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CAROLINA CERQUEIRA BARBOSA

Estudo de cenários baseados em projeções de mudanças climáticas e de uso do solo para o reservatório de Itupararanga (SP): *open access tools* no gerenciamento da qualidade das águas

São Carlos (SP)
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Tese apresentada à Escola de Engenharia de São Carlos da Universidade de São Paulo, como requisito para a obtenção do Título de Doutora em Ciências: Engenharia Hidráulica e Saneamento.

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RESUMO

BARBOSA, Carolina Cerqueira**. Estudo de cenários baseados em projeções de mudanças climáticas e de uso do solo para o reservatório de Itupararanga (SP)**: *open access tools* no gerenciamento da qualidade das águas 2022. 127f. Tese (Doutorado em Ciências: Hidráulica e Saneamento). Escola de Engenharia de São Carlos, Universidade de São Paulo, São Carlos, 2021.

Os reservatórios são ambientes de transição entre rios e lagos que possuem fragilidades inerentes à construção das barragens e que somadas aos problemas associados necessitam de monitoramento ambiental frequente. A modelagem determinística de reservatórios tem se firmado como tecnologia promissora no estudo do ecossistema aquático e qualidade das águas. Compreender as diversas interações bióticas e abióticas e suas alterações devido a forçantes externas e internas nesses ambientes é um desafio para o gerenciamento ambiental e controle da poluição das águas. Nesse sentido, a presente pesquisa introduziu novas abordagens de modelagem para estudar respostas hidrodinâmicas e de qualidade da água do reservatório de Itupararanga (SP) em face à cenários de mudanças climáticas e de modificações futuras de uso e ocupação do solo. Diferentes acoplamentos de modelos *open-source* foram utilizados para avaliar a performance das abordagens metodológicas, além de (1) projeções de aumento das emissões de CO_2 para entender como o nível de água do reservatório e o regime térmico responderiam ao final da década de 2020; (2) tendências de uso e ocupação do solo da bacia do Alto Sorocaba para proposição de cenários e análise de respostas da qualidade da água; e (3) implicações na quantidade e qualidade da água do reservatório com base em cenários de uso e ocupação do solo e projeções climáticas para a década de 2050. As abordagens de modelagem testadas foram eficientes na simulação de variáveis hidrológicas, hidrodinâmicas, biogeoquímicas e ecológicas e demonstraram as potencialidades desses modelos em estudos de gerenciamento de qualidade da água. As principais respostas obtidas foram que a alteração dos padrões hidrológicos tem interferência importante na disponibilidade hídrica do reservatório de Itupararanga e de acordo com projeções climáticas espera-se que haja redução dos volumes de precipitação nas próximas décadas. Além disso, comprovou-se que as projeções de aquecimento global têm influência nos padrões de estratificação térmica e estabilidade da coluna de água. A intensificação da estabilidade e aprofundamento da termoclina podem ser de grande risco aos usos múltiplos por alterarem a dinâmica do fitoplâncton e favorecerem a dominância de cianobactérias. Considerando cenários de uso do solo baseados em tendência esperada de ocupação para 2050, diminuição e intensificação de áreas agrícolas e expansão urbana, foram encontrados melhores respostas de qualidade da água para o cenário conservacionista, destacando a importância da conservação e recomposição da Mata Atlântica na proteção do ecossistema aquático. Os resultados dos conjuntos de cenários de projeções climáticas e alterações de uso do solo evidenciaram que ambos *drivers* são importantes para a dinâmica trófica do reservatório de Itupararanga. Apesar das projeções climáticas, os cenários de redução do desmatamento e aumento das áreas preservadas indicaram tendência de oligotrofização do reservatório. Contudo, devido às projeções indicarem aquecimento global e outras mudanças de forçantes meteorológicas seriam esperados picos mais elevados na disponibilidade de fósforo total e biomassa fitoplanctônica em comparação aos últimos anos. Os resultados apontam a urgência de esforços de manejo para controlar a expansão agrícola e urbana sem controle ambiental na bacia do Alto Sorocaba. Espera-se que os resultados da presente pesquisa possam embasar ações de prevenção à crise hídrica incentivando estratégias de operação da barragem para gestão do volume útil do reservatório, controle da qualidade da água e proteção do ecossistema aquático.

Palavras-chave: modelagem de qualidade da água, mudanças climáticas, reservatório de Itupararanga, gerenciamento de recursos hídricos.

ABSTRACT

BARBOSA, C.C. **Scenarios based on climate change and land use projections for the Itupararanga reservoir (São Paulo, Brazil)**: open-source tools applied to water quality management**.** 2022. 127 f. Dissertation (PhD) – São Carlos School of Engineering, University of São Paulo, São Carlos, 2021.

Reservoirs are transitional environments between rivers and lakes that present weaknesses inherent to the construction of dams and that, added to the associated problems, require frequent environmental monitoring. Deterministic modeling has established itself as a promising technology in the study of freshwater ecosystems and water quality. Understanding the various biotic and abiotic interactions and their changes due to external and internal forcing in those water bodies is a challenge for environmental management and water pollution control. Thus, this research has introduced new modeling approaches to study the hydrodynamic and water quality responses of the Itupararanga reservoir (São Paulo, Brazil) under climate change scenarios and alterations in land use and land cover in the watershed. Different couplings of open access tools were used to assess the performance of the methodological approaches, in addition to (1) projections of increased CO2 emissions to understand how the reservoir water level and thermal regime would respond for the 2020s; (2) trends in land use and land cover in the Alto Sorocaba basin to propose scenarios and analyze water quality responses; and (3) implications on reservoir water quantity and quality based on land use and land cover scenarios and climate projections for the 2050s. The proposed modeling approaches were efficient in simulating hydrological, hydrodynamic, biogeochemical and ecological variables and demonstrated the potential of these models in water quality management studies. The main insights of this research were that changes in hydrological patterns have an important interference in the water availability of the Itupararanga reservoir and, according to climate projections, it is expected that there will be a reduction in precipitation volumes in the coming decades. Furthermore, global warming projections have been shown to influence thermal stratification patterns and water column stability. The intensification of stability and deepening of the thermocline may threaten the reservoir's multiple uses, as they alter the dynamics of phytoplankton and favor the dominance of cyanobacteria. Considering land use scenarios based on the expected occupation trend for the 2050s, reduction and intensification of agricultural areas and urban expansion, there was an improvement in the reservoir water quality for the conservation scenario. Those results highlight the importance of conservation and restoration of the Atlantic Forest in protecting aquatic ecosystems. The results of the sets of climate projections and land use change scenarios showed that both drivers are important for the trophic dynamics of the Itupararanga reservoir. Despite climate projections, the scenarios of reduced deforestation and increase in preserved areas indicated a trend towards oligotrophication. However, as projections indicate global warming and other changes in meteorological forcing, higher peaks in the total phosphorus availability and phytoplankton biomass compared to recent years would be expected. The outcomes point to the urgency of management efforts to control agricultural and urban expansion without environmental management in the Alto Sorocaba basin. It is expected that the results of this research support management actions to prevent the water crisis, encouraging dam operation strategies to manage the reservoir volume, control water quality and protect the aquatic ecosystem.

Keywords: water quality modeling; climate change, Itupararanga reservoir; water resources management.

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CAPÍTULO 1- INTRODUÇÃO GERAL E JUSTIFICATIVA

1. Contextualização

Os reservatórios são formados pelo represamento de rios, para atender a usos múltiplos, principalmente geração de energia, regularização de vazão e abastecimento público de água. São considerados sistemas de natureza híbrida, com gradientes horizontais, semelhantes aos rios, e verticais, característicos de lagos, com relação aos fatores abióticos que governam a produção primária (Thornton et al., 1990). De acordo com Lewis (1987), para a análise das propriedades dos ecossistemas continentais tropicais é essencial o conhecimento das causas primárias e os efeitos de primeira ordem que as governam, com base na latitude.

Como causas primárias é possível relacionar as baixas latitudes à alta irradiância anual e, consequente, pouca variação sazonal (máximas e mínimas) e baixo efeito da força Coriolis, sendo igual a 0 no Equador, devido à latitude 0º. Como efeitos físicos, a diferença de temperatura entre o topo e o fundo de lagos que tendem a se estratificar aumenta com a latitude até o pico de 35º-50º, fator relacionado às temperaturas da água (Lewis, 1987). As consequências biológicas são a alta produção primária durante todo o ano.

A qualidade da água, bem como as cargas de nutrientes são influenciadas pela operação da barragem que cria pulsos e altera constantemente a dinâmica dos organismos. Além disso, fatores socioeconômicos, como o uso e ocupação do solo, captação de água, o manejo da terra e drenagem das águas pluviais, além de mudanças climáticas também se relacionam à disponibilidade e qualidade da água nesses ambientes.

A literatura tem indicado os efeitos das mudanças climáticas sobre as taxas de evaporação (Althoff et al., 2020; O'Reilly et al., 2015; Zhan et al., 2019) e padrões de estratificação térmica de lagos e reservatórios (Kraemer et al., 2017; Moras et al., 2019; Niedrist et al., 2018). Geralmente, as respostas estão associadas ao balanço hídrico e à temperatura e morfometria média dos ecossistemas. Períodos de escassez hídrica têm se tornado mais frequentes ao redor do mundo e também se relacionam ao aquecimento global (Huo et al., 2020; Zwart et al., 2017).

Alterações nos padrões de precipitação têm gerado impacto direto no fornecimento de água potável e geração de energia por hidrelétricas. Além disso, estudos observaram que as estratificações nos reservatórios estão se tornando mais estáveis, tendo como consequência termoclinas mais profundas e favorecimento das florações de cianobactérias (Huisman et al., 2018; Wells et al., 2015).

Outros *drivers* do aumento do nível trófico de lagos e reservatórios são a expansão urbana e agrícola e manejo inadequado do solo (Amorim et al., 2020; Huo et al., 2019). A eutrofização pode limitar os usos múltiplos a que os corpos de água se destinam, especialmente o abastecimento de água. Como efeitos indiretos estão os danos à saúde, incluindo toxinas e patógenos, além dos efeitos negativos no uso para recreação, como maus odores e interdição ao uso esportivo/recreativo. As florações de cianobactérias tóxicas também provocam mortandade de peixes, anoxia da coluna de água e deterioração do habitat aquático. Como consequência da eutrofização acelerada, as florações podem aumentar os gastos no tratamento de água. Os organismos podem entupir filtros, aumentar a necessidade de produtos químicos na coagulação, bem como modificar o sabor e o odor da água tratada. Alterações na composição da comunidade fitoplanctônica podem favorecer o entendimento do processo de eutrofização (Beghelli et al., 2016) e auxiliar no controle da poluição aquática.

Nas últimas décadas, o surgimento e a utilização de modelos determinísticos voltados à simulação da qualidade da água, especialmente as variáveis bióticas, em corpos hídricos continentais têm demonstrado o potencial dessas tecnologias no gerenciamento ambiental (Fragoso et al., 2010). Tais modelos podem realizar prognósticos e apontar a necessidade de aplicação de tecnologias ambientais na solução de problemas.

Complementarmente à utilização dos modelos de qualidade da água, o estudo da hidrodinâmica permite compreender a mistura horizontal e vertical das águas em lagos, estuários e reservatórios (Fragoso et al., 2009). A ligação entre os processos biogeoquímicos e hidrodinâmicos do ecossistema aquático favorece uma representação flexível e integrada da dinâmica dos organismos vivos e suas relações com as mudanças de nível trófico, variações de nível de água e ciclagem de nutrientes no meio.

Embora a literatura venha demonstrando a eficiência na utilização de modelos de qualidade da água, principalmente em regiões temperadas

(Bhagowati and Ahamad, 2019; Calamita et al., 2021), no Brasil e em outros países em desenvolvimento, há lacuna de dados de monitoramento de longo período. Isto limita a utilização dos modelos de ecossistema aquático que demandam diversos conjuntos de dados e calibração de grande quantidade de parâmetros. Apesar do aumento de instalação de estações de alta frequência para monitoramento de qualidade da água nos últimos anos, ainda existem poucos estudos com aplicação desse tipo de ferramenta em regiões tropicais e subtropicais (Soares and Calijuri, 2021).

A literatura também tem destacado o acoplamento de modelos climáticos e hidrológicos e modelos de bacia como uma tendência nos últimos anos (Soares and Calijuri, 2021) visto à interdependência de todas as variáveis e seus efeitos sobre os ecossistemas aquáticos e à qualidade da água.

Diante da demanda de estudos acerca das respostas de reservatórios de usos múltiplos em face à cenários de mudanças climáticas e tendências futuras de uso e ocupação do solo em bacias hidrográficas, o presente estudo testou o acoplamento de modelos para simulação dessas forçantes e variáveis hidrodinâmicas e de qualidade da água. A estrutura desta tese foi organizada, além dessa introdução geral e justificativa, contendo ainda objetivo geral e hipóteses, descrição da área de estudo e da importância da modelagem de ecossistemas aquáticos, em outros quatro capítulos, conforme Tabela 1.1.

Com esses quatro capítulos espera-se contribuir para a ampliação do conhecimento acerca das potencialidades dos modelos *open-source* nas investigações de cenários de mudanças climáticas e de alterações de uso do solo em bacias hidrográficas e as consequências esperadas na disponibilidade hídrica e na qualidade da água de reservatórios a fim de dar *insights* para o gerenciamento e controle ambiental e operação de barragens.

Tabela 1-1: Estrutura da Tese

CAPÍTULO	DESCRIÇÃO
2. Future projections of water level and thermal regime changes of a multipurpose subtropical reservoir (São Paulo, Brazil)	Apresenta os resultados das alterações de nível de água e regime térmico do reservatório de Itupararanga devido às projeções climáticas para o fim da década de 2020, por meio de simulações hidrológica e hidrodinâmica.
3. Modeling the Responses of Dissolved Oxygen and Nitrate Concentrations due to Land Use	Apresenta as respostas das concentrações de oxigênio dissolvido e nitrato à cenários de mudanças de uso e cobertura do solo da bacia do Alto Sorocaba

and Land Cover Change Scenarios in a Large Subtropical Reservoir	para a década de 2050 por meio de modelagem de carga distribuída de bacia e hidrodinâmica e biogeoquímica de reservatório.
4. Forecast of trophic state changes of a subtropical reservoir due to climate change and land-use change scenarios for the 2050s: an integrated climate-hydrological-biogeochemical modeling approach	Apresenta resultados do acoplamento de modelos hidrológico, termodinâmico, de carga distribuída, hidrodinâmico e ecológico para previsão do nível trófico do reservatório de Itupararanga para a década de 2050, com base em cenários de projeções climáticas e de mudanças de uso e cobertura do solo.
5. Considerações finais e recomendações	Apresenta uma síntese dos resultados dos quatro capítulos e conclusão da Tese, com considerações acerca das principais descobertas e contribuições do presente trabalho, além de fornecer recomendações acerca das metodologias propostas para estudos de qualidade da água em reservatórios

2. Objetivos e hipóteses

O objetivo principal da pesquisa foi testar o acoplamento de modelos *open-source* no estudo de respostas hidrodinâmicas e de qualidade da água do reservatório de Itupararanga (SP) em face a cenários de mudanças climáticas e de modificações futuras de uso e ocupação do solo na bacia hidrográfica.

Com base no objetivo formulado, investigou-se se o acoplamento de modelos determinísticos e técnicas implementadas em sistemas de informações geográficas (SIG) seriam eficientes para o estudo da qualidade das águas do reservatório de Itupararanga. Além disso, como tais simulações seriam úteis para analisar variações verticais e sazonais de nível de água, regime térmico, dinâmica de nutrientes e nível trófico do reservatório de Itupararanga, do período de 2009 a 2019, e proposição de cenários hipotéticos com os parâmetros estimados para avaliar o comportamento do ambiente aquático às projeções climáticas e modificações de uso e ocupação do solo em seu entorno.

3. Área de estudo

O estado de São Paulo possui 22 Unidades de Gerenciamento de Recursos Hídricos (UGRHI), definidas pela Lei nº 9.034/1994 (São Paulo, 1994). Entre estas, a UGRHI 10 corresponde à bacia hidrográfica do rio Sorocaba e Médio Tietê (SMT), localizada na porção centro-sudeste do estado.

A UGRHI 10 é dividida em seis sub-bacias hidrográficas, correspondendo: Médio Tietê Inferior, Médio Tietê Médio, Baixo Sorocaba, Médio Sorocaba, Médio Tietê Superior e Alto Sorocaba. Esta última possui uma Área de Proteção Ambiental (APA), denominada APA de Itupararanga, a qual foi criada pela Lei Estadual nº 10.100/1998 e alterada pela Lei 11.579/2003.

A APA de Itupararanga contribuiu para manter quase 41% de formação florestal devido a extratos de vegetação arbórea em 2019 na bacia do Alto Sorocaba segundo o projeto Mapbiomas (2021). Por outro lado, a agricultura ocupa a segunda posição com 40% de presença na bacia. Pastagens (12%) e áreas urbanas (3%) seguem com as maiores porcentagens de ocupação. As áreas de remanescente vegetal primitivo estão sendo afetadas pelo desmatamento nos últimos anos, devido a atividade agropecuária e construção de loteamentos (Manfredini, 2018; Taniwaki et al., 2013).

A pluviosidade média anual da bacia foi de 1572 mm/ano entre 2009 e 2018 (INMET, 2020). O clima é o *Cwa,* caracterizado com verão chuvoso e estiagem no inverno, de acordo com a classificação climática de Köppen (Kottek et al., 2006). Também na bacia do Alto Sorocaba é onde se localiza o reservatório de Itupararanga, apresentado na Figura 1.1.

O reservatório de Itupararanga é formado pelos rios Sorocabuçu e Sorocamirim, principais formadores do rio Sorocaba. O reservatório é utilizado, principalmente, para abastecimento público, sendo responsável por 63% da água destinada ao suprimento de cerca de 800.000 pessoas de diversos munícipios no entorno, entre eles Mairinque, Alumínio, Piedade, Votorantim e Sorocaba (Rosa et al., 2015) e geração de energia elétrica destinada à Votorantim Energia (antiga Companhia Brasileira de Alumínio – CBA). A UHE Itupararanga iniciou sua operação em 1914.

As dimensões, capacidade e potencial de geração de energia elétrica do reservatório são apresentados na Tabela 1.2. A planta de tomada d´água da UHE de Itupararanga é dada na Figura 1.2 e a batimetria do reservatório em metros em relação ao nível do mar é dada na Figura 1.3.

Figura 1-1: Localização da bacia do Alto Sorocaba: a.no Brasil, b.no estado de São Paulo, e c. localização do reservatório de Itupararanga.

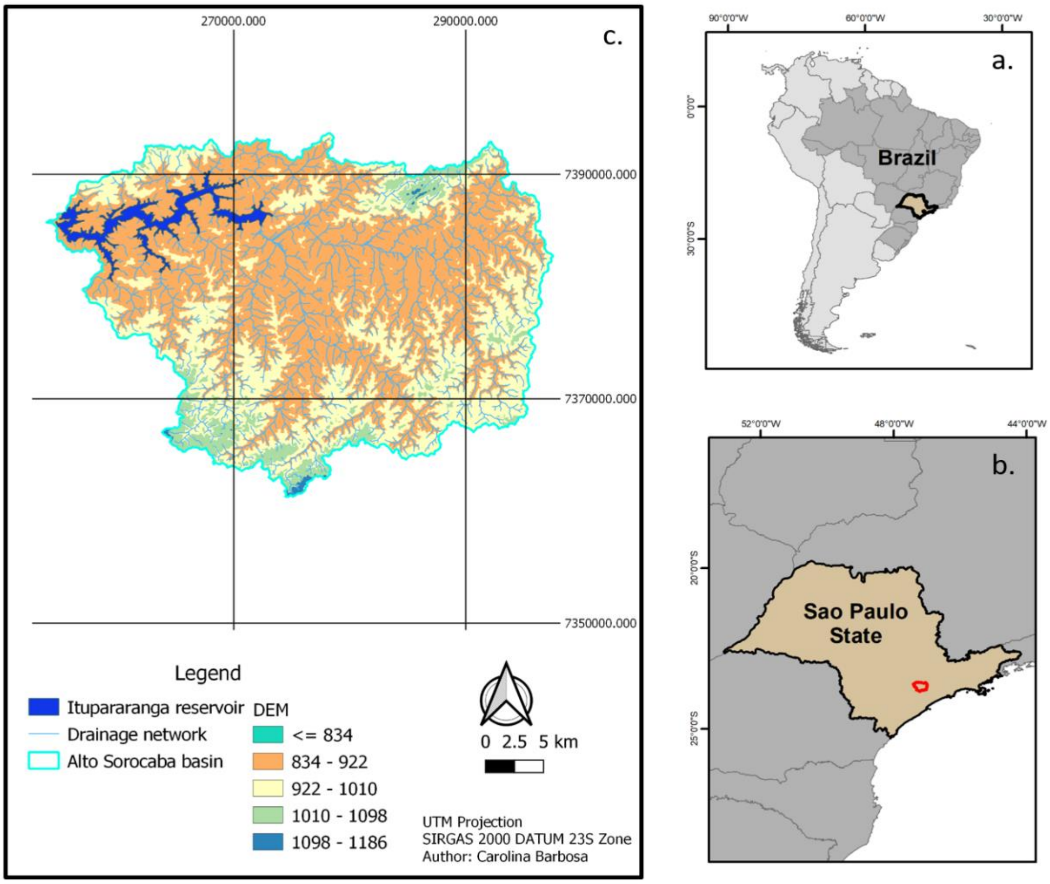
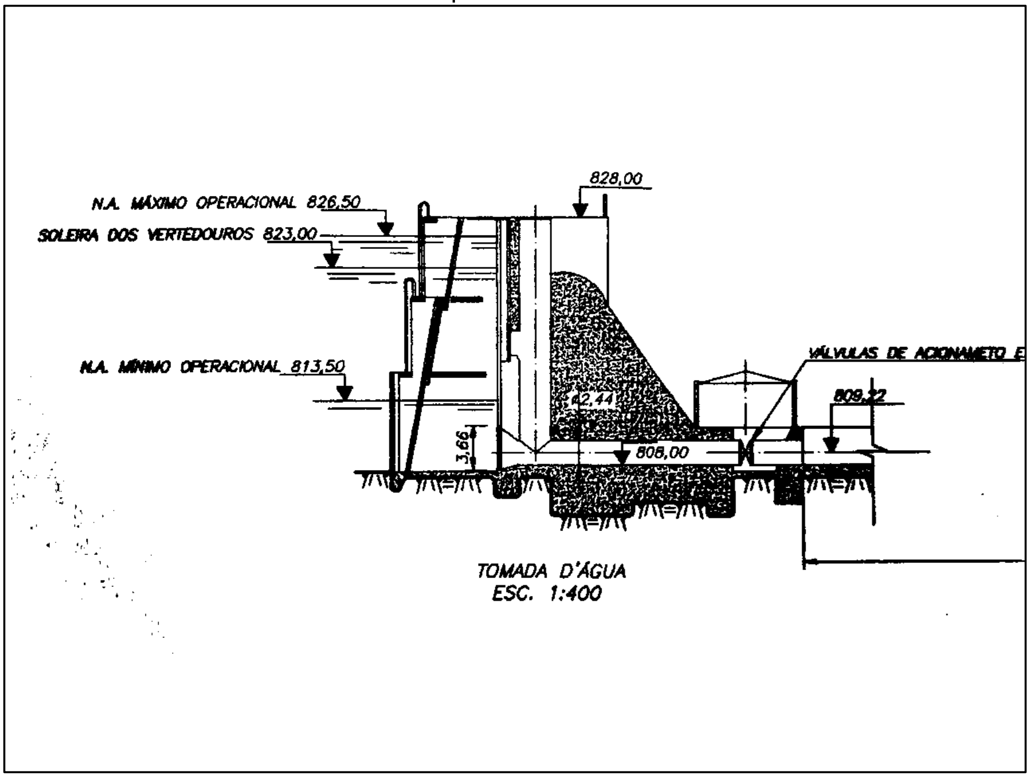


Tabela 1-2: Dimensões, capacidade e potencial de geração elétrica do reservatório de Itupararanga.

