a viable sedimentation rate; then, the external PO₄ load was reduced at incremental 5% steps until the mesotrophic condition was achieved (Table 7.4). Both methods, acting simultaneously, were able to considerably decrease the required reduction of external PO₄ load from 95% to 60%. The S7 scenario proved to be a restoration strategy to improve the water quality at a catchment scale, as both TP and chl-a concentrations decreased in all downstream reservoirs (Table 7.3), avoiding the eutrophic condition: BA reservoir was also mesotrophic, IB

was oligotrophic, and PR, NA and TI reservoirs were ultraoligotrophic (Figure 7.3). However, episodic events of algal blooms still occurred in BB and BA reservoirs.

Figure 7.3. The simulated trophic state index in the reservoirs along the cascade system for scenario S7.

Note: Each colour area corresponds to a trophic state category: blue is ultraoligotrophic, green is oligotrophic, yellow is mesotrophic, brown is eutrophic, red is supereutrophic, and purple is hypereutrophic.

7.4 Discussion

7.4.1 Restoration methods

Reducing external PO_4 loads from the catchment

Reducing external nutrient loads is a fundamental premise for lake restoration (Chorus et al., 2020; Chou et al., 2021; Liu et al., 2018), and management efforts often focus on achieving this goal. According to the model simulations, a reduction of the external PO_4 load would be effective at controlling eutrophication in the reservoirs along the Tietê River's cascade system. The primary factor sustaining high external PO_4 load into the BB Reservoir is point-source pollution from domestic sewage, due to its lack or insufficient collection and treatment: 60% of sewage collection and 44% of treatment, from which only 10% is submitted to tertiary treatment for phosphorus removal (ANA, 2012). Other point sources of external PO_4 loads are industrial effluents from more than 1,000 industries of diverse sectors, such as textile, paper pulp, food industry, and sugar plants, located at the catchment (CETESB, 2019).

Hence, the most important strategy to control external PO_4 load into the BB Reservoir is (1) to interdict raw sewage load into the reservoir's tributaries and redirect its discharge to wastewater treatment plants (WWTPs; Huang et al., 2019). Moreover, (2) the establishment of additional infra-structures increasing sewage treatment capacity within the catchment by building new WWTPs and implementing the tertiary treatment in the current ones, are required to accommodate the continuously increasing urban and agricultural activities. Additionally, (3) a river water treatment plant in the Tietê River (Coutinho, 2007) upstream from the reservoir's inlet, and (4) constructed wetlands (Paerl and Barnard, 2020) could be efficient methods to improve the inflow water quality.

Non-point sources of PO_4 loads come from fertilisers, pesticides, deforestation and improper soil management, diffuse pollution in both agricultural and urban areas, and solid waste improperly disposed (ANA, 2012). On-land strategies to reduce diffuse load should include (5) controls on fertiliser usage in crops and adoption of better agriculture practices (Marttila et al., 2020). (6) Efforts to implement reforestation and afforestation can also help to reduce the external PO_4 load, since the loss of forest cover usually increases land erosion and sediment transport (ILEC, 2005). In view of the lack of riparian vegetation in the BB Reservoir's surroundings, (7) the implementation of vegetated buffers composed by trees, shrubs and grasses alongside the water body and its tributaries could remediate direct non-point source pollution (Zhang et al., 2010). (8) Land use planning and soil conservation practices can be effective in minimizing soil loss from poor land management in agricultural areas, such as overgrazing, fallow cultivation, gully erosion, and unstabilised streambanks (ILEC, 2005). Additionally, (9) policy development and decision making for in-catchment management should be based on best management practices and legislation designed to mitigate nutrient loads (Qiu et al., 2018). Finally, (10) the financial compensation to landowners that provide ecosystem services from their land use through Payment for Ecosystem Services may be an innovative sustainable way to reduce diffuse PO_4 sources into the reservoir (Mueller et al., 2019).

Reducing internal PO₄ load by inactivation

The introduction of compounds is used to adsorb PO₄ and form a stable complex that precipitates and remains permanently bound in the sediments, ultimately being unavailable for phytoplankton uptake. Indeed, in the present study, the higher sedimentation of PO₄, reducing its internal load, strongly reduced TP concentration within the reservoir to 22% in comparison to the base scenario. In response, chl-a concentration considerably reduced to 58% of its initial value, revealing an effective bottom-up regulation of phytoplankton through TP.

