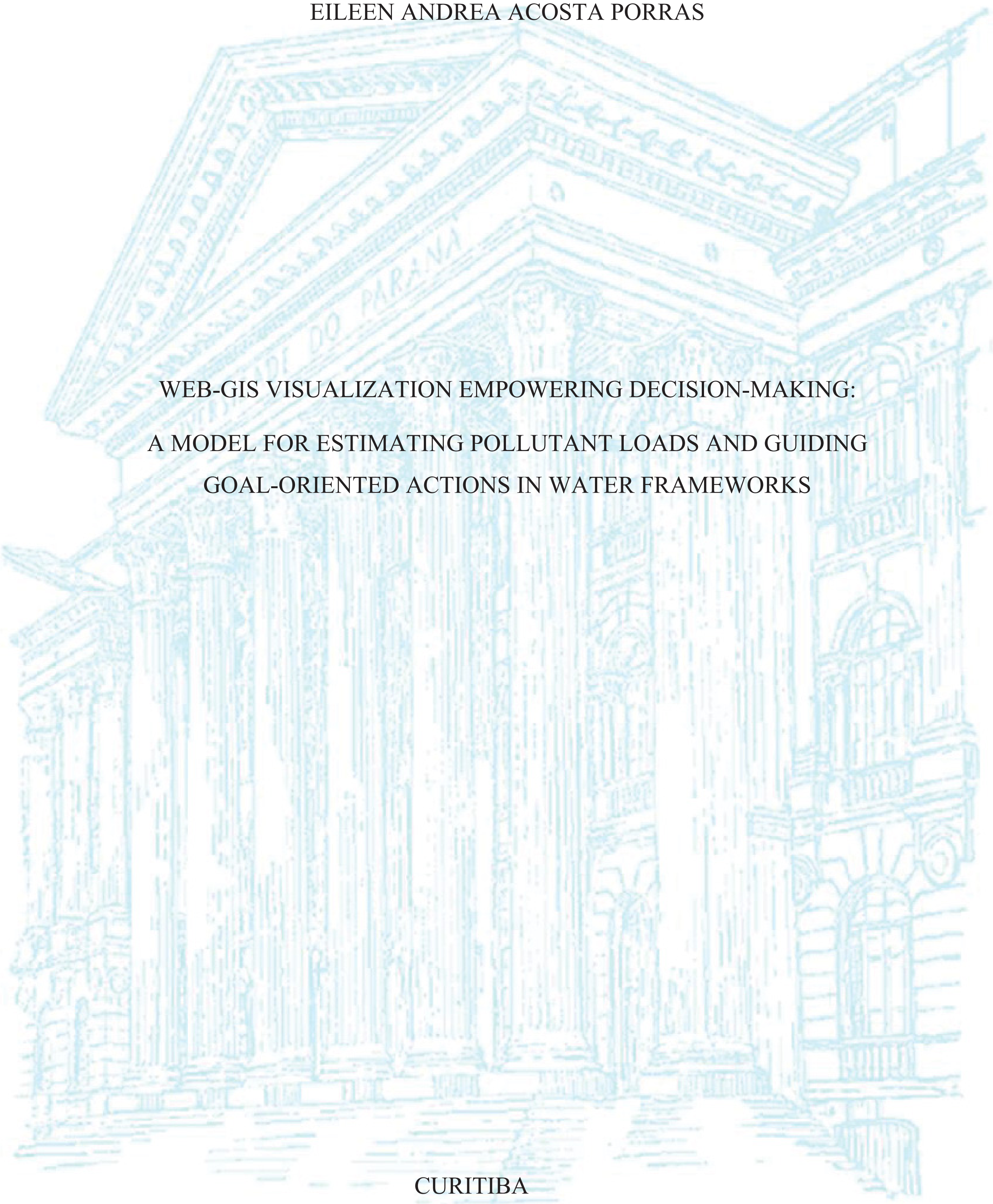

UNIVERSIDADE FEDERAL DO PARANÁ

EILEEN ANDREA ACOSTA PORRAS

WEB-GIS VISUALIZATION EMPOWERING DECISION-MAKING:
A MODEL FOR ESTIMATING POLLUTANT LOADS AND GUIDING GOAL-ORIENTED ACTIONS IN WATER FRAMEWORKS