Extensão	40 km
Área da bacia de drenagem	936,51 km^2
Área superficial do reservatório	29,9 km^2
Profundidade máxima	23 m
Canal principal	26 km
Tempo de residência médio anual	250 dias
Volume útil	286 milhões de m^3
Fetch do vento	3,1 km
Vazão média afluente	12,70 $m^3.s^{-1}$
Vazão média defluente	12,68 $m^3.s^{-1}$
Potência instalada	56 MW
Produção média anual	150 GWH

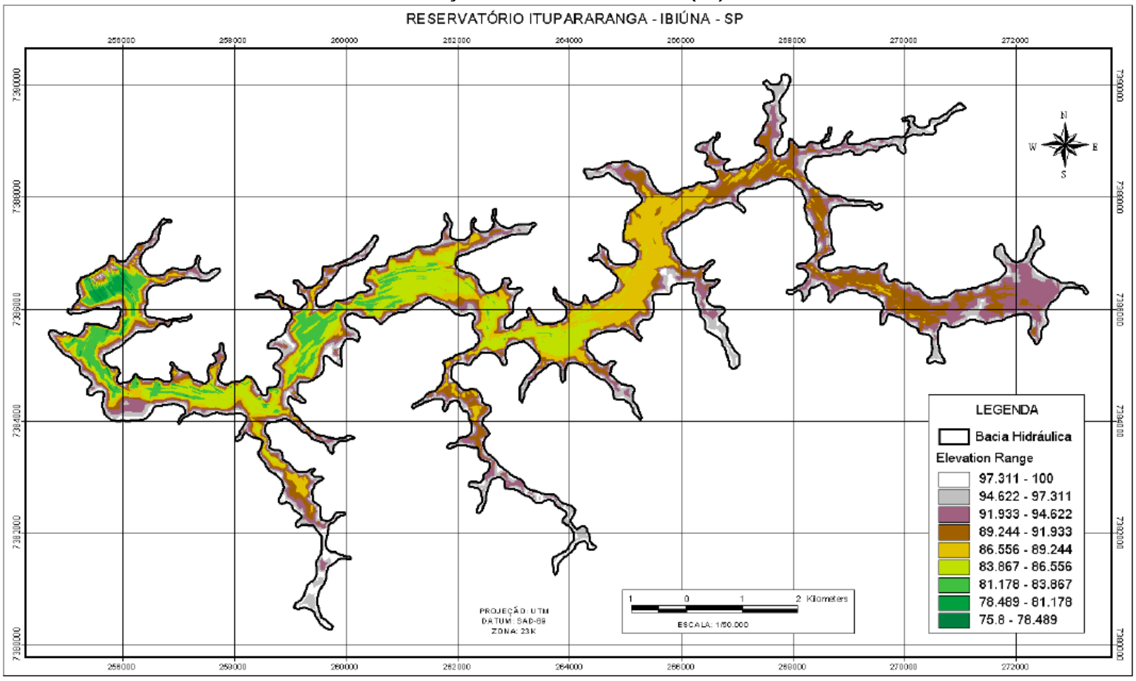
Fonte dos dados: Frascareli *et al.* (2015); INMET (2020); ANEEL (2020).

Figura 1-2: Planta de tomada d'água da UHE de Itupararanga com cotas de níveis operacionais.



Fonte: DAEE-SP

Figure 1-3: Levantamento batimétrico do Reservatório Itupararanga. Intervalo de elevação com relação ao nível do mar (m).



Fonte: CBH-SMT

Como principais atividades antrópicas que tem comprometido a qualidade das águas da represa de Itupararanga é possível citar a construção de loteamentos, como chácaras e casas de veraneio, uso intensivo de irrigação, intensa utilização de agrotóxicos e a falta de zoneamento territorial que discipline o uso e ocupação do solo (Manfredini, 2018). Outra fonte de poluição significativa são os lançamentos de efluentes domésticos com baixo ou nenhum tratamento do município de Ibiúna à montante da cabeceira do reservatório (FABH-SMT, 2018).

O estado trófico do reservatório de Itupararanga tem se modificado ao longo dos anos, apresentando atualmente características meso-eutróficas, com elevadas concentrações de nutrientes (Cunha et al., 2017; Vargas et al., 2020). A comunidade fitoplanctônica tem sido dominada por cianobactérias, em particular a espécie *Raphidiopsis raciborskii*, que tem provado ser tóxica no reservatório (Beghelli et al., 2016; Casali et al., 2017; dos Santos Machado et al., 2021; Moraes et al., 2021) e pode causar impacto nas comunidades aquáticas e cadeias alimentares ou até mesmo no abastecimento de água potável à população no futuro.

Além das cianobactérias potencialmente tóxicas observadas no reservatório de Itupararanga, espécies exóticas têm sido relatadas no ambiente, como exemplo a macrófita aquática *Urochloa sp*. (Pavão et al., 2017). A presença de espécies invasoras pode causar sérias implicações para a bacia como um todo.

4. Modelagem determinística de qualidade da água

O avanço da tecnologia e o desenvolvimento de modelos numéricos usados para simulação de ecossistemas aquáticos tem viabilizado o entendimento da dinâmica desses ambientes e a previsão de respostas futuras à forçantes ambientais e antropogênicas. Nas últimas décadas, diversos modelos de ecossistema aquático foram desenvolvidos e aplicados na simulação de variáveis bióticas e abióticas de qualidade da água, disseminando as diversas potencialidades dessas ferramentas na conservação ambiental (Fenocchi et al., 2019; Bueche et al., 2019; Ulańczyk et al., 2018; Van der Linden et al., 2015).

De acordo com Hipsey *et al.* (2015), a literatura tem empregado modelos de ecossistemas aquáticos, principalmente, para simulação da qualidade da água em escala de bacia e da biogeoquímica aquática dos sistemas individualizados, como lagos, estuários e reservatórios. Outra tendência baseia-se na integração de modelos determinísticos, simulação de cenários de diferentes aportes de nutrientes e índices de qualidade da água como ferramenta para determinar os limites das ações de gerenciamento (Gilboa et al., 2014, Soares and Calijuri, 2021).

Diversos estudos em reservatórios brasileiros aplicaram o acoplamento com modelos hidrológicos para estimativa das contribuições da bacia hidrográfica (Silva et al., 2016; Tambara et al., 2017; Munar et al., 2018; Lopes et al., 2018). Outras utilizações da modelagem determinística no país têm sido retratar os processos que ocorrem no ecossistema aquático com relação ao metabolismo (Cavalcanti et al., 2016), padrões espaciais e temporais da comunidade fitoplanctônica (Deus et al., 2013), bem como proposição de cenários e análise do comportamento do ambiente frente à possíveis impactos (Fragoso Jr *et al.*, 2011).

Os modelos matemáticos unidimensionais (1D) são ferramentas mais simplificadas para cálculos, apresentam menor número de parâmetros, devido a menor discretização espacial. A escolha de um modelo hidrodinâmico 1D na vertical (1D-V) se deve ao fato de que esses tipos de modelos conseguem simular os gradientes verticais de temperatura da água, que são maiores que os horizontais, além dos níveis de água. Modelos 1D-V conseguem simular gradientes verticais de temperatura da água e oscilações de volume, com baixo tempo de processamento computacional e alta resolução de saída espacial e temporal em relação às variáveis de estado e fluxos modelados, o que os torna adequados para realizar análises de modelagem de longo prazo.

Os modelos hidrodinâmicos levam em conta os principais componentes e funções que estabelecem as condições de contorno no funcionamento de reservatórios e cujas medidas são essenciais. Destacam-se as variáveis climatológicas e hidrológicas, tempo de residência e posição do reservatório (fluxos de entrada e saída), bem como características morfológicas do lago (batimetria) e da barragem (altura da barragem, tomada de água, profundidade máxima na barragem). Tais condições de contorno são base para simulações da qualidade de água, uma vez que a ciclagem de nutrientes e a dinâmica dos organismos estão totalmente relacionados às características citadas anteriormente.

As incertezas inerentes às variáveis de predição geradas nos modelos existem (Arhonditsis et al., 2006). Todavia, os esforços para melhorar a acurácia e previsibilidade das respostas tem crescido nos últimos anos (Robson, 2014). A tendência para a modelagem de ecossistemas aquáticos é baseada na implementação de aspectos eco-evolucionários e dinâmicas sócio-ecológicas, levando em conta o balanço das necessidades humanas com a capacidade de suporte do planeta (Mooij et al., 2018).

A comunidade científica tem buscado dar maior visibilidade aos resultados por meio do compartilhamento de algoritmos e banco de dados, dando prioridade aos modelos *open-source*, ou seja, aqueles de código aberto *e* disponíveis gratuitamente (Janssen et al., 2015). A *Global Lake Ecological Observatory Network* (GLEON-gleon.org) surgiu com o objetivo de disponibilizar dados globais advindos de sensores de alta frequência para o avanço da compreensão dos processos ecológicos em lagos (Bruce et al., 2018). O modelo *General Lake Model* (GLM) foi desenvolvido por membros da GLEON para ser disponibilizado aos usuários e flexível na manipulação das diversas variáveis hidrodinâmicas, biogeoquímicas e de qualidade da água (Hipsey *et al.*, 2017).

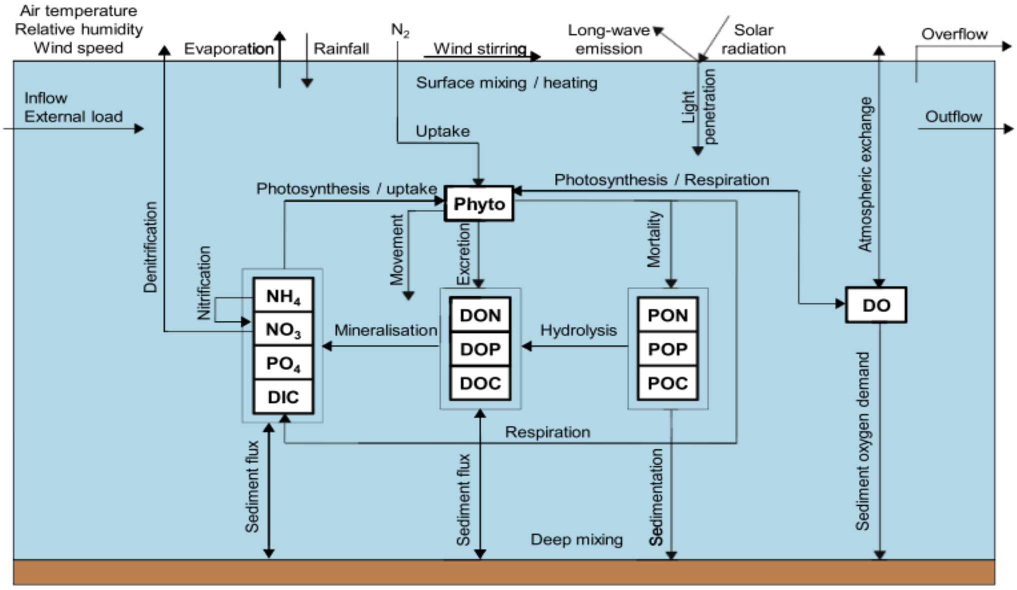
O *General Lake Model* (GLM) é um modelo determinístico 1D-V que simula balanço hídrico, balanço de energia superficial, incluindo penetração de luz, transferência de calor sensível e latente, estratificação e mistura vertical, além de fluxos montante e jusante e retiradas de água (Hipsey et al., 2019). Os algoritmos de mistura e a estrutura de camadas do GLM são baseados em modelos de ecossistemas aquáticos conhecidos, tais como o *Dynamic Reservoir Simulation Model* (DYRESM) e o *Dynamic Lake Model* (DLM). O modelo usa uma estrutura dinâmica de camada lagrangiana (Imberger and Patterson, 1981), na qual apenas a variação vertical é retida para resolver os gradientes verticais. A contração ou expansão das camadas representa alterações na densidade do lago relacionadas à mistura, estratificação e balanço hídrico.

O modelo GLM pode ser acoplado à *Aquatic EcoDynamics Model Library* (AED2; Hipsey et al., 2013) e *The Framework for Aquatic Biogeochemical Models* (FABM; Bruggeman and Bolding, 2014). Tais *libraries* permitem as simulações das variáveis biogeoquímicas e de qualidade da água. A *Aquatic EcoDynamics Modelling Library* (AED2) é uma biblioteca de módulos biogeoquímicos e de qualidade da água. Os módulos permitem a simulação individual ou conjunta dos ciclos do carbono, nitrogênio, fósforo, oxigênio dissolvido e sílica, além de matéria orgânica, fitoplâncton e zooplâncton por meio de equações de balanço de massa.

Os modelos GLM e AED têm sido amplamente aplicados para entender a dinâmica térmica de lagos (Hipsey et al., 2017; Bruce et al., 2018; Hipsey et al., 2019) e para investigar mudanças na hidrodinâmica de lagos e reservatórios sob mudanças climáticas (Bucak et al., 2018; Soares et al., 2019; Gal et al., 2020). O modelo também tem sido utilizado para aumentar a compreensão sobre as interações dos processos ecossistêmicos e ações humanas, bem como facilitar o aprendizado acadêmico sobre conceitos de mudanças climáticas (Cobourn et al., 2018; Carey and Gougis, 2016). Estudo recente comparou o desempenho do modelo GLM com modelos 2D e 3D e destacou as potencialidades e eficiência do modelo especialmente em estudos de dinâmica térmica e balanço hídrico em lagos e reservatórios (Ishikawa et al., 2021).

O GLM está implementado no software estatístico R para simular e analisar os resultados. O modelo GLM-AED2 é *open source* e *freeware,* permite manipulações em seu código-fonte e aprimoramentos em seus algoritmos, além de ser gratuito para os usuários. Dessa forma, mostrou-se viável aos objetivos propostos para esta pesquisa. Exemplo esquemático de aplicação recente do modelo acoplado por Soares e Calijuri (2021) considerou variáveis e processos semelhantes ao presente estudo e é dado na Figura 1.4.

Figure 1-4: Diagrama conceitual do modelo GLM-AED para aplicação em reservatórios tropicais.



Fonte: Soares and Calijuri (2021).

Na presente pesquisa foram utilizados os modelos GLM v.3.0 e AED v.1.2 e a manipulação dos modelos foi realizada por meio do software estatístico R para simular, analisar e calcular os indicadores hidrodinâmicos por meio dos pacotes *glmtools* (Read et al., 2016), GLM3r (Hipsey et al., 2019) e *rLakeAnalyzer* (Read et al., 2011). Uma interface de usuário para o GLM (glmGUI, Bueche et al., 2019) também foi usada para a análise de sensibilidade e auto-calibração hidrodinâmica. Detalhes das equações de balanço de massa e outras manipulações dos modelos utilizados e desenvolvidas nessa pesquisa estão apresentadas nos capítulos seguintes.

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CAPÍTULO 2 - FUTURE PROJECTIONS OF WATER LEVEL AND THERMAL REGIME CHANGES OF A MULTIPURPOSE SUBTROPICAL RESERVOIR (SÃO PAULO, BRAZIL)

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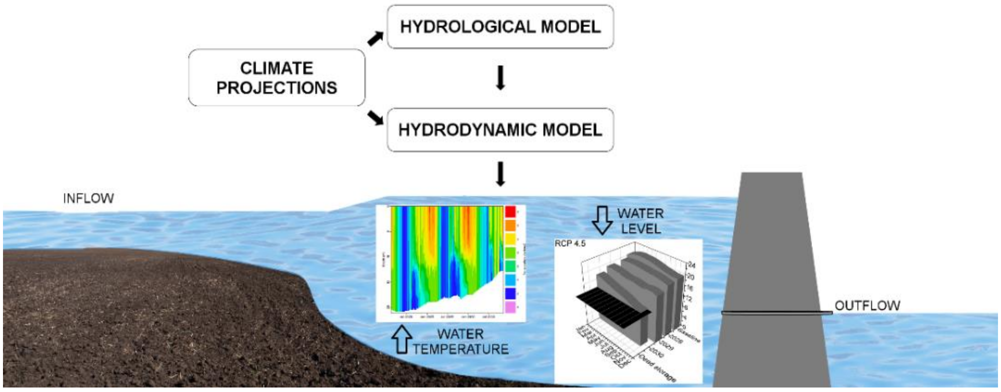
Graphical abstract



1. Introduction

Sustainable development goals have assumed a new paradigm with Earth's life-support system, society, and economy including targets for 2030 (Griggs et al., 2013). Concerns about clean water, as well as the health and production of ecosystems are intrinsically linked to climate change.

Some of the consequences of climate change are a rise in air temperatures and alterations in rainfall patterns (IPCC, 2014). The water levels of lakes and reservoirs have shifted due to the increase in the frequency of occurrence of weather extremes. More frequent drought and flood periods have been reported worldwide (Brasil et al., 2016; Soares et al., 2019; Jeppesen et al., 2015). Scientific research has focused on a relationship between volume fluctuations and water quality degradation, in particular the nutrients dynamics, trophic state, and phytoplankton community (Jeppesen et al., 2015).

There is also evidence that climate change influences the thermal dynamics of inland waters (Sahoo et al., 2016). The air temperature increase has been reported as a driver of heating surface water temperature (Zhang et al., 2020) and another consequence are alterations in the heat budgets of lakes

(Woolway and Merchant, 2019). All of those alterations can lead to cyanobacteria dominance (Kosten et al., 2012) and blooms (Wells et al., 2015; Huisman et al., 2018).

In this way, global and regionalized climate models have been applied under different concentration pathway scenarios to predict climate change impacts (Eccles et al., 2019; Fenocchi et al., 2018; Prats et al., 2018). Using this forecast data has enabled a better understanding of the global warming effects on aquatic ecosystems. Especially coupling climate models to aquatic ecosystem models has been used to predict the consequences of climate change on aquatic environments (Moe et al., 2016). Furthermore, these coupled models are used to test adaptive water management measures for the potential mitigation of negative impacts on the ecosystem (Ladwig et al., 2018).

Climate change effects have already been highlighted in global lake ecosystems (Jeppesen et al., 2017; Woolway and Merchant, 2019). However, further studies are needed to incorporate the likely impacts of climate change in vulnerability assessments and lake management efforts (O'Reilly et al., 2015). Although a water temperature increase is prospective to be felt most strongly at low latitudes (Kraemer et al., 2017), there are incipient local studies of likely impacts on lakes and reservoirs located in subtropical regions.

The present study attempts to highlight whether potential climate projections could affect the water levels and the thermal regime in a multipurpose subtropical reservoir at the end of 2020s. Data generated by a regionalized climate model was used for hydrological and hydrodynamic simulations. The overall trends of CO_2 emissions rise have led to a change in the pattern of climate forcing data and were evaluated to understand how the reservoir water level and the thermal regime would respond in the near future. This study facilitates our current knowledge of the possible implications of climate change on subtropical lakes hydrodynamics to target possible management efforts.