The most frequently used chemical agents have been aluminum salts, iron, lanthanum, and calcium (Gibbs et al., 2011; Lüring et al., 2016; Søndergaard et al., 2003). When used appropriately, these materials have proved effective and produced rapid initial response to the treatment (Huser et al., 2016a). Moreover, these geoengineering materials were found to be ecosafe because they did not promote cyanobacterial cell lysis and did not release the intra- and extracellular toxins in the water (Lucena-Silva et al., 2019). The side-effect of this method is the intrinsically PO₄ accumulation in the sediment. As BB is a polymictic reservoir, frequent mixing events may induce resuspension of the sediment P pool. Thus, associated methods are required, such as capping sediments to create a physical barrier between the sediment-water interface (Hamilton et al., 2016) or dredging bed sediments (Cao et al., 2007). Although dredging is costly and it can adversely affect benthic organisms and pose difficulties for disposing dredged sediments, this method is most feasible for reservoirs in high-use urban areas (Abell et al., 2020), as is the case of the BB Reservoir.

As the phosphorus legacy within a water body originates from the external PO₄ load, the efficiency of PO₄ inactivation is only sustainable with a concomitant control of the external PO₄ load or its association with other combined restoration methods (Barçante et al., 2020; Bormans et al., 2016; Huser et al., 2016b). Otherwise, when a large amount of nutrients still enters a reservoir by the tributaries, the accumulation of phosphorus from external sources in the sediment would still result in a return of the phosphorus release from the sediment.

Reducing phytoplankton biomass by algicides

Algicides, in particular copper sulfate, hydrogen peroxide, and potassium permanganate, have been widely used to control phytoplankton biomass (Abell et al., 2020). In the present study, increasing phytoplankton mortality proved to be an efficient technique able to reduce 87% of chl-*a* concentration on the water surface. However, considering the potential side-effects of algicides on non-target organisms such as zooplankton, mollusks and fish due to excessive release of cyanotoxins, water managers and stakeholders are usually reluctant to use chemical control (Stroom and Kardinaal, 2016). More recently, new compounds for directed suppression of uniquely cyanobacteria, which are so-called as cyanocide, show better specificity for cyanobacteria and are biodegradable or transform into non-toxic products after applications, demonstrating good prospects for sustainability (Matthijs et al., 2016). As both algicides or cyanocides treat only a symptom of eutrophication, but not its root-cause, resulting in a temporary effectiveness when they are the unique restoration method (Moss, 2007), they must be applied in parallel with the reduction of external nutrient loads.

Reducing phytoplankton biomass by sedimentation

The application of flocculants are intended to aggregate algal biomass and sink them with a ballast to the bottom (Lüring et al., 2016). In the present study, simulations of increasing the sedimentation rate of the phytoplankton achieved a high removal rate of 87%. Removal efficiencies of 60–90% were found for *Microcystis aeruginosa* in freshwater (Li and Pan, 2013). Traditional flocculants did not used to be environmental friendly or cost effective (Zou et al., 2006). Fortunately, in recent years, efforts have been made to develop flocculants based on natural and nontoxic clays, such as montmorillonite, kaolinite and phosphatic (Pan et al., 2006) or on the soil particles from a bank near the water body modified by adding a small amount of biodegradable natural polymers or proteins such as chitosan (Pan et al., 2011), therefore representing a lower risk to human and environmental health. For instance, flocculants were found to not affect metal residuals, thus not threatening the aquatic ecosystem (Yuan et al., 2016). Hence, reducing phytoplankton biomass by sedimentation can be a welcome technique combined with nutrient control methods for eutrophication management.