CURITIBA

2023

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Tese apresentada como requisito parcial para obtenção do Título de Doutor no Programa de Pós-Graduação em Engenharia de Recursos Hídricos e Ambiental, Setor de Tecnologia, Universidade Federal do Paraná. Área de Concentração: Engenharia Ambiental. Linha de pesquisa: Gestão, Monitoramento E Modelagem De Sistemas Ambientais

Orientador: prof. Drª. Regina Tiemy Kishi
Coorientador: PD Dr.-Ing. Stephan Fuchs

CURITIBA
2023

DADOS INTERNACIONAIS DE CATALOGAÇÃO NA PUBLICAÇÃO (CIP)
UNIVERSIDADE FEDERAL DO PARANÁ
SISTEMA DE BIBLIOTECAS – BIBLIOTECA DE CIÊNCIA E TECNOLOGIA

Porras, Eileen Andrea Acosta
Web-gis visualization empowering decision-making: a model for estimating pollutant loads and guiding goaloriented actions in water frameworks / Eileen Andrea Acosta Porras. – Curitiba, 2023.
1 recurso on-line : PDF.

Tese (Doutorado) - Universidade Federal do Paraná, Setor de Tecnologia, Programa de Pós-Graduação em Engenharia de Recursos Hídricos e Ambiental.

Orientador: Regina Tiemy Kishi
Coorientador: Stephan Fuchs

1. Água-Qualidade. 2. Paranapanema, Rio, Bacia (SP e PR). I. Universidade Federal do Paraná. II. Programa de Pós-Graduação em Engenharia de Recursos Hídricos e Ambiental. III. Kishi, Regina Tiemy. IV. Fuchs, Stephan. V. Título.

Bibliotecário: Leticia Priscila Azevedo de Sousa CRB-9/2029

MINISTÉRIO DA EDUCAÇÃO
SETOR DE TECNOLOGIA
UNIVERSIDADE FEDERAL DO PARANÁ
PRÓ-REITORIA DE PESQUISA E PÓS-GRADUAÇÃO
PROGRAMA DE PÓS-GRADUAÇÃO ENGENHARIA DE
RECURSOS HÍDRICOS E AMBIENTAL - 40001016021P0

TERMO DE APROVAÇÃO

Os membros da Banca Examinadora designada pelo Colegiado do Programa de Pós-Graduação ENGENHARIA DE RECURSOS HÍDRICOS E AMBIENTAL da Universidade Federal do Paraná foram convocados para realizar a arguição da tese de Doutorado de **EILEEN ANDREA ACOSTA PORRAS** intitulada: **Web-GIS Visualization Empowering Decision-Making: A Model for Estimating Pollutant Loads and Guiding Goal-Oriented Actions in Water Framework**, sob orientação da Profa. Dra. REGINA TIEMY KISHI, que após terem inquirido a aluna e realizada a avaliação do trabalho, são de parecer pela sua APROVAÇÃO no rito de defesa.
A outorga do título de doutora está sujeita à homologação pelo colegiado, ao atendimento de todas as indicações e correções solicitadas pela banca e ao pleno atendimento das demandas regimentais do Programa de Pós-Graduação.

CURITIBA, 11 de Dezembro de 2023.

Assinatura Eletrônica
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This thesis is dedicated to all the moms who work hard to find their spot in science, juggling many tasks and responsibilities in their lives.

To my children Mati and Wara.

To my husband Maciel Batista Paulino who accompanied me and didn't let me give up.

ACKNOWLEDGMENTS

First and foremost, I would like to express my profound gratitude to Regina Tiemy Kishi, my advisor, your patience, and encouragement were fundamental to the success of this work. To Stephen Fuchs, my coadvisor, whose knowledge was vital throughout the research process.

I also extend my thanks to the members of my examining committee, Cristovão Fernandes, Tobias Bleninger, Gabriel Pereira, Marcelo Souza and Se Jong Cho, for dedicating their time and expertise to evaluate this work and provide valuable insights and suggestions. Not just scientific but also encourage me when I needed it the most.

Furthermore, I would like to acknowledge my project colleagues and collaborators, whose contributions and discussions enriched my work and broadened my understanding of the subject: Specially to Alana, Gabriel and Tiago, not forgetting to mention also Julio, Alexei, João, Dani, Bruna, Camila, Arthur, and other teachers that helped us to coordinate this special challenge.