2. Material and Methods

2.1 Input data availability

The daily hydrological data were collected at one station located in the dam (*62510080*) since 2005. In combination with outflow data, this monitoring data were used to calculate reservoir inflows, water levels and volume.

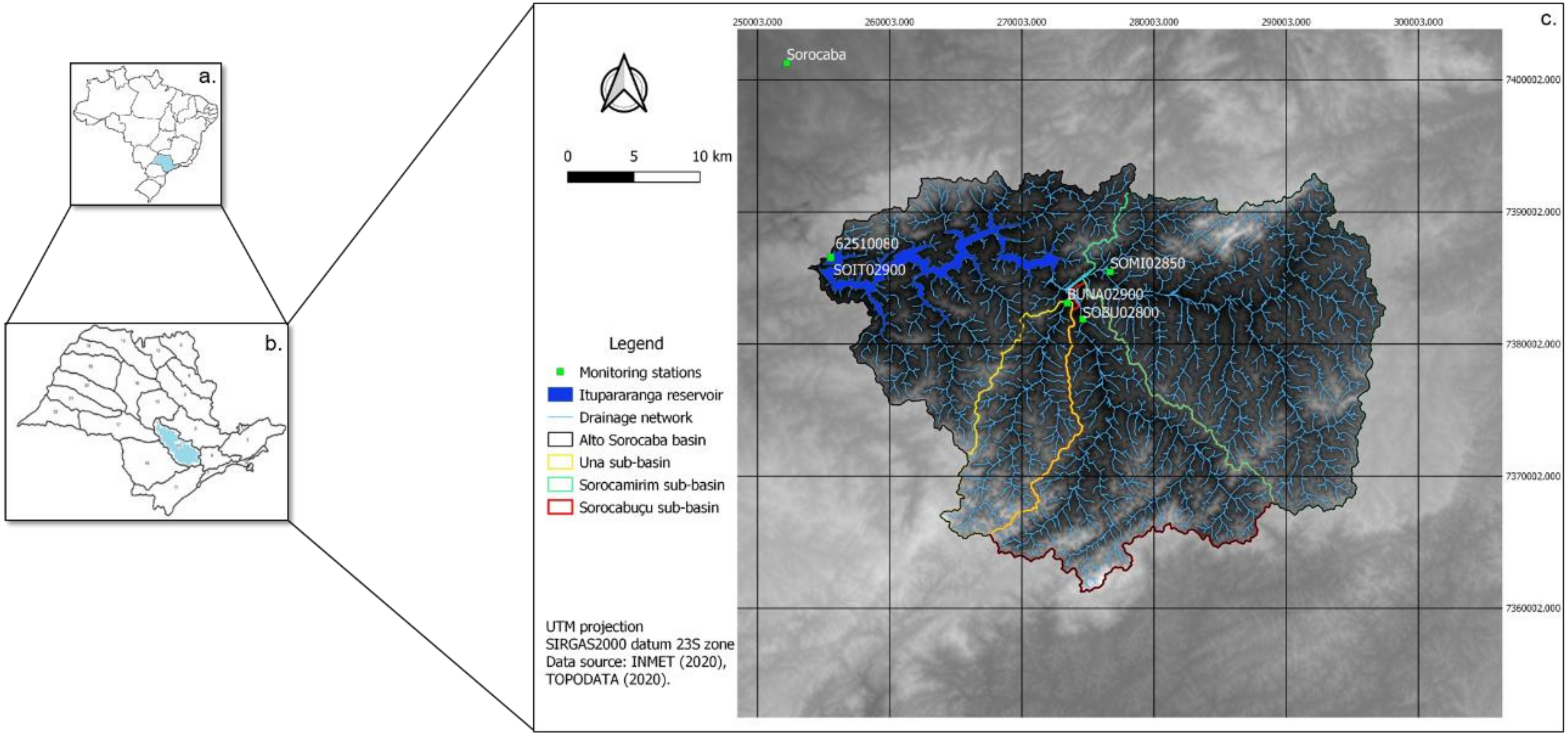
The meteorological data were collected from Sorocaba meteorological station by National Institute of Meteorology (INMET) located 29 km from the reservoir. This station is the only source for meteorological data close to Itupararanga reservoir and it has had an automatic hourly meteorological monitoring since 2006. In order to reduce bias related to those data, we performed a sensitivity analysis and calibration for model meteorological parameters.

The Environmental Company of the State of São Paulo (CETESB) has performed surface sampling every 2 months since 1998 at *SOIT02900* station, near to the dam, and since 2005 at Sorocabuçu (*SOBU02800*), Sorocamirim (*SOMI02850*) and Una (*BUNA02900*) streams. The monitoring variables include water temperature and electrical conductivity measurements. The location of Alto Sorocaba basin, its tributaries, and the monitoring stations are presented in Figure 2.1.

Previous data were collected nearby the SOIT02900 station (FAPESP Projects: 2008/55636-9, 2016/09405-1) and represent measurements in the water column every 50 cm in 2009-2011, 2013-2015, and 2017-2019.

The reservoir bathymetry, which corresponds to the storage, elevation, and area relationships, were processed by a project held at the University of São Carlos's (UFSCAR-Sorocaba). This was performed by an Ecobathymetr Bathy 500-MF and the Hypack Max Software to plan, navigate, collect, and process data.

Figure 2-1: Alto Sorocaba basin: a. São Paulo State location; b. Alto Sorocaba basin location; c. Ituparaganga reservoir location, its tributaries and monitoring station.



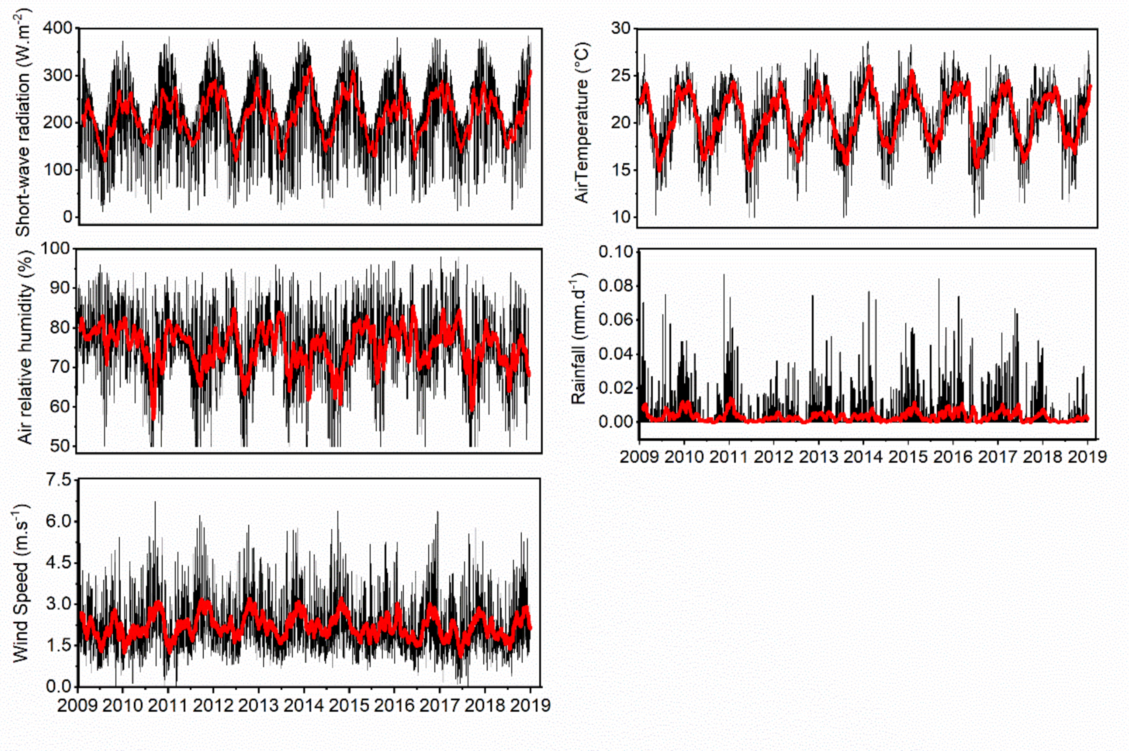
Fonte: Author

2.2 Data processing and modeling setup

Meteorological variables used in this study included short-wave radiation, air temperature, wind velocity, rainfall, and air relative humidity on an hourly time step (Figura 2.2). Long-wave radiation was estimated from relative air humidity and air temperature (Abramowitz et al., 2012).

There is one outlet used for water withdrawal located near the bottom of the reservoir (withdrawal depth of 5.7m). The outflow is partly used for hydroelectric power generation and partly for the local water supply. Periods of overflow occur through the reservoir spillway crest (>20.7m elevation). The water withdrawal and the overflow were set up as separate outflows to not increase uncertainty at hydrodynamic simulation.

Figure 2-2: Meteorological and hydrologic inputs in the simulation period. The red lines highlight a simple moving average for each hydro-meteorological forcing data.



The incoming daily streamflow was calculated using hydraulic balance calculations by the private company that operates the dam. The streamflow conductivity was converted to salinity (Hornung, 2002). To complete missing data in the salinity time series, a mass balance calculation was performed using data from the three tributaries. Meanwhile, few electrical conductivity measurements were available. Thus, the average conductivity between the three tributaries (70.8µScm^{-1}) was used to estimate a mean salinity concentration that was used in the entire period (0.06 PSS). Electrical conductivity variations have not been correlated to changes in the reservoir density flow regime; instead, the freshwater reservoir's density stratification is dominantly driven by changes in water temperature (see similar inflow data and conclusions in Ryu et al., 2020).

The inflow water temperature was estimated by a weighted average of the water temperature and flows of the Sorocabuçu, Sorocamirim and Una streams. Missing data were approximated using linear interpolation on a daily time step.

We applied an automatic sensitivity analysis and calibration technique using the glmGUI v.1.0 (Bueche et al., 2019). Here, the sensitivity analysis was first conducted on water level fluctuations and secondly on changes in water temperature. Results from the sensitivity analysis guided the automatic calibration for the period from January 2009 to December 2013 (1826 days). The validation period was from January 2014 to March 2019 (1916 days).

The parameters related to minimum (h_{min}) and maximum layers thickness (h_{max}) were manually calibrated according to the reference values. The glmGUI calculates the sensitivity index (SI) for the parameters of surface dynamics, mixing parameters, and hydrological and meteorological factors The SI's considered low (0<SI<0.05) were disregarded and those considered as medium or high (0.05<SI<0.2; 0.2<SI<1) were submitted to the calibration process (Lenhart et al., 2002).

Based on field observations between 2018 and 2019, indicated by four Secchi-disk measurements, the average radiation extinction coefficient (K_w) value was used as model input (0.94 m^{-1}). Hydrodynamics indicators were calculated to evaluate thermal regime at Itupararanga reservoir, e.g. annual average water level (AAWL), maximum vertical density gradient (DG), the average surface and bottom water temperature difference (SBD), retention time (RT), number of stratified days (NSD) and the Schmidt Stability Index (SSI) (Idso, 1973).

The RT, in days, was calculated from the daily flushing rate for each year. The SSI measures the energy required to mix the entire lake to a uniform temperature without the addition or subtraction of heat. As the highest SSI values were observed in the wet season, maximum SSI in the wet season (MSSw) was also calculated.

Water density was calculated by the rLakeAnalyzer package and the DGs were manually calculated between adjacent layer cells. According to Lewis (2000), for tropical lakes, a difference of 2ºC between the top and the bottom of the water column is sufficient to classify the water column as being stratified. Based on field surveys in Itupararanga reservoir, a high correlation was found between SBD and DG (r=0.91). In this way, the thermal stratification was defined when the SBD > 2ºC and consequently the DG > 0.13 kg.m³.m^{-1}.

The model performance to simulate water level and water temperature was evaluated through Pearson’s correlation coefficient (r) and the root mean squared error (RMSE) according Equation 1:

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N} \quad (Si-Oi)^2}{N}} \tag{1}$$

Where: N= number of observations, S= simulated data and O= observed data for each “i” time step.

2.3 Hydrodynamic scenarios under climate projection

2.3.1 Data availability and processing

Data from Climate Change Projections for South America regionalized by the ETA Model (PROJETA) were used to simulate the climate change scenarios in the Itupararanga reservoir.

The global climate model (GCM) chosen was The Hadley Centre Global Environmental Model (HadGEM2-ES). The regionalization of the HadGEM2-ES projections from 2006 to 2099, carried out by the ETA model (Eta-HadGEM2-ES), had a resolution of 20 km and covers South America, Central America, and the Caribbean. The Eta-HadGEM2-ES has proved to be more sensitive to greenhouse gas (GHG) emissions and it generates improved estimations than the ETA nested in MIROC5 (Chou et al., 2014).

The scenarios were based on two GHG representative concentration pathways (RCP), which correspond to different radiative forcing scenarios of 4.5 Wm^{-2} (RCP 4.5) and 8.5 Wm^{-2} (RCP 8.5), respectively (Chou et al., 2014).

The first one is an optimistic scenario corresponding to a CO2 increase of about 650 ppm and the other a pessimistic scenario where CO_2 exceeds 1000 ppm in 2100.

Climatic time series by Eta-HadGEM2-ES RPC 4.5 and 8.5 included daily short-wave and long-wave radiation (W.m^2), air temperature (°C), air humidity relative (%), rainfall (mm) and wind speed (m/s) from 2026 to 2030. A bias correction was performed to adjust historical data and correct the future projections using 1-decade data as control period (2009-2018). The long-wave radiation series was not corrected, due to the lack of observation data.

For air temperature and rainfall correction, we applied the linear and the variance scaling methods (LS/VS, Lenderink et al., 2007; Chen et al., 2011; Teutschbein and Seibert, 2012) inside of the Climate Change for Watershed Modeling tool (CMhyd, Rathjens et al., 2016). The LS method is a simple approach based on the average difference between monthly observed data and historical time series of climate models over the same period of the observed series. The VS corrects both the mean and the variance of time series. The same methods were applied to manually correct the other projected meteorological data.

2.3.2 Inflow simulation

To predict the future reservoir inflow from the climate scenarios the Soil Moisture Accounting Procedure (SMAP) was applied based on precipitation and evaporation data from the climate model.

The SMAP model uses a simple structure of reservoirs that represents the storage and water flow in the basin with continuous time series and uses the Soil Conservation Service - SCS (1964) method for the separation of runoff. The input data are the total precipitation and evaporation heights on a daily time step, the drainage area, and the initial conditions of the basin. For calibration, the following parameters needed to be adjusted (Lopes et al., 1982): soil saturation capacity (Str), constant runoff recession (K2t), underground recharge parameter (Crec), initial abstraction (Ai), field capacity (Capc) and constant of recession of basic outflow (Kkt).

The version used in the present study was the Smap.Net version 1.0.0.0, which is freely available from the Laboratory of Decision Support Systems

(LabSid-USP). The model runs and generates runoff for a limit of 1000 consecutive days.

The rainfall-runoff model was manually calibrated for 300 days, from 2010-06-23 to 2011-04-18. It was given as the initial conditions the drainage area (669 km²), the initial soil moisture level (65 mm mm^{-1}), and the initial base streamflow (7 m³.s^{-1}).

The goal of the calibration was to reduce the percent bias (PBIAS) for streamflow to be considered satisfactory (± 25%, Moriasi et al., 1983). The calibrated model was used to estimate the reservoir future inflows based on estimated rainfall and air evaporation by Eta-HadGEM2-ES RCP 4.5 and 8.5. The air evaporation data were bias corrected using the previously cited bias correction.

The 1000 days period chosen for the simulation of the climate projections scenarios was from 2028-02-14 to 2030-11-09, which represents an exemplary time period in the near future to evaluate potential impacts of climate change on water management decisions. For the hydrological simulation, we assumed the initial base streamflow as the mean observed flow between 2009 and 2018 (13.5 m³.s^{-1}).

As reservoir initial conditions for the hydrodynamic simulation, we used the monthly mean water temperatures of the last decade as daily input and the vertical salinity profiles assumed constant. Further, we used the mean lake level value and mean water temperature value for the month of January based on historical data series (2005 to 2018).

The present study did not take into account the various possibilities of water withdrawal for power generation and water supply, for simplification only a minimum daily withdrawal was considered (6.024 m³.s^{-1}) based on the historical series (2005-2018). Overflows were not observed in those periods. Thermal condition indicators were calculated to quantify the climate change impact on the reservoir thermal regime.

3. Results

3.1 Model performance

The Sensitivity analysis for water level and water temperature presented variations between the parameters and the evaluated multiplicative factors

(Figura 2.3). The water level had high sensitivity to the inflows and outflows factors (SI=0.54 and 0.69, respectively) and medium sensitivity to the rain factor (SI=0.15).

Regarding water temperature, the sensitivity analysis highlighted the model's medium sensitivity to the wind factor (SI=0.18) and high sensitivity (SI=0.21) to the latent heat transfer coefficient (c_e). Sensitive parameters were automatically calibrated, and the minimum and maximum layer thickness were manually adjusted (Table A2).

The calibrated and validated water level and water temperature of the Itupararanga reservoir showed good model fit criteria (Figure 2.4, Table 2.1). For calibration, Pearson correlation results showed higher values at 5m, 10m, and 15m than in the top surface layer. On the other hand, for the validation period, the highest Pearson correlation was found at 5m, followed by top surface layer, and the simulated bottom waters were warmer than the observations.

Figure 2-3: Sensitivity index for water level and water temperature. Kw=light extinction coefficient; Non-neutral bulk-transfer coefficients: ch= sensible heat transfer, ce= latent heat transfer, cd= momentum; Mixing parameters: C_K= efficiency of convective overt

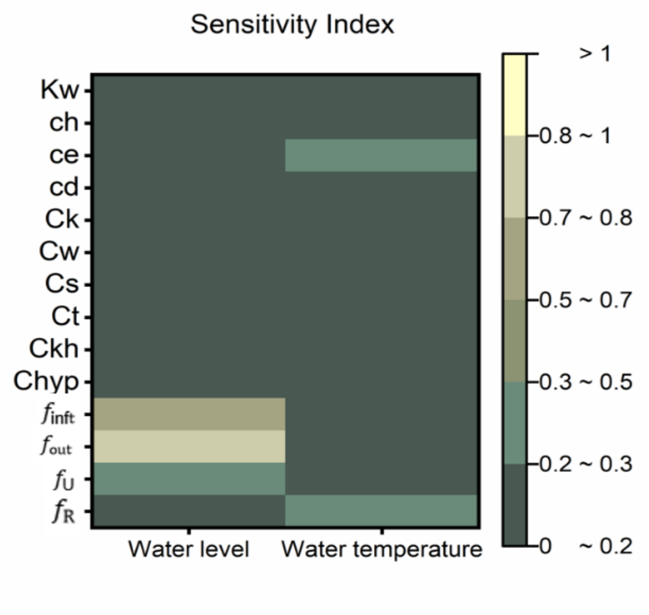


Figure 2-4: Observed and simulated water level

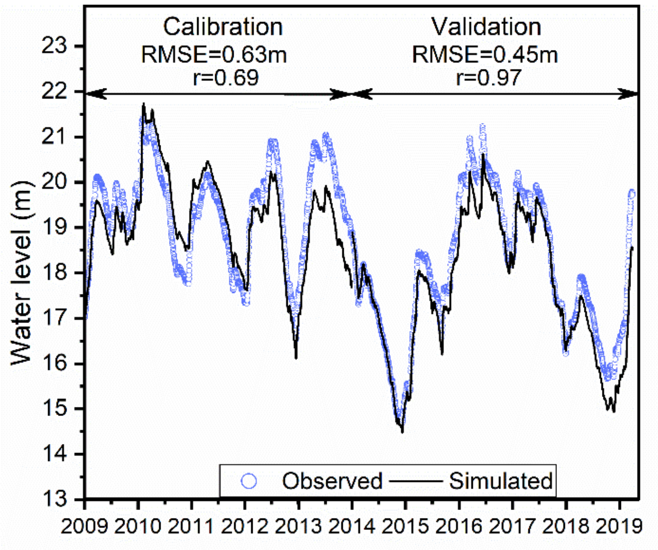


Table 2-1: Model performance metrics in four specific depths and water columns over the simulation period.

	Calibration					Validation				
Depths (m)	0	5	10	15	Water column	0	5	10	15	Water column
RMSE (ºC)	1.74	0.67	2.41	1.36	1.30	1.73	0.69	1.85	2.0	1.34
r	0.84	0.98	0.91	0.97	0.83	0.90	0.97	0.81	0.78	0.81

The simulated thermocline depths were compared with field observations to evaluate the model performance to observed mixing dynamics in the Itupararanga reservoir (Figure A1). The thermocline depths were usually measured between 6.5-14m and the simulations achieved a range between 6-16.5m, highlighting a thermocline deepening bias (PBIAS = -17).

3.2 Hydrodynamics indicators

The hydrodynamics indicators of Itupararanga reservoir in the simulation period are given in Tabela A3.

A lower NSD was identified in 2014 (72 days) compared to the entire simulated period. On the other hand, after the rising lake level in the year 2015, the SBD achieved 1.79 ºC and the NSD increased (136 days). Besides, the highest MSSw was accounted at 2018-12-21 (135.9 J.m^{-2}), followed by 116 J.m^{-2} at 2015-01-12 (shortly after the drought period).