Hypolimnetic withdrawal

Withdrawal of nutrient-rich water from the hypolimnion is a low cost technique often used in reservoirs discharging water for hydropower generation that frequently leads to a decrease in phosphorus and chlorophyll-a concentrations in the epilimnion, increases water transparency, and decreases phosphorus concentration as well as anoxia in the hypolimnion (Jilbert et al., 2020). However, in the present study, alterations on TP and chl-a concentrations were smaller than 1% relative to the base scenario. The main cause of the inefficiency of this method is attributed to the polymictic behaviour in the BB Reservoir. The frequent mixing events homogenise the water column, thus nutrient concentration is quite vertically uniform. For this reason, this method is best suited for deep water bodies that exhibit stable stratification. Most importantly, the hypolimnetic withdrawal in the BB Reservoir is not recommended because the withdrawal of nutrient-rich waters will be the input for the BA Reservoir, which is the next one in the cascade system. Hence, this technique transports the nutrient problem downstream, posing negative effects along the cascade system due to the discharge of water with potentially higher nutrients, ammonia, hydrogen sulfide or other toxic compounds (Bormans et al., 2016).

Hypolimnetic aeration and oxygenation

Hypolimnetic aeration can be achieved by adding oxygen to bottom waters using mechanical agitation, direct injection of pure oxygen, and direct injection of air (Bormans et al., 2016) to promote oxic conditions at the sediment–water interface aiming at suppressing the sediment release. Previous studies reported that the hypolimnetic aeration promoted sufficient DO at the bottom, but no effect on P reduction and phytoplankton biomass was achieved, suggesting that aeration induced the mineralisation of organic matter and the phosphorus recycling (Niemistö et al., 2016; Taipale et al., 2020). Similarly, the simulated scenario of hypolimnetic aeration did not affect TP and chl-a concentrations within the reservoir, despite the increase of DO concentration at the bottom layers. As the parameters of the GLM-AED model are constant over the simulation period, the sedimentation flux for DO ($F_{sed}^{O_2}$) could not be increased only during specific hypoxic events. Thus, the mean DO at the bottom was quite high, 10 mg L⁻¹, but during some days its concentration was below the hypoxic threshold (2 mg L⁻¹). This is a limitation of the simulated scenario that impairs a reliable assessment of the effects of

hypolimnetic aeration on TP and chl-a concentrations, which merits further investigations in future studies.

7.4.2 *Managing highly degraded reservoirs along a cascade system*

The current hypereutrophic condition in BB and BA reservoirs prevents any use of these water bodies for water supply or recreational purposes and impairs ecosystem services they may provide. In addition, IB and PR reservoirs are currently under eutrophication, and a progressive downstream degradation is forecasted reaching NA and TI reservoirs. Hence, it is urgent to implement restoration actions in order to maintain TP and chl-a concentrations below critical thresholds and mitigate the severe degradation in reservoirs at the basin catchment scale. The present study provides evidence that efforts to treat the root-cause, i.e., the external PO₄ load through the Tietê River must be a priority to eliminate issues of water quality impairment not only in the uppermost reservoir, but also in the downstream ones along the cascade system.

More than three decades have passed since the recognition of environmental degradation in the BB Reservoir (Calijuri, 1988; Matsumura-Tundisi and Tundisi, 2005). At that point, the current trophic state will be difficult to reverse due to established land use activities and high content of nutrients within the water body (Mueller et al., 2015). Indeed, the accomplishment of the required 95% reduction of external PO₄ load into the BB Reservoir, if it would be the only restoration method, would demand enormous efforts in terms of planning and management, infrastructure resources, and financial investment, ultimately being almost prohibitively feasible. Similarly, a reduction in the external nitrogen load by 70% was required to meet the water quality standards in a meso- eutrophic reservoir in China (Chou et al., 2021).

When a water body receives extreme phosphorus inputs for an extended period of time, its recovery may become irreversible, i.e., it cannot be restored by input controls alone (Carpenter et al., 1999). Indeed, the legacy of the internal phosphorus content may be very persistent due to its accumulation and subsequent release, resulting in biogeochemical lags that delay improvements in water quality following the reduction of external PO₄ load (Abell et al., 2020). Water quality can therefore remain poor for years, even after external loads have been remarkably reduced. For example, time recovery can extend from 2–4 years (Hanson et al., 2017) to 10–15 years where there is a highly enriched bottom sediment (Jeppesen et al., 2005).