In the summer of 2014, the monthly mean precipitation was 140.7 mm (INMET, 2020). In January 2014, the measured rainfall was 85 mm, the lowest accumulated between 2008 and 2018. There was an increase in rainfall in the wet season of 2015 and this led to changes in the reservoir's thermal regime. Between 2014 and 2015 the daily reservoir volume was below the mean volume observed from 2008 to 2018 that corresponded to 204.10^6 m³ (INMET, 2020). The daily average minimum volume was 115.10^6 m³ in December 2014.

3.3 Bias-corrected climate series and simulation of inflows

We corrected the simulated historical climate data from the global climate model HadGEM2-ES regionalized by the ETA model under two downscaling scenarios (RCP 4.5 and 8.5) using the linear and variance scaling approach. After the observed and simulated historical climate data had been compared and the identified biases, parameterized bias correction based on the mean and the variance of times series was used to correct historical and future climate data. (Table A4).

The forecasted climate data showed significant differences regarding the baseline period (see Figure A2). A slight future increase in shortwave radiation and wind speed are expected for the two GHG increase scenarios.

The projections indicate an average air temperature increase of 2.5 ºC (RCP 4.5) and 3.3°C (RCP 8.5) relative to the baseline for the end of this decade and beginning of the next one. On the other hand, the average rainfall and relative humidity showed a downward trend.

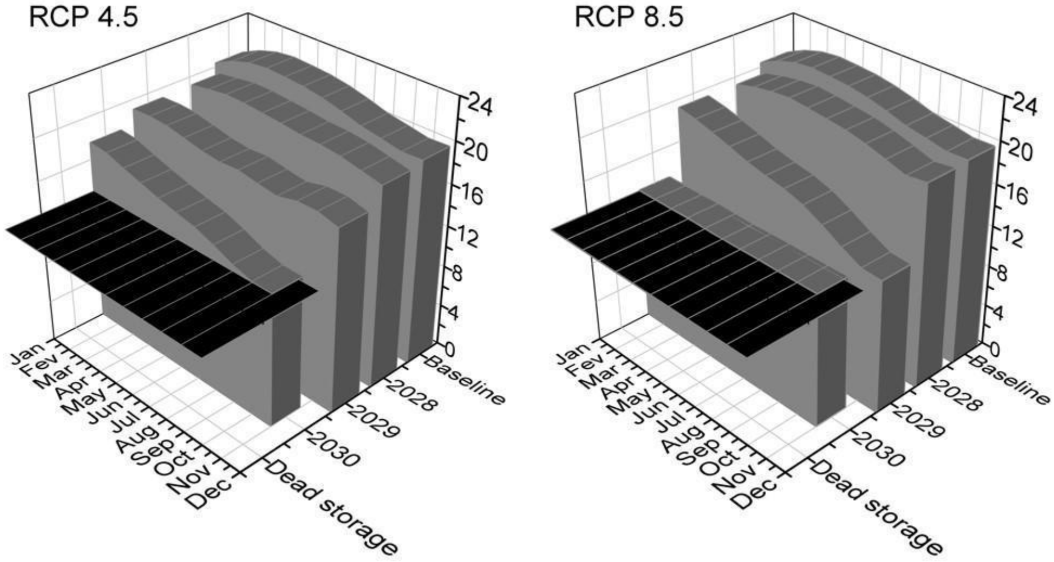
The calibrated parameters of the hydrological model are shown in Table A5. Although the observed inflow peak (January 2011) was overestimated by 37% compared to the simulation in the calibration (see Figure A3), the SMAP presented satisfactory performance (PBIAS=18%; ±15 ≤ PBIAS < ±25, Moriasi et al., 1983) to predict minimum and mean inflows.

After the calibration, the SMAP model was able to simulate representative future inflows from 2028-02-14 to 2030-11-09 (Figure S4). In the pessimistic scenario, the average daily inflows were well below (2.6 m³.s^{-1}) the historical baseline (13.5 m³.s^{-1}), despite a simulated peak in November 2028 (52.2 m³.s^{-1}) that exceed the baseline flow. On the other hand, for the optimistic scenario, the simulated inflows showed a similar behavior of decreasing discharges during the drought period observed in 2014 and during the wet period in 2018 (Figure S4).

3.4 Climate scenarios for the Itupararanga reservoir

The annual average water level showed a declining trend in the optimistic scenario (Figura 2.5; 20.5 m, 18.4m and 15.4m for the years of 2028, 2029 and 2030, respectively). In 2014, the Itupararanga water level has reached a historical minimum of 16.7m. On the other hand, in the pessimistic scenario, the water level declined with a higher rate than the optimistic scenario (20.7m in 2028, 16.3m in 2029, reaching and remaining at dead storage in the whole year of 2030).

Figure 2-5: Water levels under RCP 4.5 and 8.5 scenarios in 2028, 2029 and 2030. Baseline: monthly average depth from 2009 to 2018.



The warming of the top layer was evident in both scenarios; the annual average water temperature reached 22.6 ºC in the pessimistic scenario (Table 2.2). The SBD was higher in the RCP 4.5 scenario than in the RCP 8.5 one. This higher difference between surface and bottom temperatures results in an increased water column stability.

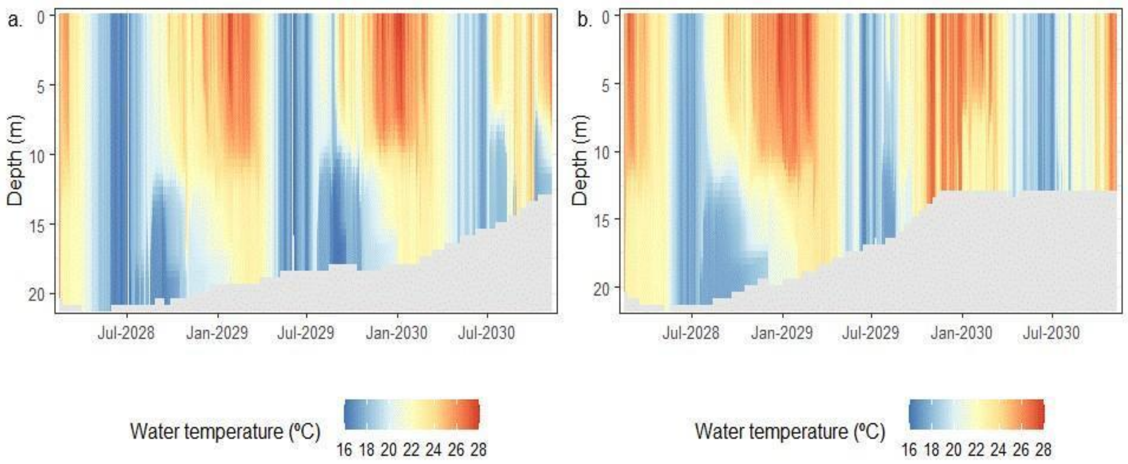
Table 2-2: Comparison between thermal conditions indicators for calibration and validation period and future optimistic (RCP 4.5) and pessimistic (RCP 8.5) scenarios.

Thermal conditions indicators	2009-2013	2014-2018	2028-2030	
			RCP 4.5	RCP 8.5
Average surface temperature (ºC)	21.0	21.6	22.2	22.6
Average bottom temperature (ºC)	20.1	20.8	19.6	20.4
SBD (ºC)	0.9	0.8	2.6	2.2
Percentage of stratified days (%)	24	30	53	36

The minimum annual depth of the thermocline was at 6m from the surface for the optimistic scenario and at 4m for the pessimistic one. The maximum depth was at 18m for both scenarios. On the other hand, in the period of reservoir dead storage, the thermocline remained shallower (10m<RCP4.5<11m; 6m<RCP8.5<10m).

The SSI values increased in both scenarios (MSSW > 150 J.m^{-2}) when compared to the baseline (Table A3 and Figure A5). The thermal stability of the Itupararanga reservoir will increase (Figura 2.6) and stratification periods would start earlier (before spring).

Figure 2-6: Simulated water temperature: a. RCP 4.5 scenario b. RCP 8.5 scenario.



4. Discussion

4.1 Evaluation of model performance and hydrodynamics features of Itupararanga reservoir

The water level simulation results suggest a good fit with the observations (RMSE<0.63m, r>0.8). Previous studies using 1D models have shown similar agreements (0.2m<RMSE<0.74m; Fadel et al., 2017; Melo et al., 2019, Bueche et al. 2019). Furthermore, the model showed a good capability to predict short-term water fluctuations, especially between 2014 and 2015, when the reservoir volume decreased to ~29% of its normal capacity (Figure 3.4).

The achieved model fit for temperature profile simulation can be evaluated as very satisfactory (RMSE<1.4 ºC, Table 2.1). The literature reports to the whole water column an acceptable range of RMSE between 0.9 ºC and 1.5 ºC (Bueche and Vetter, 2014; Fenocchi et al., 2017; Prats et al., 2018).

Recently, Farrell et al. (2020) showed that the uncertainties associated with water temperature simulations from manual and buoy data were similar and have a low influence on projections. Additionally, the study highlighted that the thermal simulations were better in the epilimnion than the hypolimnion. In the present study, when water temperatures at certain specific depths (surface, 5, 10, and 15m) were evaluated, the error adjustments increased (RMSE~1.7ºC) suggesting a trend to overestimate water temperature in the bottom and underestimate water temperatures in the surface layers. This highlights the influence of the meteorological boundary conditions on the model performance.

In the same way, a warm bias for the hypolimnetic temperature simulations had previously been reported (Bruce et al., 2018), as well as a bias in the prediction of the thermocline depth (Bruce et al., 2018, Bueche et al., 2017). In the present study, the simulation of thermocline depth achieved a satisfactory agreement compared to observations (Figure A1).

Another important finding was that in the drought period (2014-2015), the outflow was reduced, which eventually increased the hypothetical RT (453 days) to maintain a secure power generation and drinking water supply (see Table A3). In the same period, the water level dropped, and it influenced the thermal conditions of the Itupararanga reservoir (NSD=72 days and MSSw=75.9 J.m^{-2}). Similar behavior was identified in the Serra Azul reservoir, MG-Brazil, between 2014 and 2015, with a decrease of the number of stratified days due to a decrease in water level (Soares et al., 2019).

Prior studies have identified that lakes and reservoirs respond rapidly to climate change (Adrian et al., 2009) and the shifts on rainfall regime favors intensification of lake levels fluctuations (Reichstein et al., 2013). A recent decrease in the annual average rainfall was recorded in 2018 (INMET, 2020) leading to a decline of water level and a raise of MSSw (135.9 J.m^{-2}). This may be a consequence of increased air temperature and consequentially the heating of the surface layer (Darko et al., 2019).

4.2 Climatic data bias correction and hydrological calibration

Technical improvements of the output data from RCMs and their application to study the hydrological impacts of climate change has developed in the last decade (Chen et al. 2011; Chen et al., 2013). However, data bias corrections are still used to reduce the uncertainties of the simulations.

Climate projections were corrected using current data and bias correction techniques. The linear and variance scaling techniques, based on simple statistical methods (mean and variance), showed good agreement (Table A4) within the range of results available in the literature (Li et al., 2019, Eccles et al., 2019; Teutschbein and Seibert, 2012).

The calibration of a simple hydrological model was performed to simulate future inflows to the Itupararanga reservoir. Despite that the observed maximum discharge (54.4 m^3 s^{-1}) has been overestimated by 27% in the model (Figure 5), generally the SMAP model showed a good accuracy (r=0.67) to replicate the inflow dynamics. Additional monitoring stations for discharges would need required to improve the simulation results.

Similar results were achieved by Cavalcante et al. (2020) calibrating measured flash flood from eight rain gauges in the mountainous region of Rio de Janeiro, Brazil. Despite the calibration limitations, a previous study reported that the SMAP model was capable to predict future inflows for a hydroelectric plant based on data from an RCM, especially after the rainfall bias correction (da Silva et al., 2019).

4.3 Water supply implications for the Itupararanga reservoir at the end of this decade

Two scenarios (based on optimistic (RCP 4.5) and pessimistic (RCP 8.5) climate projections concerning GHG) were simulated using the hydrodynamic model. To run these scenarios the bias-corrected climate projections and the simulated inflows were set as boundary conditions to GLM.

The decrease in the air evaporation rates and the average daily rainfall in the analyzed period led to a decrease in the future inflows, assuming historical minimum outflow conditions in the reservoir (Figure A2 and A4). Bucak et al. (2018) also reported a trend of decreasing future total inflows under RCP 4.5 and 8.5 conditions in 2030 and 2060 based on land-use changes for a large lake in Turkey.

Our simulations suggest that the local water supply from the reservoir works will be scarcely limited by October 2030 in the optimistic scenario due to future lower daily rainfall in the watershed and the, although low, withdrawal within the reservoir itself. On the other hand, in the pessimistic scenario, the reservoir may not be able to provide enough water already beginning in December 2029 as it had reached dead storage (Figure 2.5).

The generalizability of the achieved results is subject to certain limitations. For instance, we are limited in predicting future outflow changes as well as shifts in the land-use of the catchment, which could cause feedback reactions on the reservoir's volume and thermal dynamics. In another study, under current land-use conditions and the HadGEM model under RCP 4.5 data, predictions until 2030 of the Lake Beyşehir had indicated a drop in the water level and for the RCP 8.5 scenario a slight increase (Bucak et al., 2018).

The simulated scenarios highlight that the water management needs to avoid future water losses in the Itupararanga reservoir water supply. During the drought period (2014 to 2015), management used the reservoir dead storage, however it was not possible to supply drinking water to the almost 1 million inhabitants and there was a need for water rationing in some cities. Due to a decrease in the volume of the Itupararanga reservoir in 2018, the population was advised to save water to avoid new rationing.

Despite the fact that a lake's water storage can be influenced by climate change, there exist a large regional variability that interacts with it (Woolway et al., 2020, Shatwell et al., 2019). For example, strong seasonal variations regarding rainfall regime (dry and wet periods in the region), as well as lake-specific factors, such as morphometry. Further, reservoirs operation can play an important role to maintain appropriate water levels.

4.4 Consequences in the reservoir thermal regime based on climate projections

In both simulated scenarios the average surface water temperature increased compared to model calibration and validation periods (RCP 4.5: +1.1ºC (2009-2013), RCP 8.5: +1.6ºC (2009-2013), RCP 4.5: +0.6°C (2014-2018), RCP8.5: +1.1ºC (2014-2018)). The literature has reported that lake surface temperatures have raised worldwide similarly to air temperature trends (O'Reilly et al., 2015; Woolway et al., 2019; Farrell et al., 2020).

The heating trend along the water column has also been reported (Pilla et al., 2018; Shatwell et al., 2019, Mi et al., 2020). In Itupararanga reservoir, the SBD measured was -1ºC between 2008 and 2018 and for the optimistic and pessimistic scenarios, it will increase by +2ºC for the period between 2028 and 2030 (Table 2.2), which would increase thermal stratification. Due to climate change, many lakes across the world may mix less frequently and alter their thermal regimes (Woolway and Merchant, 2019).

The optimistic scenario projects future stratification from October to mid-July/August (53% of stratified days in the entire simulated period, see Figure 6a). This occurs in conjunction with rainfall regime changes (an increase of 38% between July and September compared to the historical time series).

On the other hand, the percentage of stratified days was lower for the pessimistic scenario (36%) compared to the RCP 4.5, prolonging the number of mixing days (Figure 3.6b). This downward trend in stratified days may be related to the decrease in water level (shown in Section 4.1) that favors the heating of the total water column and vertical mixing of water masses (Magee and Wu, 2017).

The simulated thermocline depth has also shifted in both scenarios. Higher GHC emission scenarios predicted thermocline deepening. Similar behaviors have been forecasted for Lake Maggiore and Lake Tegel, with an intensification of the summer stratification period and an increase of thermocline depth (Fenocchi et al., 2018; Ladwig et al., 2018).

The stratified days and the thermocline depth are projected to increase in Itupararanga reservoir, as well as the water column stability (Figure A5). Our model also predicted that the lakes thermal stability (SSI) is projected to increase in the future, resulting in strengthened stratification and reduced vertical exchange between surface and bottom layers (Darko et al., 2019; Niedrist et al., 2018).

The literature has highlighted cyanobacteria predominance in the last 20 years in the Itupararanga reservoir (Beghelli et al., 2016; Cunha and Calijuri, 2011). Such dominance was driven by high water temperatures, especially in the summer, and high concentrations of ammonium and nitrate available in the reservoir (Cunha et al., 2017). Casali et al. (2017) also showed evidence of correlation between high concentrations of dissolved nutrients and higher densities of *Raphidiopsis raciborskii* (Cyanobacteria), as well as concentrations of saxitoxins in the water.

A recent study highlighted that the RCP 8.5 projections are closer to historical projections and have been predicted as the best combination for 2030 and 2050 based on current GHG emission policies (Schwalm et al., 2020). Further investigation needed to be done to better assess the impacts on reservoir water quality by water level fluctuations. Periods of drought have been related to the increase in trophic state and consequent blooming of cyanobacteria (Tundisi et al., 2015; Brasil et al., 2016; Mantzouki et al., 2018).

Under surface water heating, thermal stability intensification and a lengthening of the stratification duration, water quality could potentially deteriorate (Gray et al., 2019; Huisman et al., 2018). A potential trophic level increase may prevent some reservoir uses, such as navigation and fishing, and generate high costs to improve drinking water treatment. Therefore, water management needs to assess likely future impacts and decision-making needs.

5. Conclusion

The current study investigates the impacts of future scenarios on the hydrodynamics of a Brazilian multipurpose reservoir. Meteorological projections based on a one low CO_2 emissions (RCP 4.5) scenario and a high-emission pathway with no climate policy (RCP 8.5) scenario were incorporated in a simple hydrologic model and a process-based hydrodynamic model.

In two scenarios of GHG emissions and minimum water withdrawal by the reservoir management, the water level was projected to decrease and fall to the reservoir dead storage. Consequently, there could be a future lack of water supply and decrease of power generation for a region with a population of almost 1 million of people. The intensity of CO_2 emissions has been shown to have a strong correlation with the meteorological variables. The daily rainfall projections were lower for 2028-2030 in comparison to the long-term historical data, showing a negative correlation with the GHG emissions raise. In the RCP 8.5 scenario, the dead volume would be reached in 2029, while in the optimistic scenario, the reservoir would become unusable 10 months later.

On the other hand, air temperature projections had a positive correlation with the CO_2 emissions scenarios. Consequently, surface water temperatures tend to increase in both simulated scenarios. Furthermore, longer periods of thermal stratification and a projected rise of water column stability are expected and may generate harmful consequences for aquatic biota and water quality.

Further research should focus on determining climate effects on the aquatic ecosystem, especially regarding harmful cyanobacteria that can cause many issues. The insights gained from this study may be of assistance to support management measures to ensure the maintenance of reservoir uses and water quality considering future climate projections.

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Anexo I

Figure A1: Simulated and observed thermocline depths in the simulated period

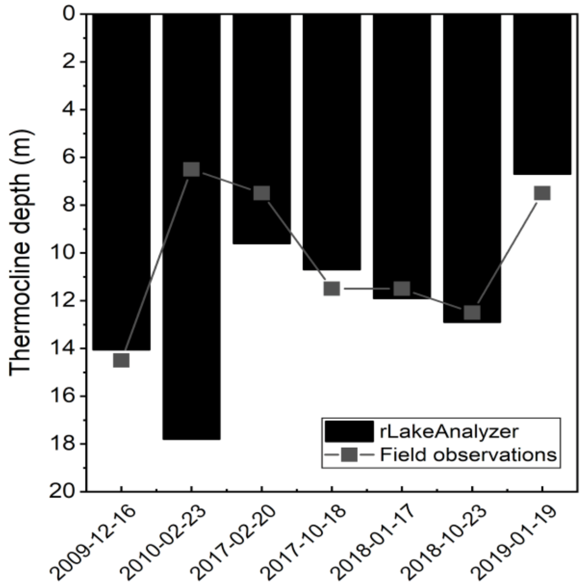


Table A2: Calibrated physical parameters and factors, their range values and references.

Physical parameter/ Factor	Unit	Description	Calibrated value/ Range	Reference
h_{min}	m	Minimum layer thickness	0.27 (0.25-0.5)	Hipsey et al., 2014; Bueche et al., 2017; Fadel et al., 2017
h_{max}	m	Maximum layer thickness	3.0 (1.5-3.5)	Bayer et al., 2013; Hipsey et al., 2014; Bueche et al., 2017
c_e	-	Bulk aerodynamic coefficient for latent heat transfer	0.001625 (0.0013)	Fischer et al, 1979; Bruce et al., 2018; Hipsey et al., 2019
Wind	-	Wind multiplication factor	2.025	Calibrated
Inflow	-	Inflow flow rate multiplier	0.475	Calibrated
Outflow	-	Outflow flow rate multiplier	0.475	Calibrated
Rain	-	Rain multiplication factor	0.8	Calibrated

Table A3: Simulated hydrodynamic indicators of Itupararanga reservoir.

YEAR	AaWL (M)	RT (DAYS)	NSD (DAYS PER YEAR)	MSSW ($J.m^{-2}$)	SBD (°C)
2009	19.3	197	77	85.4	0.7
2010	19.6	190	77	94.0	0.5

2011	18.9	340	82	102.2	0.5
2012	19.1	263	105	89.7	0.9
2013	19.9	243	103	87.1	1.0
2014	16.7	453	72	75.9	1.0
2015	17.6	246	136	116.0	1.8
2016	19.9	177	128	72.7	1.1
2017	18.9	208	88	60.7	0.8
2018	16.7	356	100	135.9	0.3

Figure A2: Baseline (2009-2018) and future climate data (2026-2030).

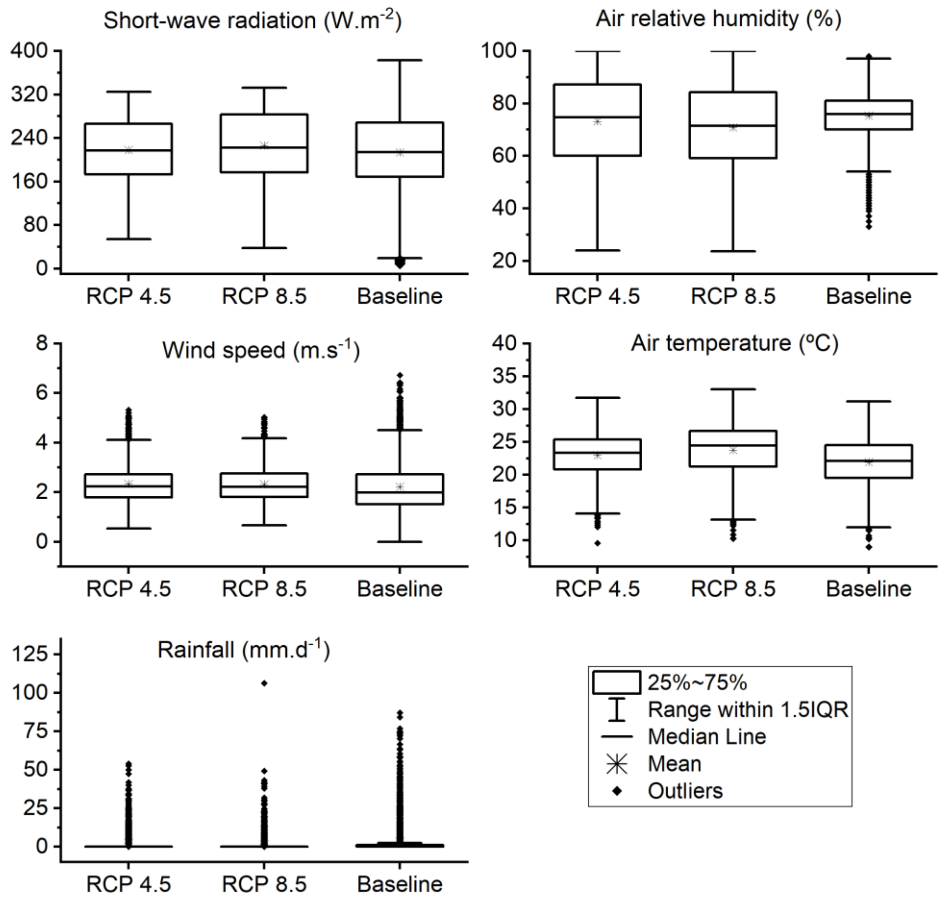


Table A5: Calibrated values and their ranges.

Parameter	Unit	Optimum value	Range
Str	mm	160	100-2000
Crec	%	20	0-20
Kkt	days	64	30-180
K2t	days	4	0.2-10
Ai	mm	2	2-5
Capc	%	40	30-50

Figure A3: Measured and simulated flows by the SMAP.

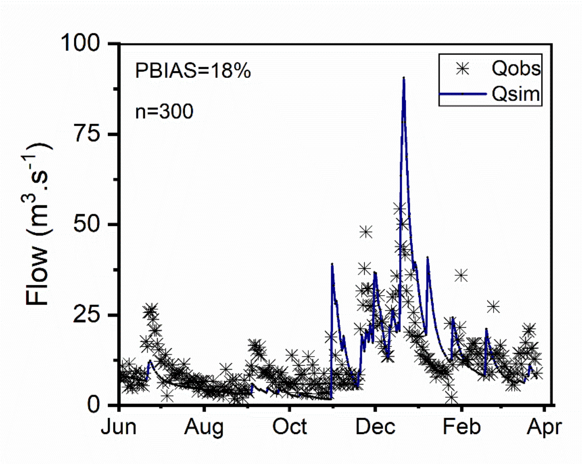


Figure A4: Comparison between observed inflows and projections. The red circles highlight drought periods at Itupararanga reservoir.

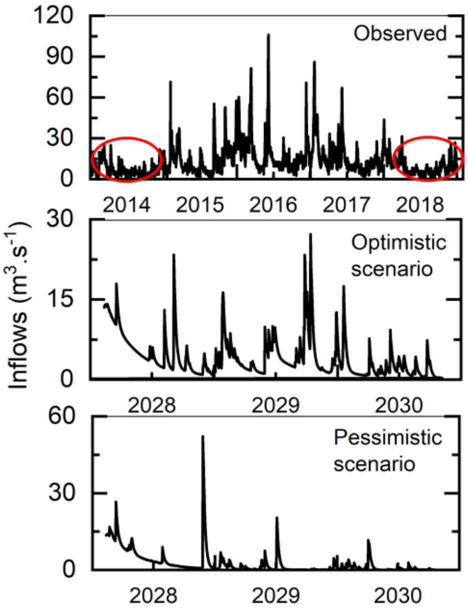
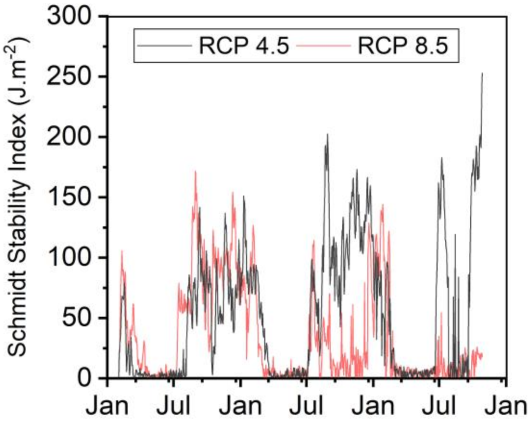


Table A4: Statistics metrics for Eta-HadGEM2-ES RCP 4.5 and RCP 8.5 projections and after bias-corrections. Rain – rainfall, WS – wind speed, AirT – air temperature, SW – short-wave radiation, RH – air relative humidity, Evap – air evaporation.

	RCP 4.5						*RCP 8.5*					
	Rain	WS	AirT	SW	RH	Evap	Rain	WS	AirT	SW	RH	Evap
Statistics	**Eta-HadGEM2-ES projections**											
MBE	-0.74	2.02	-0.7	46.1	-14	-0.8	1.25	2.03	-2.2	45.9	-9.8	-0.4
PBIAS	22.47	-91.18	-0.4	-21.6	19.3	21.9	-38.3	-91.6	2.9	-21.6	13.1	11.2
	Bias-corrected values											
MBE	-6. 10^{-3}	-2.10^{-5}	-0.4	1.1$10^{-5}$	-0.3	7. 10^{-5}	6.2. . 10^{-3}	7.5. 10^{-5}	-0.7	- 2. . 10^{-5}	-7. . 10^{-2}	8. . 10^{-5}
PBIAS	0.17	0.014	-0.6	-5. 10^{-6}	0.46	-2. . 10^{-3}	-1.92	12. . 10^{-3}	-0.5	9. . 10^{-6}	9. . 10^{-2}	-2. . 10^{-3}

Figure A5: Schmidt Stability Index for each simulated scenario.



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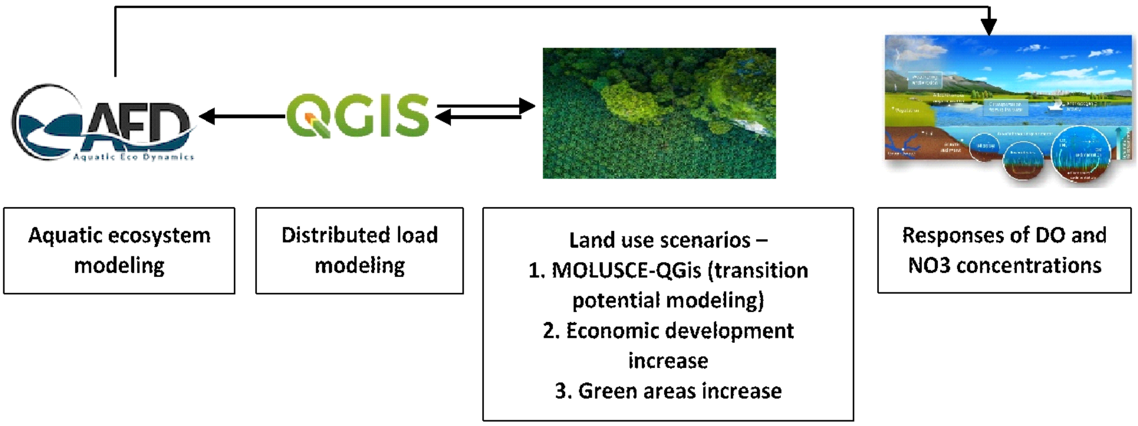
Capítulo 3 - MODELING THE RESPONSES OF DISSOLVED OXYGEN AND NITRATE CONCENTRATIONS DUE TO LAND USE AND LAND COVER CHANGE SCENARIOS IN A LARGE SUBTROPICAL RESERVOIR

Manuscrito submetido à periódico revisado por pares em setembro de 2021.
Autores: Barbosa, C.C., Calijuri, M.C., Anjinho, P.S., dos Santos, A.C.A.

Graphical abstract



1. Introduction

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

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

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

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

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

2. Methods

2.1 Study site

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

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

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

2.2 Database processing

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

Using data from previous studies (Cunha, 2012; Rôdas, 2013; Garcia 2013), it was possible to calculate that the dissolved oxygen (DO) loads in the

Sorocaba River upstream of the reservoir were statistically coincident (linear adjustment, r2 =0.85 (n=20)) with the sum of the flows and DO loads of the Sorocabuçu and Sorocamirim rivers measured ~ 3 km from the head of the Sorocaba River. Although upstream Sorocaba River receives effluents from the ETE Ibiúna, this has not sufficiently caused water quality deterioration due to the low flow.

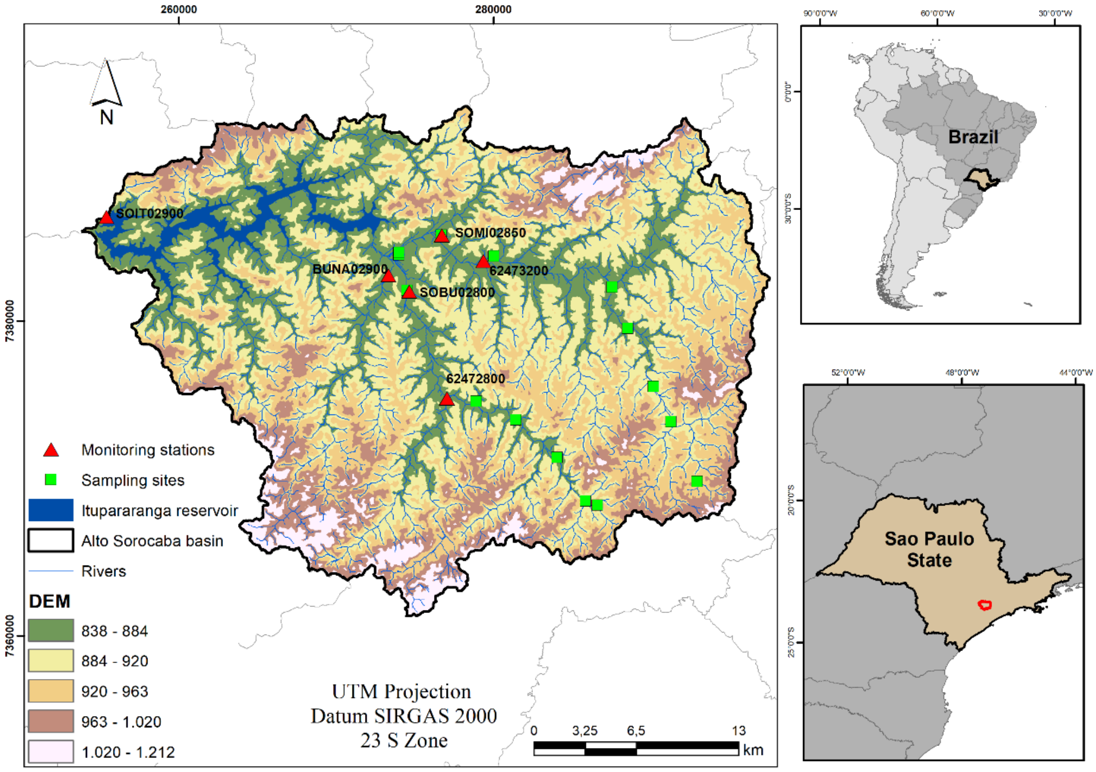
We used flow data along the Sorocabuçu and Sorocamirim streams adopting studies carried out by Rôdas (2013) and Garcia (2013) from July 2011 to April 2012 to support the flow calculation per km in the streams through the equations of two exponential functions (adjustment = r2> 0.91, dry season and r2>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

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

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

The location of the sampling sites and the monitoring stations are given in Figure 3.1: the green squares correspond to the 17 sampling sites measured at bimonthly time-step by Rôdas (2013) and Garcia (2013) and the red triangles refer to the 5 monitoring stations - monthly water quality time series (SOBU02800, SOMI02850, BUNA02900) and daily flows time series (62472800, 62473200).

Figure 3-1: Sampling sites performed by Rôdas (2013) and Garcia (2013), and monitoring stations operated by CETESB and ANA



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

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

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

The median values of reservoir inflow concentrations are shown in Table 3.1. As the water quality time-series by the CETESB did not have available data for particulate organic carbon (POC), organic nitrogen and all phosphorus and nitrogen pools, we had to estimate the required input data from the available biogeochemical time-series. As input for the GLM-AED2, 14 inflow time-series were used as follows: water temperature, pH, and concentrations of DO, DOC, POC, NH4, nitrate (NO3), DON, PON, FRP, ASRP, DOP, POP, and chlorophyll-a (Chla).

Table 3-1: Median values of inflow nutrient concentrations.

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

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

2.3 Biogeochemical modeling

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

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

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

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

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

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

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

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

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

2.3.1 Calibration and validation

The model parameters were calibrated following the bottom-up principle: firstly, the water level and water temperature were previously calibrated as described in Barbosa et al. (2021), and then the parameters regarding the concentrations of DO and NO3. Due to the low water quality data availability compared to the water level and water temperature historical time-series, the chosen calibration and validation period were shorter for the present study compared to the previous one. Firstly, we used 3 months (Jan 2009 to March 2009) to spin up the model. Then, we performed 936 days (April 2009 to Dec 2011) for the calibration and 784 days (Jan 2017 to Feb 2019) for the validation.

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

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

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

2.4 Basin distributed load modeling

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

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

The mean annual TN and TP loads were simulated based on the export coefficients established in the Mathematical Model of Correlation between Land Use and Water Quality (MQUAL), v. 1.5 (SMA, 2010) that were developed for the Guarapiranga Basin located also in São Paulo State and presenting a similar LULC to the Alto Sorocaba Basin (Table 3.2). We used the LULC GEOTiff data published by the MapBiomas project (MapBiomas, 2020) to determine the specific areas of the basin (km^2) covered by each LULC to calculate the nutrient export coefficient regarding each of them. Load values were converted from $kg.km^{-2}.y^{-1}$ to $kg.pixel^{-1}.y^{-1}$ and then the flow accumulation algorithm was used to generate the accumulated nutrient load model.

Table 3-2: MQUAL 1.5 export coefficients (SMA, 2010; Anjinho et al., 2021).

LULC	TP LOAD (KG $KM^{-2}Y^{-1}$)	TN LOAD (KG $KM^{-2}Y^{-1}$)
AGRICULTURE	126.29	1076.75

FOREST FORMATION	14.24	219
PASTURE	10.22	182.5
RURAL AREA	18.25	328.5
SILVICULTURE (FOREST PLANTATION)	14.24	219
URBAN AREA	12.41	465.01

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

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

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

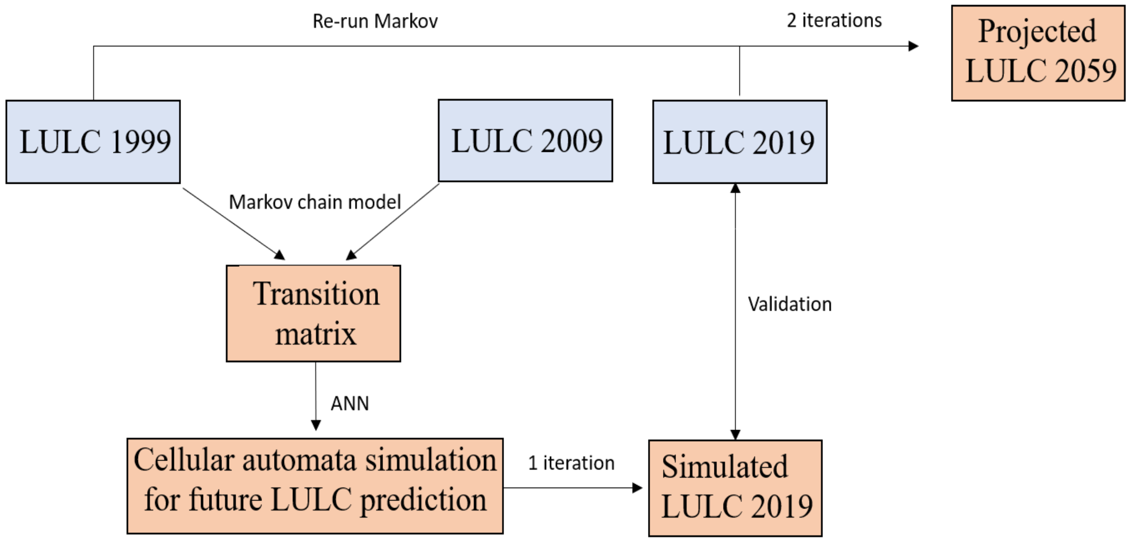
In order to assess the model performance, we performed a double validation approach which consisted of using the long-term historical time-series of flows (Q), TP and TN in the first step (Validation 1) for the three streams' monitoring stations: 12 years for the Sorocamirim stream, 8 years for the Sorocabuçu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

2.5 Transition potential modeling of the Alto Sorocaba catchment

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

The module can use ANN, Multi Criteria Evaluation (MCE), Weights of Evidence (WoE) and Logistic Regression (LR) methods to model LULC transition potential. The ANN method is a learning algorithm which analyzes the accuracy on training and validation sets of samples based on neighbor pixels and three learning parameters. The MOLUSCE module analyzes the transitional potential to predict LULC patterns in the future using the cellular automaton model (Burnham et al., 1973). The model integrates the spatial rules of cellular automaton with the transition of the Markov chain (CA-Markov) to simulate maps based on two images from different dates. The Ca-Markov is a stochastic model that reproduces changes in LULC by transition and information matrix based on the current state. The MOLUSCE methodology framework is shown in detail in Figure 3.2.

Figure 3-2: Flow chart for the MOLUSCE methodology. Pink boxes refer to the MOLUSCE outputs.



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

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

2.5.1. Land use scenarios for the 2050s

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

The potential transition scenario (MOLUSCE) was used as a first scenario for future modification actions in the basin. The other two scenarios were formulated based on the simulated LULC for 2059 considering the increase in preservation areas, focusing on the restoration of permanent preservation areas, and reducing agricultural uses (Green Scenario) and increased economic development of the basin focusing on agriculture, pasture, soy and urbanization (ED scenario) (Table 3.3).

Table 3-3: Percentage of changes regarding the MOLUSCE scenario.

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

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

3. Results

3.1 Biogeochemical simulations

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

The biogeochemical sensitive parameters and their respective values calibrated in the present study are compared with the reference values and shown in Table S1. Overall, the biogeochemical modeling showed good fit criteria compared with the observations for simulation of the DO concentrations (Table 3.4). The DO simulation was able to catch the small changes between wet and dry season, especially in the calibration which has a longer period of simulation compared to validation (Figure 3.3).