For this reason, the inactivation of PO_4 from the water column can be a valuable method in parallel to the reduction of external PO_4 load into the BB Reservoir, comprising a combination of in-lake and on-land treatments to reinforce the reservoir's recovery. Besides, additional interventions to treat eutrophication symptoms, including the reduction of phytoplankton biomass by both algicides and sedimentation are recommended since they proved to be efficient methods to decrease TP and chl-a concentrations within the BB Reservoir. It is important to emphasise that neither on-land management nor in-lake controls alone are capable of completely mitigating the eutrophication at the basin catchment scale, but rather they are useful complimentary strategies to recover water quality. Long-term effects of in-lake treatments can, however, be difficult to achieve, and in many cases, lake restoration may need to be conducted on a regular basis, rather than a 'once and for all' solution (Søndergaard et al., 2007). As part of a management plan, research and educational programs are always helpful to foster citizens' engagement with environmental protection. Finally, long-term monitoring campaigns at higher spatial and temporal resolution to obtain data records at a higher frequency are highly recommended.

7.4.3 Limitations

The configuration of the GLM-AED model prevented the simulation of some restoration methods because there is not an associated parameter that could be altered to simulate certain methods. For instance, the dredging of sediments is envisaged as a required method in the BB Reservoir, especially following the inactivation of PO_4 by chemical agents and the sedimentation of phytoplankton by flocculants. Moreover, the physical removal of surface phytoplankton scum by superficial skimming also requires further investigation. As the model does not simulate high levels of biodiversity, such as macrophytes and fish, biomanipulation methods, involving the introduction of species that affect the food web in a beneficial way, could not be included in the present study. Besides the limitation of the model, the study sites lack a detailed knowledge of the aquatic ecology of the reservoirs and the long-term presence of ecological monitoring. Finally, other hydrologic restoration strategies, such as water level alterations, were not implemented because they are incompatible with the reservoirs' operation.

7.4.4 *Restoration challenges in a changing climate*

Increasing temperature in a future climate will likely act to negatively impact lake water quality (Me et al., 2018) leading to an intensified impact in high-nutrient ones (Farrell et al., 2020). Previous studies (Chang et al., 2015; Rolighed et al., 2016; Ficker et al., 2017) suggest that in-lake phosphorus availability is expected to be enhanced by higher mineralisation rates and release from bottom sediments triggered by higher water temperatures. In addition, more frequent large storm events arising from climate change will likely result in increased exports of both dissolved and particulate phosphorus from agricultural lands in the catchment (Dolph et al., 2019). Considering the ongoing significant warming in the BB Reservoir since 1993 with heating rates as high as 1.02 °C per decade on the surface (Soares et al., 2021b), it is likely that more rigorous mitigation efforts may be needed to accomplish an even higher reduction of external nutrient load beyond current restoration targets to counteract the deterioration (Bucak et al., 2018). In face of complex interactions and many controlling factors of eutrophication within lakes and reservoirs, a dynamic coupled atmospheric-land-lake modelling approach has the potential to provide more realistic strategies for reducing PO₄ load from the catchment and move toward a holistic prediction of restoration management scenarios (Sharma et al., 2018).

7.5 Conclusions

The GLM-AED model was a valuable tool to assess the response of a reservoirs' cascade system to different restoration methods over the 2009–2016 period. Whereas many studies evaluated restoration methods to a single water body, as the authors are aware, this is the first study evaluating the propagation of water quality improvements taking into account the feedback from one water body to the next. In summary, the major findings of the present study were: (1) the reduction of both external and internal PO₄ loads is highly recommended as they treat the root-cause of hypereutrophy in the BB Reservoir. Besides, the adopted model approach revealed the bottom-up control of cyanobacteria and the propagation of improvements in all downstream reservoirs along the cascade system; (2) the reduction of phytoplankton biomass proved to be a successful method to improve the trophic state in the BB Reservoir, however it did not support positive effects along the cascade system; (3) no effects were promoted by hydrological methods

due to the polymictic behaviour in the BB Reservoir; and (4) the required 95% reduction in the external PO_4 load, when this method is applied alone, would demand huge financial investment and commitment, and is almost practically impossible to achieve. Hence, the effective restoration at a basin catchment scale must comprise a combination of on-land and in-lake restoration techniques to make the recovery more feasible in highly degraded reservoirs.