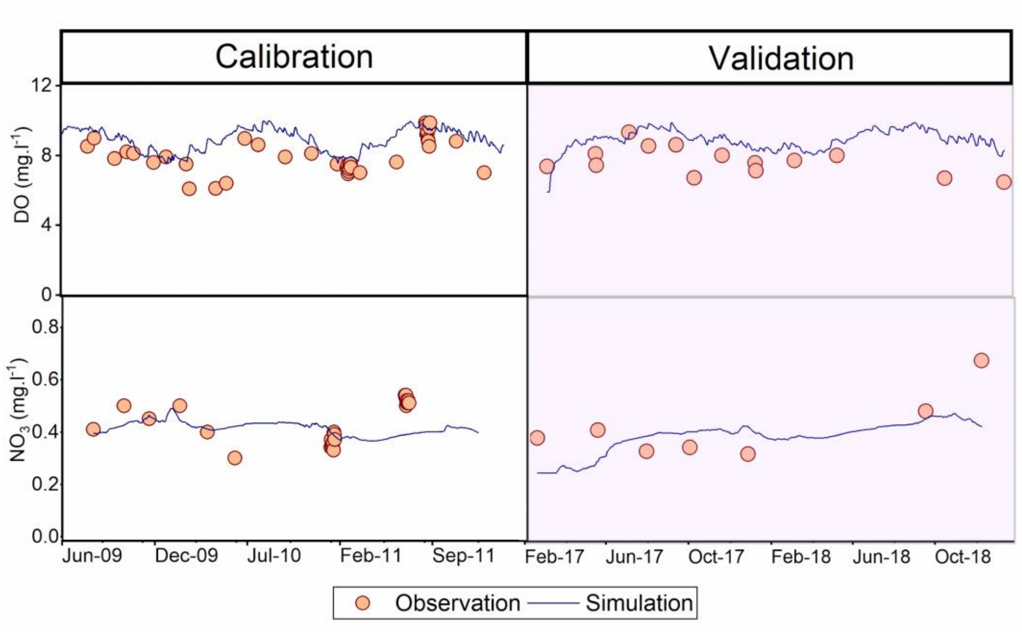
On the other hand, the simulated NO3 concentrations presented reasonable fit criteria. Although the NO3 validation showed RMSE and r values much lower than the calibration (Table 4), the performance metrics are similar with range values from previous studies (0.05 mg. l^{-1}<$RMSE_{NO3}$< 1.2 mg. l^{-1}, Ladwig et al., 2018; Weng et al., 2020) and the model also represented the median values of the observations in both simulation periods (Figure 3.3).

Table 3-4: Performance metrics of the DO and NO3 calibration and validation

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

NO_3	**Epilimnion**	42	0.04	0.38	0.03	0.4	0.32	7	0.13	-0.03	0.09	-0.1	-0.14

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



3.2 Distributed load and transition potential modeling of Itupararanga reservoir

The distributed load modeling was able to represent the flows (Q) and concentrations of TP and TN along the Itupararanga headwaters compared with the reference values from Moriasi et al. (2007) highlighted in Table 3.5.

Table 3-5: Results for the distributed load modeling.

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

	Very good		Good		Unsatisfactory

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

The validation results of the transition potential for the Alto Sorocaba basin in 2019 using 1999 and 2009 LULC data according to each land use/land cover are presented in Table 6 in relation to the total area (km^2) of the Alto Sorocaba basin.

Table 3-6: Validation of the transition potential in 2019 (km^2).

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

Overall, the model had a satisfactory performance ($r=0.99$, $r2=0.99$, $K=0.73$) to represent the LULC evolution in the basin despite underestimating forest plantation, urban, soybean and other temporary crops areas. The simulation of the transition potential of the Alto Sorocaba basin in 2059 shown in Figure 3.4 and the built scenarios related to the 2019 baseline are shown in Figure 3.5.

Figure 3-4: Comparison (%) of gains and losses for the Alto Sorocaba basin between the historical baseline LULC and simulated LULC for 2059.

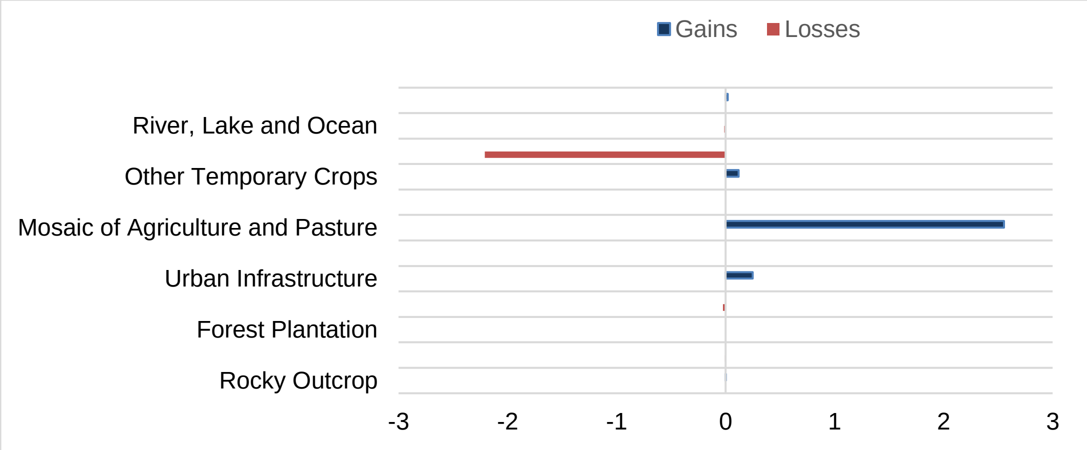
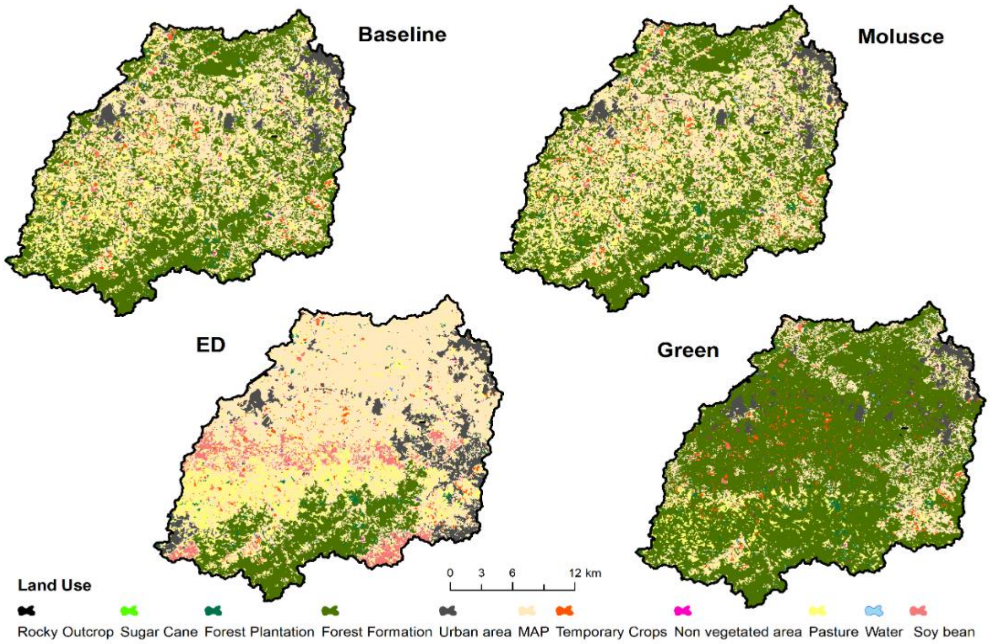


Figure 3-5: LULC scenarios used in the present study compared to the 2019 baseline.



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

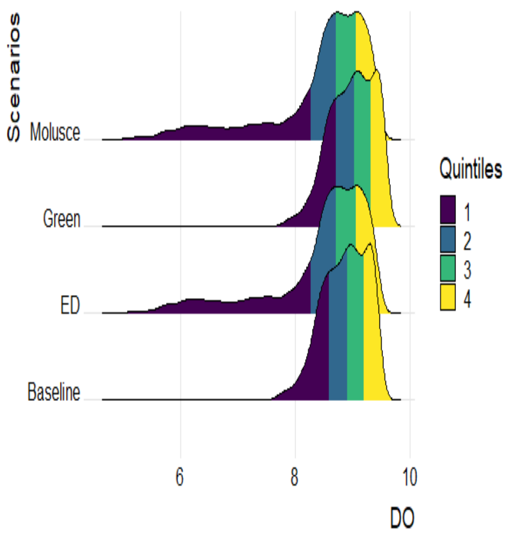
The DO concentrations from the three scenarios slightly changed compared to the historical baseline (2009-2011 and 2017-2019), as shown in Table 3.7 and Figure 3.6a. As expected, the mean DO concentration decreased in the MOLUSCE and ED scenarios due to an increase in O2 consumption by nitrification. On the other hand, changes in inflow NO3 and PO4 concentrations led to a greater influence on the NO3 simulations in the reservoir, which may be associated with the greater impact of allochthonous loads in the reservoir due to changes in land use (Figure 3.6b). The simulated Chla concentrations for each scenario were shown to be influenced by such changes of the inflow dissolved nitrogen and phosphorus concentrations (Figure 3.6c).

Table 3-7: Mean and standard deviations of the DO and NO3 simulations.

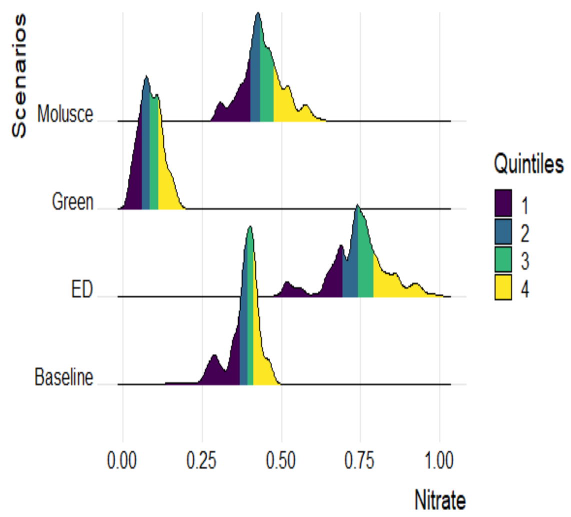
Scenario	DO concentration (mg. l-1)	NO3 concentration (mg. l-1)
Baseline	8.87 (0.38)	0.38 (0.05)
MOLUSCE	8.45 (0.90)	0.44 (0.06)
Green	8.98 (0.38)	0.09 (0.03)
ED	8.45 (0.90)	0.74 (0.09)

Figure 3-6: Quintiles based on the kernel density estimation (KDE) for a. DO, b. NO3 and c. Chla concentrations in each simulated scenario.

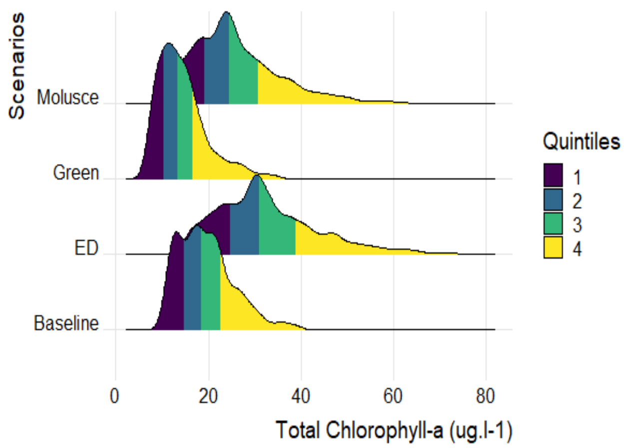
a.



b.



c.



4. DISCUSSION

4.1. Performance of models

The biogeochemical modeling was able to represent the average DO and NO3 concentrations on the Itupararanga reservoir. Model performance metrics for 936 days of calibration and 784 days of validation showed similar results along the surface and epilimnion depths with values in the range of previous studies (0.96mg.l^{-1}<$RMSE_{DO}$<3.6 mg.l^{-1}, Burger et al., 2008; Farrell et al., 2020; 0.05 mg.l^{-1}<$RMSE_{NO3}$< 1.2 mg.l^{-1}, Ladwig et al., 2018; Weng et al., 2020).

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

The distributed modeling validations of TN and TP concentrations along the Alto Sorocaba Basin based on the nutrient loads exported from the catchment (Johnes, 1996) can highlight the potentialities of this GIS approach to assess the LULC impacts on the streams and the Itupararanga reservoir. The simulated TP and TN concentrations in the watercourses showed good fit criteria compared with the reference values from Moriasi et al. (2007). Another recent study applied a catchment-scale nutrient model with a similar modeling fit compared to the results shown in Table 3.5 (Messina et al., 2020).

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

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

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

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

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

4.3 Novel open science framework based on coupled models

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

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

We assess water quality changes focusing on reservoir DO and NO3 concentrations in response to the proposed scenarios based on land use forecasts for 2059. The first scenario was simulated based on the potential LULC conditions for the Alto Sorocaba basin in 2059 and the second and third ones took into account an increase in green areas and an increase in economic development of the Alto Sorocaba basin. The results of the basin transition potential simulation show that even though the K coefficient value (K=0.73) corresponds to a moderate agreement between the reference map and the simulated map (Mienmay, 2018), the r and r2 values (>0.9) have shown satisfactory performance.

The simulated scenarios were able to indicate future biogeochemical changes in the Itupararanga reservoir and also the water quality deterioration in an environmental degradation scenario (ED). A 31% increase in NO3 and FRP concentrations in the inflow in the ED scenario compared to the MOLUSCE scenario has led to an increase in O2 consumption by nitrification and a decrease in the DO concentrations. On the other hand, in the green scenario, a 64% decrease in input NO3 and FRP concentrations compared to the MOLUSCE scenario can have led to a decrease in O2 consumption by nitrification and an increase in DO concentrations. Likewise, a 4% increase in the same concentrations in the MOLUSCE scenario performed similarly.

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

5. CONCLUSION

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

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

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

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Anexo II

Figure A1: Input time-series of pH and DO, TOC, TP and TN concentrations used in the biogeochemical simulations.

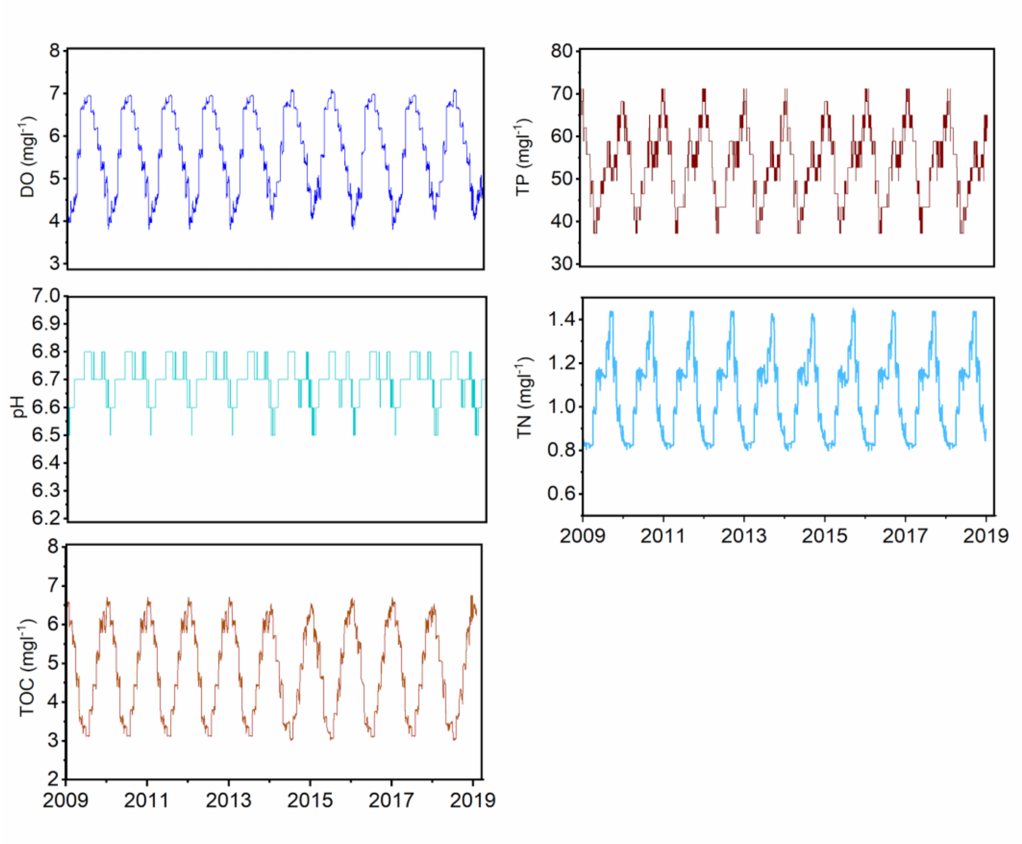


Table A1: Sensitive parameters and their respective calibrated values.

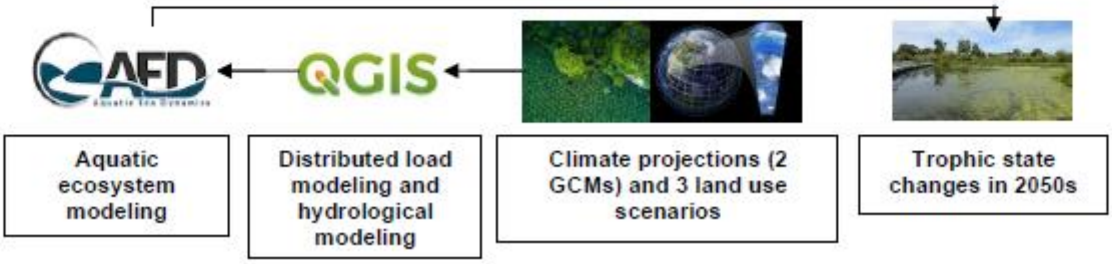
Symbol	Description	Reference (Hipsey et al., 2013)	Present study
	Oxygen		
Fsed_oxy	Sedimentation flux for dissolved oxygen (mmol m^{-2} d^{-1})	-100	-137.94
Ksed_oxy	Half saturation constant of oxygen sediment flux (mmol m^{-3})	10-100	42.98
theta_sed_oxy	Temperature multiplier for oxygen sediment flux	1.04-1.12	1.09
Kpom_hydrol	half saturation constant for oxygen dependence on particulate decomposition rate (mmol O2 m-3)	47-78	68.09
Kdom_minerl	half saturation constant for oxygen dependence on aerobic mineralisation rate (mmolO2.m-3)	47-78	67.837
	Nitrogen		
Fsed_nit	Sedimentation flux for nitrate (mmol m^{-2} d^{-1})	-21.4-7.14	-5.34
Rnitrif	Maximum reaction rate of nitrification at 20 °C (d^{-1})	0.03-0.05	0.038

Rdenit	Maximum reaction rate of denitrification at 20 °C (d^{-1})	0.01-0.04	0.01
Knitrif	Half saturation constant for oxygen dependence of nitrification (mmol m^{-3})	62.5-93.7	85.97
Kdenit	Half saturation constant for oxygen dependence of denitrification (mmol m^{-3})	12.5-15.6	12.5
Ksed_amm	Half saturation constant of ammonium flux (mmol m^{-3})	1.56-15.6	12.37
Ksed_nit	Half saturation constant of nitrate flux (mmol m^{-3})	2.14-15.6	14.99
theta_denit	Temperature multiplier for temperature dependence of denitrification	1.05	1.10

Capítulo 4 - FORECAST OF TROPHIC STATE CHANGES OF A SUBTROPICAL RESERVOIR DUE TO CLIMATE CHANGE AND LAND-USE CHANGE SCENARIOS FOR THE 2050S: AN INTEGRATED CLIMATE-HYDROLOGICAL-BIOGEOCHEMICAL MODELING APPROACH

Manuscrito submetido à periódico revisado por pares em fevereiro de 2022.

Graphical abstract



1.Introduction

Climate change impacts on lakes and reservoirs have been extensively studied in recent years (Jeppesen et al., 2017; Ladwig et al., 2018; Magee and Wu, 2017; Sahoo et al., 2016). Changes in rainfall and climate patterns on different continents have generated immediate responses in the biogeochemical and ecological dynamics of lakes and their respective basins and, consequently, in the aquatic ecosystem (Adrian et al., 2009). The release of nutrients is being influenced by such changes (Sinha et al., 2017) and, thus, it has also driven the development, proliferation and maintenance of cyanobacteria blooms (Wells et al., 2015).

Eutrophication is a growing problem that can compromise the water quality and its related uses due to the intensification of external nutrient availability in many agricultural and urban watersheds. Several studies have investigated this process using data science and modeling approaches (Rigosi et al., 2014; Fernández et al., 2015; Hu et al., 2016; Fadel et al., 2017; Dalu and Wasserman, 2018).

The increase in the trophic state of lakes and reservoirs can lead to the growth of potentially toxic cyanobacteria, causing several damages to multiple uses, especially in the drinking water supply. Global warming has also been pointed out as another driver of this process. The increase in water temperatures, modification of stratification patterns and thermal regime and changes in climatic forcing are some of the consequences already observed (Paerl and Huisman, 2008, Moe and Couture, 2016). On the other hand, even with the expected intensification of urbanization rate for the next decades, restoration efforts have shown to have effectiveness in the water quality control of some catchments (Fu et al., 2021).

Land use and land cover (LULC) shifts have also driven eutrophication and have been investigated in order to improve water quality of inland waters. Deterministic modeling approaches have been used to understand impacts of climate and LULC changes in lake ecosystems (Messina et al., 2020; Moe et al., 2016; Pace et al., 2021) and give insights for water management (Liu et al., 2018). Long-term analysis has shown that climatic pressure and nitrogen limitation contributed to the high variability of cyanobacterial blooms in a shallow temperate reservoir (Moal et al., 2021).

In the present study, different couplings of open access tools for aquatic research were used to assess the methodological approaches performance to study the water availability and water quality responses. Following this, we draw conclusions on the implications of trends in water level and water quality for reservoir operation to prevent eutrophication and not impair the drinking water supply.

2. Methods

2.1 Driver data

The data availability and the processing of meteorological and hydrological time-series and the inflow water quality concentrations used in the simulation steps are detailed in the second and third chapters of this Dissertation.

2.2 Climate projections

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

The first GCM used in the present study was the Model for Interdisciplinary Research on Climate, version 5 (MIROC5). The MIROC5 is a Japanese coupled ocean-atmosphere model of resolution of about 150 km in horizontal and 40 levels in vertical. Another GCM used in the present study was the HadGEM2-ES which was already described in the Chapter 2 of this Dissertation, as well as the radiative forcing scenarios of 8.5 $W.m^{-2}$ (RCP 8.5). We performed our scenario simulations using only the RCP 8.5 emission curve for the HadGEM2-ES and the MIROC5 climate projections. Our choice was based on RCP8.5 to be the best match out to mid-century greenhouse gases emissions and stated environmental policies as reported by Schwalm et al. (2020).

The time-series of climate projections were biased-corrected to adjust historical data and correct the future projections using 1-decade data as control period (2009–2018). Details of bias correction methods are given in the Chapter 3 of this Dissertation.

2.3 Hydrological simulation

The SMAP model was used to simulate the future inflow in the Itupararanga reservoir. Details about the SMAP are presented in Chapter 2. In the scope of this present study, we performed a new calibration and validation for the model considering a longer temporal time-series. We used 1000 days (June 23, 2010- June 23, 2013) for the calibration and 700 days (June 29, 2016- Sept 07, 2018) for the validation.

The statistics metrics used to assess the model performance were the percent bias (PBIAS) (Gupta et al., 1999) which measures the average tendency of the simulated data to be larger or smaller than their observation, and the Pearson correlation coefficient (r). We ended the calibration efforts when the model was able to achieve a range of PBIAS considered satisfactory ($\pm15 < PBIAS < \pm25$) according to Moriasi et al., 2007, and we were able to identify good agreement between simulated and observed discharge by visual inspection. After the calibration and validation of the SMAP model, we have estimated future daily discharges from January 2050 to December 2059 using the HadGEM2-ES and MIRO-C5 projections for air temperature and evaporation. Those data were used as input to the distributed load basin model and the lake ecosystem model.

2.4 Catchment TN and TP simulations and land use scenarios

The chapter 3 of this Dissertation describes the watershed-process based lake modeling approach and the land use and land cover (LULC) scenarios built for the Itupararanga reservoir in 2059. Thus, this modeling approach was used to simulate future nutrients loads in the reservoir based on the three LULC future scenarios proposed and mean estimated flows for the two climate models.

We have calculated the long-term average discharge of the HadGEM2-ES and MIROC5 projections for the 2050s to use in the estimation of TP and TN loads in the same future period. For that, we have considered the same three LULC scenarios proposed in Chapter 4, adopting the mean estimated flows for the 2050s. We have performed the estimate using each LULC area and its respective export coefficient divided for the two long-term average discharges to find the average annual nutrient concentrations upstream of the Itupararanga reservoir.

2.4 Water temperature prediction using Air2stream

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

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

After manually testing each set of parameters and quantifying the minimum value for the objective function based on RMSE metric, we have chosen a set of five parameters as the best option for our calibration. We calibrated the air2stream model using the daily air temperature, the reservoir daily inflow and the water temperature estimated in the chapter 2 from 2009 to 2013 and we validated from 2014 to 2019. The mean absolute error (MAE) and r were calculated to assess the model performance to fit observation and simulation.

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

2.5 Lake Ecosystem modeling

The vertical one-dimensional model GLM-AED2 which couples hydrodynamic, biogeochemical, and ecological processes in lakes was used to simulate total nitrogen (TN), total phosphorus (TP) and total chlorophyll-a (TCHLA) in the Itupararanga reservoir.

The TN and TP concentrations are based on the sum of nitrogen and phosphorus pools considering dissolved, particulate, organic and inorganic forms, as well as internal nitrogen and phosphorus stores in the phytoplankton community (Equation 1 and 2).

The TCHLA concentrations are calculated as an indicator of phytoplankton abundance (Equation 3) using a carbon mass balance equation based on processes of uptake, excretion, mortality, respiration and vertical movement in the water column (Equation 4). Grazing was not taken into account in the model equations as we did not have available zooplankton data.

$$TN = NO_3 + NH_4 + DON + PON + \sum_a^{N_{PHY}} PHY_{Na} \tag{1}$$

$$TP = PO_4 + PO_4^{ads} + DOP + POP + \sum_a^{N_{PHY}} PHY_{Pa} \tag{2}$$

$$TCHLA = \sum_a^{N_{PHY}} PHYa_{Xc:Chla}\, PHY_{Ca} \tag{3}$$

$$\frac{dPHY_{Ca}}{dt} = +f_{uptake}^{PHYCa} - f_{excr}^{PHYCa} - f_{mort}^{PHYCa} - f_{resp}^{PHYCa} - f_{set}^{PHYCa} \tag{4}$$

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

The global sensitivity analysis and the calibration and validation of TP, TN and TCHLA have followed the same methodological approach presented in the Chapter 4. We have performed an automatic and manual calibration technique. As we did not identify any temporal patterns and due to the coarse resolution in the measured data, the focus of our calibration was representing expected annual patterns based on the observed median of TP, TN and TCHLA concentrations. Thus, we have chosen five goodness-of-fit (GOF) metrics using the hydroGOF package (Zambrana-Bigiarini, 2017) in R to assess the model's performance in minimize differences between observations and simulations: the root mean squared error (RMSE), r, MAE, PBIAS and Kling-Gupta efficiency (KGE).

The target of the calibration was to represent the median values in order to simulate their future trends and be able to calculate the trophic state changes over the years. When the ecosystem model was able to capture the median, maximum and minimum concentrations of TP, TN and TCHLA, we performed simulation of future scenarios using the two climate projections and the three LULC scenarios.

2.6 Coupled hydrological-hydrodynamic-biogeochemical models

We used a coupled modeling framework to assess six scenarios based on the HadGEM2-ES and MIROC5 climate projections and LULC scenarios proposed in Chapter 2. We simulated all combinations of LULC and climate scenarios, for a total of 6 simulations. The methodological framework is shown in Figure 4.1 and detailed in Table 4.1.

Figure 4-1: Methodological framework. Drivers in black color; Model input estimated by climate projections and LULC scenarios in red color; Model input estimated by climate projections in purple color.

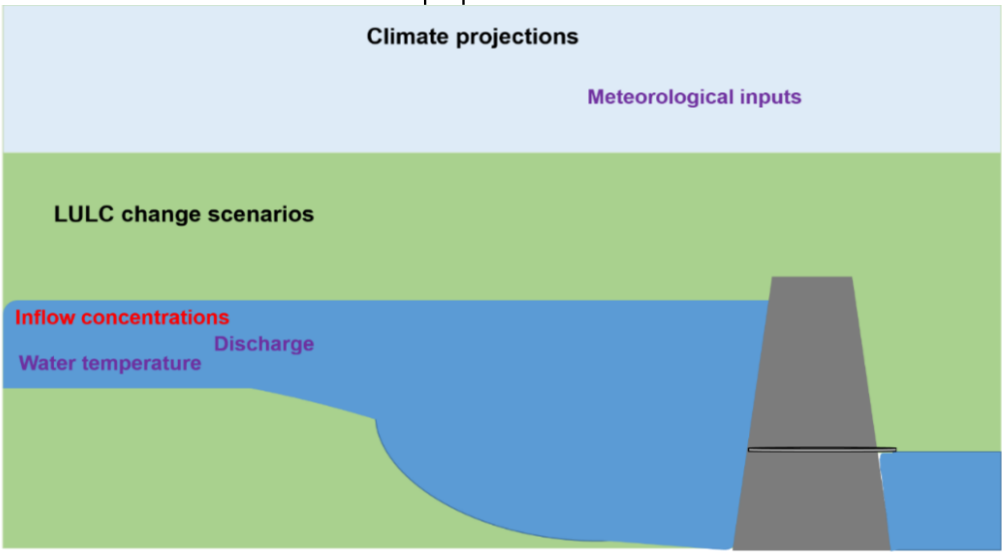


Table 4-1: Models and input and output data for each of them used for the scenario's simulation from 2050 to 2059.

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

The previously presented calibrated and validated models were used to perform analysis of water quality and water level in the Itupararanga reservoir based on future projections of climate data and LULC for the 2050s. We have used observed time-series of water level and TP and TCHLA concentrations as baselines to compare likely changes based on the proposed scenarios. In order to assess the future consequences on the water quality of Itupararanga reservoir, we have also calculated the trophic state index for tropical/subtropical reservoirs (TSI_{tsr}) proposed by Cunha et al (2013) and described below in Equation 5:

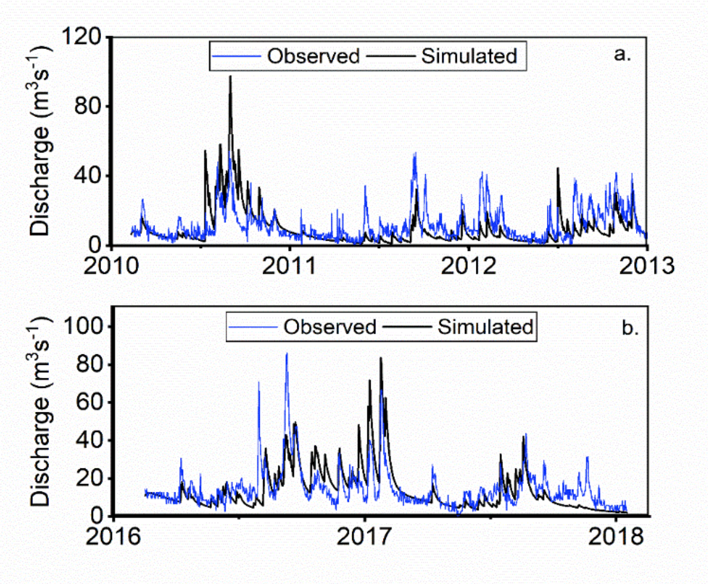
$$TSI_{tsr} = \frac{TSI(TP)_{tsr} + TSI(Chla)_{tsr}}{2} \quad (5)$$

3. Results and Discussion

3.1 Calibration and validation of the SMAP, Air2stream and AED2 model

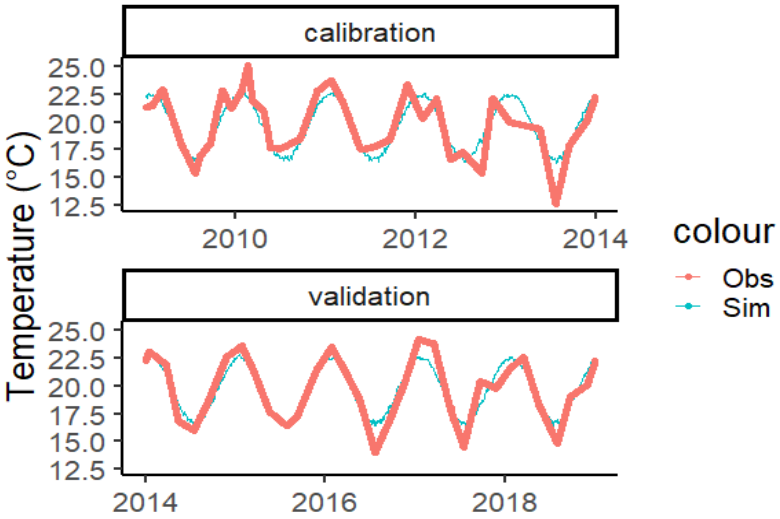
The SMAP model was used to simulate daily flows upstream from the Itupararanga reservoir. The hydrological model reasonably represented seasonality differences and captured flow peaks from the daily observed rainfall and evaporation data (Figure 4.2). The PBIAS metric was 19% and r=0.52 in the calibration period and PBIAS=4% and r=0.69 in the validation one. Those values were considered satisfactory for calibration and in very good agreement for validation according with Moriasi et al., 2007. The values of the calibrated parameters are shown in Table A1.

Figure 4-2: Comparison between: a. calibration and b. validation results of the SMAP model.



The air2stream model was used to simulate the daily temperatures of the headwater of the Itupararanga reservoir as shown in Figure 4.3. Simulated water temperatures were similar to observed water temperatures in the calibration (MAE=-0.039, r=0.88, RMSE=1.11ºC) and validation (MAE= -0.011, r=0.95, RMSE=0.89ºC) periods. Those results are in the range found in previous studies using the Air2stream model (0.86ºC<RMSE<1.52ºC, Fenocchi et al., 2017; Toffolon & Piccolroaz, 2015b).

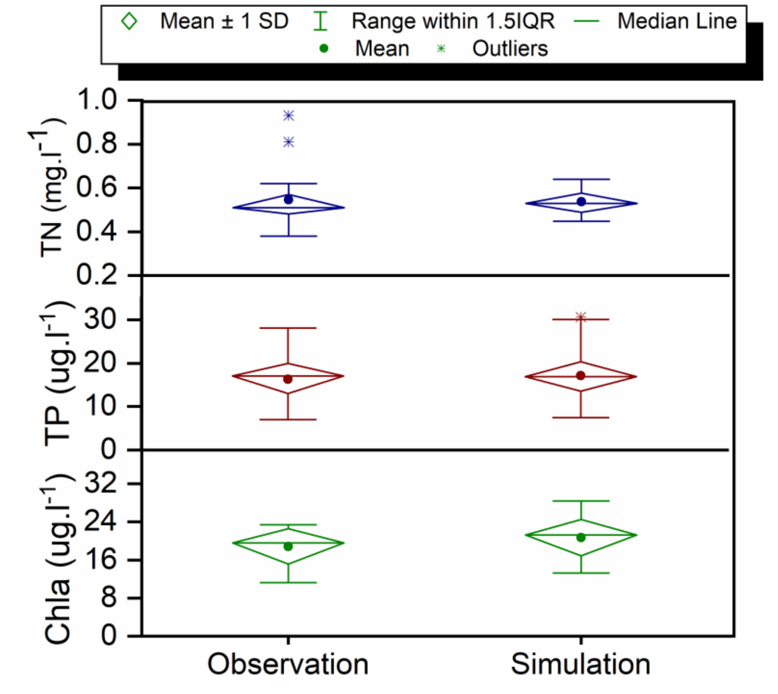
Figure 4-3: Comparison between observed and simulated water temperatures for the calibration and validation periods.



A coupled hydrodynamic-ecological model was used to represent the median concentrations of TP, TN and TCHLA observed in the Itupararanga reservoir from 2009 to 2011 (calibration) and from 2017 to 2019 (validation). An automatic and manual calibration was performed to identify suitable values of the parameters. A comparison between the calibrated values and the literature range values is shown in Table A2 in the Supplementary material.

The AED2 was able to simulate median and mean values of the nutrient's concentrations. On the other hand, the simulated median of the TCHLA concentrations was slightly overestimated, as well as the simulated maximum and minimum concentrations as shown in Figure 4.4. The GOF metrics of the surface and epilimnion and hypolimnion depths are presented in Table 5.2. Our calibration approach aimed to reproduce essential patterns instead of seemingly exact numerical values, as suggested by Jachner et al. (2007) for ecological simulations.

Figure 4-4: Diamond plots of the simulated and observed TN, TP and TCHLA concentrations.



The simulated TP and TN concentrations were better represented in the epilimnion (TP: 5µg.l^{-1}<RMSE<9µg.l^{-1}, TN: 110 mg.l^{-1}<RMSE<170mg.l^{-1}) compared to the hypolimnion (TP: RMSE=9 µg.l^{-1}, TN: RMSE=250µg.l^{-1}). A recent study found a similar range and the same trend for the TP and TN simulations using the GLM-AED2 (Farrell et al., 2020). The PBIAS values for the TP, TN and TCHLA simulations were considered good and very good (PBIAS<±40) according to the classification given by Darko et al. (2019) and Moriasi et al. (2007).

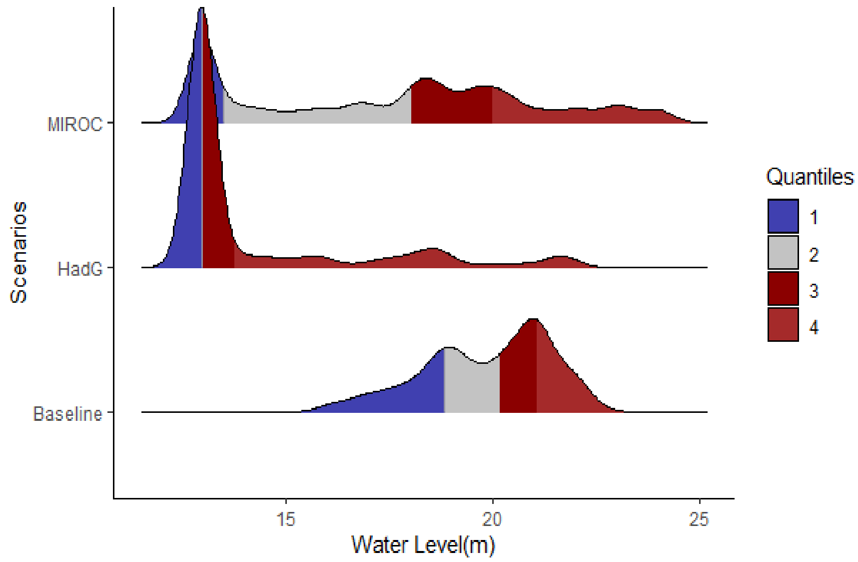
Tabela 5-2: GOF metrics for TP, TN and TCHLA simulations at surface (0m), epilimnion (Ep) and hypolimnion (Hip) depths.

Variable	Depth	Calibration						Validation					
		n	**RMSE**	**r**	**MAE**	**PBIAS**	**KGE**	**n**	**RMSE**	**r**	**MAE**	**PBIAS**	**KGE**
TP (µg.l^{-1})	**Surface**	42	6.0	0.51	0.004	-6.3	0.250	15	9.0	-0.300	0.007	27.1	-0.470
	Epilimnion	42	5.0	0.62	0.004	-9.4	0.460	15	9.0	-0.300	0.007	25	-0.500
	Hypolimnion	25	9.0	0.55	0.008	-22.5	-0.020	5	9.0	0.87	0.21	13.9	-0.93
TN (mg.l^{-1})	**Surface**	42	0.08	0.2	0.06	1.3	0.35	15	0.18	-0.65	0.13	-4.8	-0.66
	Epilimnion	42	0.11	0.03	0.09	2.9	0.11	15	0.17	-0.62	0.11	-8.3	-0.6
	Hypolimnion	25	0.25	0.05	0.21	-18.6	-0.15	7	0.25	-0.4	0.15	-19.2	-0.7
TCHLA (µg.l^{-1})	**Surface**	42	4.95	-0.08	3.68	9.9	0.11	14	8.02	-0.03	7.14	34.3	-0.04
	Epilimnion	42	4.55	-0.12	3.36	6.8	0.15	14	8.18	-0.03	7.05	35.7	-0.1

3.2 Water quality of the Itupararanga reservoir for the 2050s under climate and LULC scenarios

We have used the SMAP model with the calibrated parameters to predict future daily flows upstream from the Itupararanga reservoir. For that, we used climate projections from MIROC5 and HadGEM2-ES models from 2050 to 2059. Mainly due to the downward trend in both rainfall projections, in comparison to the long-term annual flow (13.53 m³.s^{-1}), the flows would decrease ~18% (11.06 m³.s^{-1}) in the MIROC5 projections and ~57% (5.86 m³.s^{-1}) in the HadGEM2-ES climate projections. Likewise, Sarmento et al. (2013) have predicted rainfall decrease for tropical South America based on the IPCC projections for this century. Such a reduction in inflows and the air temperature increase would directly influence the water level in Itupararanga reservoir, leading to a water level decrease for the 2050s, as shown in Figure 4.5.

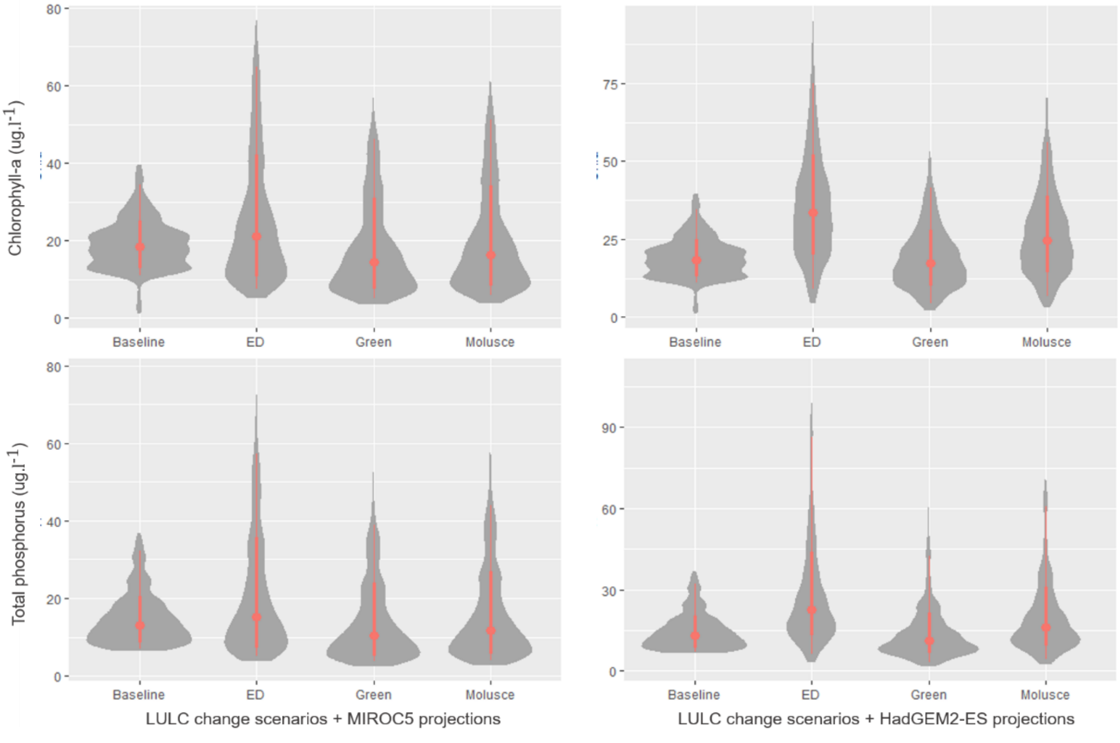
Figure 4-5: Quartiles of water level data in baseline and climate projections for the 2050s.