The present study provides a methodology to investigate restoration methods that result in positive effects not only in the reservoir itself but also promoting an overall improvement in water quality at a basin catchment scale. A restoration program of the aquatic ecosystems in the Tietê River's cascade system is still absent even after thirty years since the recognition of eutrophication in the BB Reservoir envisioning a downstream degradation. The presented findings have important implications for the studied system but can also be applied for other situations where lakes and reservoirs are located in cascade systems, especially in highly anthropogenic impacted catchments.

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8

Concluding remarks and future directions

8.1 Synthesis

The Tietê River's cascade system is a prominent representative of subtropical reservoirs constructed along a single river and was used as a study case to provide a deep understanding of their physical limnology. The uppermost reservoir in the system, Barra Bonita, was intensively reported in former studies. Despite the importance of the downstream reservoirs, they were poorly studied since their construction. To overcome the limited information from the tropics, deterministic modelling is central to understand reservoirs' internal processes and expanding our knowledge of how ecosystems react to altered boundary conditions. In the present thesis, a coupled hydrodynamic-biogeochemical modelling was applied for the first time for these reservoirs. As identified in Chapter 2, a consistent protocol of good practices was followed by applying an open-source model and by conducting sensitivity analysis, calibration, validation, and multiple metrics for performance assessment. The model has proved its power for addressing science questions in a broad morphometric range (maximum depth from 19.2 to 45.6 m, hydraulic residence time from 15 days to 1.2 years, and surface area from 46 to 654 km²) and water quality gradient (from hypereutrophic to oligotrophic).

In the first part of this thesis, hydrodynamics were studied to quantify the thermal processes within the reservoirs aiming at a better understanding of internal dynamics and their implications to biogeochemical cycles. In Chapter 3, a hindcast simulation applying the GLM model was calibrated and validated to reconstitute the thermal structure and stratification patterns

over the 2009–2016 period. The first original contribution of this work is the parameterization strategy applied to accomplish a better simulation by the estimation of potential sensitive parameters through regression curves to overcome the challenge of exploring hydrodynamics in two reservoirs with a lack of measured temperatures. This procedure enhanced the current knowledge of hydrodynamics for reservoirs where field measurements were recorded in a scarce frequency (every two months), beyond to provide the first representation of the thermal characteristics of reservoirs that have never been monitored. Without the applied parameterization strategy, the thermal behavior of such reservoirs would remain unclear. Future work to test the parameterization curves for other reservoirs is strongly recommended to critically frame the obtained results.

Chapter 4 represents an important keystone of this thesis because the impacts of climate change on subtropical reservoirs were not intensively studied in the recent literature. It was demonstrated from hindcast modelling the effects of increasing air temperature and decreasing wind speed on the hydrodynamics of Barra Bonita Reservoir, which would be difficult to analyze using only field data. It is envisioned that other polymictic reservoirs in the subtropics are facing warming as well, however future work devoting efforts to model other subtropical water bodies are recommended towards a deeper understanding of their response to a changing climate.

The second part of this thesis placed the focus on biogeochemical processes. Chapter 5 supplied a better understanding of the governing ecosystem dynamics, providing the parameters that control the dynamic behavior in each reservoir according to their thermal regime and trophic state. The second original contribution of this work is the sequential modelling approach that fully links reservoirs' processes, in which alterations in the boundary conditions are propagated through one water body to the next. Chapter 6 proved that the hypothesis of a synergistic interaction among reservoirs triggering a domino effect along the cascade system, thus affecting the water quality further downstream, is true. This finding is of great scientific interest as it allows the identification of the most strategic reservoir to devote management actions, especially in developing countries where resources, infrastructure, and preparedness are frequently scarce.

In face of the increasing pressure posed on the reservoirs from poor environmental protection in combination with climate change, resulting in water quality severe degradation, Chapter 7 supplied scenarios of classical restoration methods to guide optimized restoration

efforts at a basin catchment scale. In the Tietê River's cascade system, the effective restoration must comprise a combination of on-land and in-lake techniques to make the recovery more feasible due to the high degradation of the uppermost reservoirs. This finding may be of primary interest to water managers for establishing an efficient restoration program and ensuring water security for future generations, as water quality degradation is expected to exacerbate in face of cumulative stressors such as population growth, agricultural development, deforestation, urbanization, and climate change. It is expected that the main messages of the present study also apply to other interconnected lakes and reservoirs worldwide, providing relevant information for increasing water resources sustainability and aquatic biodiversity.

8.2 Major findings

The major scientific outcomes obtained from modelling results are summarized below:

- **The warming of Barra Bonita Reservoir in response to climate change is already under way**

A warming signal was detected in Barra Bonita Reservoir along the water column over the 1993–2018 period. Simulation results from Chapter 4 showed that deepwater warming was primarily enhanced by intrinsic characteristics of human-made and human-operated aquatic systems, such as the outlet structure and the high water level fluctuation. Water temperature warming has implications for many processes that affect biogeochemical cycling and suggests that the current eutrophication-related problems will probably become more drastic, adding further stress to the ecosystem, ultimately requiring more rigorous mitigation efforts to counteract deterioration.

- **Management efforts should be devoted to the uppermost reservoir along a cascade system due to the synergistic interaction among them**

Modelling results from Chapter 5 indicate that the reduction of external nutrient loads in the uppermost reservoir was propagated through one reservoir to the next, triggering a domino effect along the cascade system. A synergistic interaction was caused by the retention capacity of

nutrients in each reservoir, corroborating that the modelling of connected systems is worthwhile given that the feedback from one system to the next is an important driver of the resulting state of the next system. It is expected that this finding from the Tietê River case study applies to cascade systems in general because the physical mechanisms of nutrient retention are valid to any water body.

- **Numerical modelling is a powerful tool for water resources management**

The outcomes of this thesis demonstrated the importance of a numerical model as a tool to elucidate ongoing effects from both climate and anthropogenic pressures on hydrodynamics and water quality in six reservoirs. Indeed, modelling results brought new information that allowed to (i) achieve a deep understanding of the mechanisms that govern ecosystem functioning in the study sites, (ii) fill temporal gaps and accomplish a daily data set instead of measurements at a bi-monthly frequency, and (iii) conduct virtual experiments to simulate restoration techniques. We advocate for the use of numerical models for decision-making to assist in planning mitigation and adaptation strategies for ensuring the security of water storage, ecological balance, goods, and ecosystem services that reservoirs provide to society.

8.3 Recommendations for future research

The outcomes of this thesis identified scientific gaps that warrant further research. In the following paragraphs, possible directions for future research routes are addressed. While simulation results give evidence that Barra Bonita Reservoir is warming in response to climate change, future modelling studies could investigate impacts over a broad range of reservoirs. Expanding the number of reservoirs to be modelled can be useful for identifying patterns across a diverse range of reservoirs, providing further information on reservoir response in low-latitudes.

One of the research limitations in this thesis was the low frequency of field monitoring. Historically, measurements conducted by environmental agencies in Brazil were taken every two months, and episodically scientific monitoring campaigns have been taken at a higher frequency, but during short periods. We recommend a future application of high-frequency monitoring that performs measurements of vertical profiles at additional points to overcome the scarcity of field

data aiming. Such field data would be hugely beneficial in reducing sources of uncertainty and refining our understanding of the internal processes, besides being a powerful tool for enabling 2D and 3D models applications. In addition, satellite data can be calibrated by in-situ measurements, which may offer large opportunities, especially in a scarce data context.

Finally, I expect and encourage the application of the GLM-AED model, calibrated and validated, for the reservoirs in the Tietê River's cascade system for future work to address other matters of interest. While phytoplankton dynamics were not the focus of the present thesis, it is a key area with several environmental implications that merits further studies. Additionally, the holistic evaluation of on-land restoration scenarios by coupling lake and catchment models is strongly advisable to investigate how changes in land use, nutrient loading, rainfall and streamflow might affect reservoir ecosystems. Another area of interest would be the simulation of future scenarios, which is of particular importance to ensure water security in face of a more variable climate.

9

Publication list

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Soares, L.M.V., Calijuri, M.C., Silva, T.F.G., Novo, E.M.L.M, Cairo, C.T., Barbosa, C.C.F., 2020. A parameterization strategy for hydrodynamic modelling of a cascade of poorly monitored reservoirs in Brazil. *Environ. Model. Softw.* 134. <https://doi.org/10.1016/j.envsoft.2020.104803>

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