The median water level of the HadGEM2-ES and MIROC5 projections are going to be 18m and 13.8m, which means a reduction of 10% and 31% compared to the median water level observed between 2009 and 2018 (20m). The downward trend of the water level in the Itupararanga reservoir was also reported for 2028-2030 in Chapter 2. Some studies have been highlighted the consequences of previous drought periods in the water quality of tropical and subtropical lakes and reservoirs (Brasil et al., 2016; da Costa et al., 2016; Tundisi et al., 2015).

The trends in the TP and TCHLA concentrations for each simulated scenario are shown in Figure 4.6. Overall, there is a pattern of increase in such concentrations in comparison with the baseline. As noted earlier, the HadGEM2-ES climate projections tend to be more significant and have direct consequences on reservoir productivity. Even in the green scenario, which considers a reduction in deforestation and an increase in preserved areas, the median concentrations would decrease but it would have higher peaks of phosphorus availability and phytoplankton biomass compared to recent years in the coupled climate-land use projections.

Figure 4-6: Comparison between the baseline TP and TCHLA concentrations and for each climate projection (MIROC5 and HadGEM2-ES) plus LULC change scenarios.



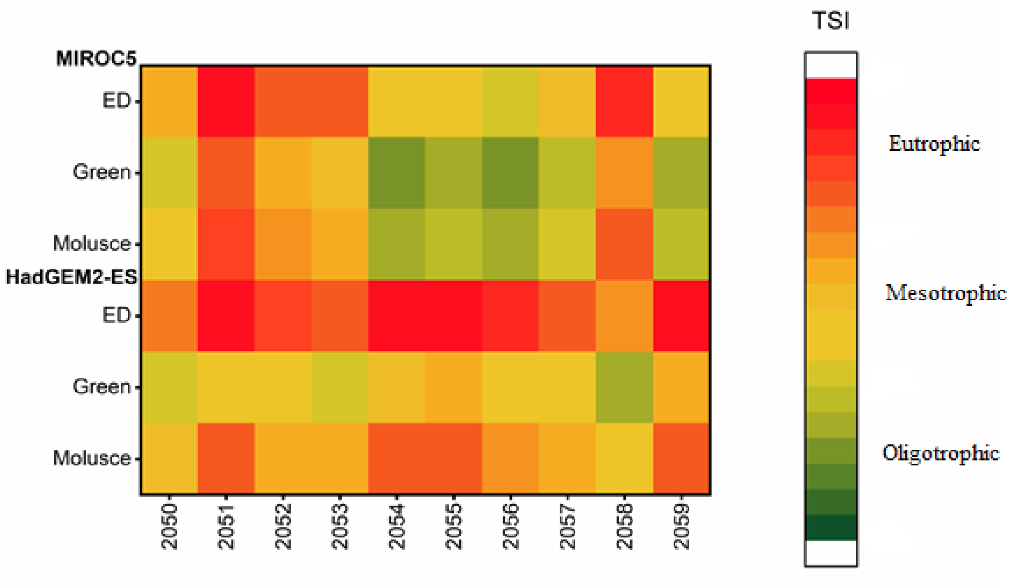
Total phosphorus has been well established as a predictor of phytoplankton in lakes, especially in the Itupararanga reservoir (Beghelli et al., 2016; Melo et al., 2019). Recently, it has been reported that TP have nearly equal importance to that of climate in predicting water quality in lakes on a global scale (Shuvo et al., 2021). Itupararanga reservoir has already been reported as a nutrient sink (Cunha, 2012) and also it has a self-purification function which contributes to release in the outflow a higher quality of the water (Melo et al, 2019). According to Brazilian legislation (CONAMA 2012), the chlorophyll-a limit for continental class II water bodies is 30 µg.L. If the TCHLA concentration limit is exceeded, Itupararanga water should not be used for swimming or irrigation (Beghelli et al., 2016).

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

The trophic state index (TSI) was calculated for each year in the 2050s considering all the six simulated scenarios (Figure 4.7, Table A3). In the climate projections plus green scenario it was possible to identify an oligotrophication trend. Such outcomes are in agreement with the reduction of the simulated median concentrations of TP and TCHLA which were used to calculate the annual values of the TSI. On the other hand, the main consequences of the other climate-land use scenarios were the trophic state increase in the Itupararanga reservoir due to climate warming and higher agricultural and urban impacts.

As expected, there was an increase in the trophic state in the ED scenario in both climate projection. Such high productivity is related to the increase in the impervious areas in the watershed and greater release of external loads in the reservoir compared to the current LULC. Previous studies have identified an increase in the TSI values in dry periods in the Itupararanga reservoir mainly due to the land use in the Alto Sorocaba basin (Cunha et al., 2017; Pedrazzi et al., 2013). Likewise, Itupararanga reservoir has been identified as having external loads more significant than internal turnover (Barbosa et al., 2021, under revision). Such increase in trophic state is not only due to climate change and exploratory management actions, but also an importance of the allochthonous inputs in the water quality of Itupararanga reservoir (Barbosa et al., 2021, under revision). Sarmento et al. (2013) considering climate change consequences in large tropical lakes mainly driven by internal loads indicates oligotrophication rather than eutrophication as a result of the increased water column stability.

Figure 4-7: Trophic state index (TSI) calculated for each year in the 2050s, considering climate projections + LULC change scenarios.



The more productive moment for Itupararanga reservoir was 40-50 years after the dam construction, also paleolimnology analysis indicated an improvement in Itupararanga water quality after 1970s (Wengrat et al., 2019) The authors reported that Itupararanga reservoir have remained mesotrophic over time and the phytoplankton species found in the sediment suggested fluctuation of water quality in the last decades.

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

4. Conclusion

The present study aimed to use a coupled modeling framework to perform forecasting of water quality in the Itupararanga reservoir for the 2050s. We have chosen open-source tools implemented in R and GIS to foster the reproducibility of the modeling approach.

Projections of two climate models forced by the greenhouse gases representative concentration pathway of 8.5 $W.m^{-2}$ showed rainfall decrease and air temperature increase in the Alto Sorocaba basin. The water level of the Itupararanga reservoir would fall between 20% and 60% of its average volume for both climate models.

The outcomes also suggest water quality deterioration due to warming climate and three LULC change scenarios. The optimistic land use scenario plus climate projections, which predicted a reduction in deforestation and an increase in preserved areas, highlighted a decrease in the median concentrations of TP and TCHLA and a trend towards oligotrophication. However, there would be higher peaks in phosphorus availability and phytoplankton biomass in the Itupararanga reservoir compared to recent years. On the other hand, the main consequences of the other climate-land use scenarios were the trophic state increase due to climate warming and higher agricultural and urban impacts.

Therefore, not only advanced water treatment plants must be installed in the Alto Sorocaba basin in the near future, but also management efforts must be made to control agricultural lands without environmental protection actions. Another alternative could be to develop strategies for the reservoir operation to save water for drinking supply, control water quality and protect the aquatic ecosystem.

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Anexo III

Table A1: Calibrated values and their ranges in the calibration of the SMAP model.

Parameter	Unit	Optimum value	Range
Str	mm	100	100-2000
Crec	%	20	0-20
Kkt	days	60	30-180
K2t	days	4	0.2-10
Ai	mm	2	2-5
Capc	%	30	30-50

Table S2: AED2 parameters values.

Symbol	Description	Initial value	Range (Hipsey et al., 2013)	Present study
	Oxygen			
Fsed_oxy	Sedimentation flux for dissolved oxygen (mmol m^{-2} d^{-1})	6	-100	-137.94
Ksed_oxy	Half saturation constant of oxygen sediment flux (mmol m^{-3})	15.6	10-100	42.98
theta_sed_oxy	Temperature multiplier for oxygen sediment flux	1.08	1.04-1.12	1.09
Kpom_hydrol	half saturation constant for oxygen dependence on particulate decomposition rate (mmol O2 m-3)		47-78	68.09
Kdom_minerl	half saturation constant for oxygen dependence on aerobic mineralisation rate (mmolO2.m-3)		47-78	67.837
Rdom_minerl			0.5	
	Carbon			
Fsed_dic	sediment CO2 flux	4.0		4.0
Ksed_dic	half-saturation oxygen concentration controlling CO2 flux	30.0		7.0
Theta_dic	Arrhenius temperature multiplier for sediment CO2 flux	1.0		1.08
Rpoc_hydrol	Maximum rate of decomposition of POC at 20C (d^{-1})	0.07	0.01-0.08	0.0156
Fsed_doc	sediment DOC flux	10	1-50	5.99
	Nitrogen			
Fsed_amm	Sedimentation flux for ammonium (mmol m^{-2} d^{-1})	3.00	1.35-6.42	3.00
Fsed_nit	Sedimentation flux for nitrate (mmol m^{-2} d^{-1})	-14.00	-21.4—-7.14	5.34
Rnitrif	Maximum reaction rate of nitrification at 20 °C (d^{-1})	0.03	0.03-0.05	0.038
Rdenit	Maximum reaction rate of denitrification at 20 °C (d^{-1})	0.01	0.01-0.04	0.01
Knitrif	Half saturation constant for oxygen dependence of nitrification (mmol m^{-3})	62.5	62.5-93.7	85.97
Kdenit	Half saturation constant for oxygen dependence of denitrification (mmol m^{-3})	15.6	12.5-15.6	12.5
Ksed_amm	Half saturation constant of ammonium flux	15.6	1.56-15.6	12.37

	(mmol m^{-3})			
Ksed_nit	Half saturation constant of nitrate flux (mmol m^{-3})	15.6	2.14-15.6	14.99
theta_nitrif	Temperature multiplier for temperature dependence of nitrification	1.08	1.03-1.08	1.05
theta_denit	Temperature multiplier for temperature dependence of denitrification	1.05	1.05	1.10
theta_sed_amm	Temperature multiplier for sediment ammonium flux	1.08	1.04-1.10	1.08
theta_sed_nit	Temperature multiplier for sediment nitrate flux	1.08	1.04-1.10	1.08
	Phosphorus			
Fsed_frp	Sediment PO4 flux (mmol m^{-2} d^{-1})	0.12	0.08-0.125	0.11
Ksed_frp	Half saturation constant of phosphate flux (mmol m^{-3})	15.6	15.6	197
theta_sed_frp	Temperature multiplier for sediment phosphate flux	1.08	1.04-1.10	1.04
Rpop_hydrol	Maximum rate of hydrolysis/breakdown of particulate organic phosphorus (d^{-1})	0.03	0.01-0.03	0.08
Fsed_dop	sediment DOP flux (mmol m − 2 day − 1)	0.12	-	0.08
	Phytoplankton			
Xcc	carbon to chlorophyll ratio (mg C/mg chla)	50	-	50
R_growth	Phyto max growth rate 20°C (/day)	1.0	-	2.0
I_K	Half saturation constant for light limitation of growth (microE/m^2/s)	130	-	130
I_S	saturating light intensity (microE/m^2/s) used if lightModel=1	150	-	150
R_resp	Phytoplankton respiration/metabolic loss rate (degC)	0.085	-	0.05
Theta_resp	Arrhenius temperature scaling factor for respiration (-)	1.05	-	1.12
K_N	Half-saturation concentration of nitrogen (mmol N/m^3)	1.0	-	1.0
X_ncon	Constant internal nitrogen concentration (mmol N/ mmol C)	-	-	0.048
K_P	Half-saturation concentration of phosphorus (mmol P/m^3)	0.05	-	0.15
X_pcon	Constant internal phosphorus concentration (mmol P/ mmol C)	-	-	0.0015

Table S3: TSI values. Pink colour: eutrophic state.

	HadGEM2-ES			**MIROC5**		
	Molusce	Green	ED	Molusce	Green	ED
2050	54.7	53.7	56.0	54.3	53.8	55.3
2051	56.2	54.5	57.4	56.7	56.3	57.7
2052	55.4	54.1	56.6	55.5	55.1	56.5
2053	55.1	53.6	56.3	55.4	55.0	56.4
2054	56.3	55.0	57.6	53.0	52.5	53.9
2055	56.4	55.1	57.7	53.3	52.8	54.2
2056	55.8	54.4	57.0	52.9	52.4	53.8
2057	55.3	54.0	56.5	53.7	53.3	54.7
2058	54.4	53.1	55.7	56.2	55.8	57.2

2059	56.5	55.1	57.7	53.4	53.0	54.4

Capítulo 5 - CONSIDERAÇÕES FINAIS E RECOMENDAÇÕES GERAIS

Considerações finais

A presente pesquisa testou as potencialidades do acoplamento de *modelos open-source* nas investigações de cenários de mudanças climáticas e de alterações de uso do solo em um reservatório subtropical multiuso. Estudos recentes que identificaram tendência de aumento da temperatura das águas devido ao aquecimento global também correlacionaram aumento da biomassa de fitoplâncton, especialmente as cianobactérias. Com essa motivação e a fim de investigar outras forçantes que impactam o ecossistema aquático, o segundo capítulo apresentou consequências das projeções climáticas nos níveis da água e regime térmico do reservatório de Itupararanga no final da década de 2020.

De acordo com projeções climáticas baseadas em emissões de gases de efeito estufa otimistas (RCP 4.5) e pessimistas (RCP 8.5) foi estimada uma redução significativa no nível de água do reservatório para ambos os cenários de 35% em relação às condições atuais. Previu-se que a temperatura da água superficial aumentaria 0,6 °C e que, por outro lado, haveria um resfriamento do hipolímnio (RCP 4,5 = -0,3 °C; RCP 8,5 = -1,2 °C). Outra consequência seria o aumento da duração dos períodos de estratificação que iniciariam mais cedo no período de estiagem (entre julho e agosto), bem como a intensificação da estabilidade da coluna d'água (+ 43% em relação às condições atuais) e um aprofundamento da termoclina.

Além das mudanças climáticas, outro *driver* muito importante de degradação da qualidade das águas é o manejo do solo nas bacias hidrográficas, identificado pelo uso e ocupação do solo nas sub-bacias e principalmente à montante de lagos e reservatórios. A fim de investigar como diferentes cenários de uso do solo impactariam a qualidade da água do reservatório de Itupararanga, o terceiro capítulo objetivou testar a modelagem de carga distribuída de bacias para gerar cenários de uso do solo usados na modelagem biogeoquímica. Considerando três cenários baseados em: tendência esperada de ocupação para 2050, diminuição e intensificação de áreas agrícolas e expansão urbana na bacia do Alto Sorocaba, foi constatado que mesmo que as concentrações de oxigênio dissolvido e nitrato não aumentassem acima dos limites permitidos pela legislação brasileira para todos os cenários, as concentrações de clorofila-a aumentariam significativamente, o que poderia representar uma séria ameaça ao uso do reservatório de Itupararanga como fonte de abastecimento de água. A modelagem proposta também foi capaz de representar a importância das áreas de formação florestal na conservação da qualidade da água do reservatório.

Por fim, para fazer previsões realistas da qualidade da água do reservatório de Itupararanga na década de 2050 com base em projeções climáticas e mudanças de uso do solo, no quarto capítulo foi proposto um acoplamento de modelos hidrológico, termodinâmico, de carga distribuída de bacia e hidrodinâmico-biogeoquímico para analisar a influência dos resultados no balanço hídrico e nos níveis tróficos do reservatório de Itupararanga.

Dessa forma, no capítulo quatro foram considerados três cenários de uso do solo e dois cenários climáticos com base em projeções regionalizadas de dois modelos climáticos globais e cenário pessimista de gases de efeito estufa (RCP 8.5). Os principais resultados foram que o nível da água do reservatório cairia entre 20% e 60% do seu volume médio para cada modelo climático e que na maioria dos cenários haveria aumento do estado trófico da represa devido ao aquecimento do clima e maiores áreas agrícolas e urbanas na bacia. Por outro lado, nos cenários de redução do desmatamento e aumento das áreas preservadas e projeções climáticas houve diminuição nas concentrações de fósforo total e clorofila-a e tendência à oligotroficação. No entanto, haveria picos mais elevados na disponibilidade de fósforo e biomassa fitoplanctônica no reservatório em comparação aos últimos anos provavelmente relacionados ao aquecimento global.

Os resultados do capítulo quatro sugerem que não apenas estações avançadas de tratamento de água devem ser instaladas na bacia do Alto Sorocaba em um futuro próximo, mas também esforços de manejo para controlar a expansão agrícola sem práticas de controle ambiental. Outra alternativa poderia ser o desenvolvimento de estratégias de operação do reservatório para economizar água para o abastecimento, controlar a qualidade da água e proteger o ecossistema aquático.

Os acoplamentos de modelos *open-source* propostos na presente pesquisa foram eficientes para gerar respostas hidrodinâmicas e de qualidade da água necessárias ao gerenciamento futuro de qualidade da água do reservatório de Itupararanga e podem servir como base metodológica para estudos semelhantes em outros reservatórios e lagos subtropicais, pois todos os modelos utilizados são disponibilizados por seus desenvolvedores e permitem alterações e melhorias em seus códigos-fonte.

As incertezas inerentes ao acoplamento de modelos determinísticos existem e devem ser minimizadas com base nos parâmetros a serem calibrados. Contudo os dados de entrada de cada modelo também são fonte de incertezas para as simulações e devem ser avaliados cuidadosamente em etapa anterior. Devido a inconsistências nas séries temporais observadas de qualidade da água, nos dois últimos capítulos, os períodos de calibração e validação do modelo biogeoquímico foram reduzidos em comparação aos períodos utilizados na calibração hidrodinâmica do segundo capítulo. Apesar da limitação de séries de dados de longo período, o modelo acoplado GLM-AED2 respondeu satisfatoriamente à alteração em diferentes forçantes externas e evidenciou as consequências esperadas na qualidade da água do reservatório de Itupararanga em comparação aos últimos anos.

Recomendações

As seguintes recomendações são propostas para estudos futuros:

- Instalação de boias de monitoramento frequente de alta resolução no reservatório de Itupararanga ao longo do eixo longitudinal para estudos mais detalhados de heterogeneidade espacial e temporal;
- Testar modelos bidimensionais ou tridimensionais no estudo da qualidade das águas do reservatório de Itupararanga por considerar também variações do gradiente horizontal importantes na dinâmica do ecossistema aquático;
- Utilização das metodologias propostas para formulação de estratégias de controle e restauração ambiental considerando redução de cargas internas e externas de fósforo dissolvido, redução de biomassa de fitoplâncton e retirada de água e/ou aeração do hipolímnio;

- Simulação de grupos ou espécies de fitoplâncton com foco em cianobactérias para avaliar respostas dos indivíduos aos cenários e prováveis mudanças na dinâmica das espécies.

Lista de publicações oriundas da presente pesquisa

Publicado

BARBOSA, C. C.; CALIJURI, M. C.; SANTOS, A. C. A.; LADWIG, R.; OLIVEIRA, L. F. A.; BUARQUE, A. C. S. Future projections of water level and thermal regime changes of a multipurpose subtropical reservoir (São Paulo, Brazil). *Science of the Total Environment*, v. 770, p. 1-11, 2021.

Submetido

BARBOSA, C. C.; CALIJURI, M. C.; ANJINHO, P. S., SANTOS, A. C. A. Modeling the Responses of Dissolved Oxygen and Nitrate Concentrations due to Land Use and Land Cover Change Scenarios in a Large Subtropical Reservoir. Environmental Modelling & Software.

Resumos apresentados em eventos científicos internacionais

BARBOSA, C. C.; CALIJURI, M. C.; ANJINHO, P. S., SANTOS, A. C. A. Modeling the Responses of Dissolved Oxygen and Nitrate Concentrations due to Land Use and Land Cover Change Scenarios in a Large Subtropical Reservoir *(Apresentação oral).* In: AGU Fall Meeting, dezembro de 2021, New Orleans-EUA.

BARBOSA, C. C.; SOARES, L. M. V.; CALIJURI, M. C. Climate change projections and water level decrease in a Brazilian multipurpose reservoir. In: 1st IAHR Young Professionals Congress, 2020, *Anais do the 1st IAHR Young Professionals Congress*. Madrid-Spain, Beijing-China: International Association for Hydro-Environment Engineering and Research –IAHR, p. 1-237, 2020.

BARBOSA, C. C.; SOARES, L. M. V., CALIJURI, M. C. Simulation of hydrodynamic alterations in a Brazilian reservoir at the 2050s by two climate projections models. In: GLEON 21.5 Virtual Meeting, *Book of Abstracts*, 2020.

BARBOSA, C. C.; MOUTINHO, F. H. M.; CALIJURI, M. C. Influence of Reservoir Volume Alterations Under Climate Change and Impacts on the Trophic State of the River-Lake Transition Zone. In: 2020 NALMS International Symposium, 2020, Virtual Presentation *Abstracts*, 2020.