Obviously, I need to thank the institutions and people that made the project possible for Elaboration of Study of Implementation and Application of Hydrodynamic and Quality Models of Surface Waters of Federal Domain as support for Decision Making in Framework Proposal, the UFPR, and the National Water Agency (ANA). Including the people behind the conception of the whole project: Irani Santos and Cristovão from UFPR, and Marcelo Souza and Diana Cavalcanti from ANA.

To PPGERHA, the program that accepted me and allowed me the opportunity to pursue and advance this research in modeling.

I cannot express enough gratitude to my husband, Maciel, who dedicated uncountable hours to reviewing my English, offering great advice, and providing emotional support and encouragement throughout my research journey, especially during the most challenging periods. His devoted belief in me inspired me to follow ahead.

To my work colleagues who helped and supported me during the time I was balancing between my PhD life and my work: Izabela, Maitê, Bruna, Mari, Milena, Ariane, Marilia, Enaylle, Fronza, Arley, Petry, Silvia, Edenise, and everyone I worked with The Nature Conservancy during this time.

I wish to express my appreciation to my unconditional friends (almost family)

who stayed with me and inspired me and supported me to reach the end of my journey: Patricia, Oranys, Nico, Viviane, Edson, Ive, Geovani, Liara, and Alan.

Also, to my friends that were an inspiration in one or more stages of my research: Maria José, Luis, Joelma, Nocy, Jaime, Se Jong, Bárbara, Luci, and Steph.

Last, but not least, I wish to express my acknowledge to my parents, my sisters Cin y Karo, my brother David, and my kids Wara and Matias.

RESUMO

Garantir o equilíbrio entre a demanda e o fornecimento de água de qualidade através do planejamento de bacias é fundamental para o bem-estar da população. O verdadeiro desafio está em compreender a origem da poluição pontual e difusa, assim como na identificação dos mecanismos pelos quais as substâncias alcançam os corpos d'água. Embora muitos estudos tenham sido realizados com o intuito de aprimorar metodologias que garantam um ambiente ecologicamente saudável, persistem desafios significativos para as comunidades científicas, tanto na modelagem quanto na precisão dos diagnósticos para embasar decisões de gerenciamento ambiental. Para aprofundar a compreensão das vias de poluição, o presente trabalha apresenta um estudo de caso, onde se aplica uma modelagem simplificado, baseado em dados, para estimar as cargas difusas e pontuais na bacia do rio Paranapanema, abrangendo os estados do Paraná e São Paulo. Esse modelo utiliza dados biofísicos, informações de licenciamento, dados de campo, censos, atlas e taxas per capita para calcular as cargas totais que podem afetar o corpo d'água. Os resultados da pesquisa mostram fornecem uma visão das quantidades de carga por unidade de análise, contribuindo para a priorização de ações e identificação das principais fontes e vias de poluição. Além disso, os resultados foram processados e apresentados num sistema WEB-GIS que permite que a avaliação de diferentes cenários de intervenção e possibilitam uma compreensão mais precisa pelos tomadores de decisão e instituições governamentais. Portanto, o objetivo primordial desta pesquisa foi desenvolver um modelo para estimar as cargas de poluentes, permitindo a identificação de suas fontes, sejam elas difusas ou pontuais. Este modelo pode servir como uma ferramenta crucial na definição e monitoramento de metas de conformidade, além de auxiliar na priorização de ações necessárias para manter ou atingir a qualidade desejada em cada segmento do corpo d'água.

Palavras-chave: enquadramento da qualidade da água; Bacia do Paranapanema; Cargas difusas e pontuais; Modelagem regionalizado de emissões (MoRE); WEB-GIS; Sistema de suporte à decisão.

ABSTRACT

Ensuring the balance between the demand and supply of quality water through basin planning is fundamental for the well-being of the population. The real challenge lies in understanding the origin of both point and diffuse pollution, as well as in identifying the mechanisms through which substances reach water bodies. Although many studies have been conducted to improve methodologies that ensure environmentally healthy surroundings, significant challenges persist for scientific communities, both in modeling and in the accuracy of diagnoses to support environmental management decisions. To intensify the understanding of pollution pathways, this work presents a case study where a simplified data-based modeling approach is applied to estimate diffuse and point loads in the Paranapanema river basin, covering the states of Paraná and São Paulo. This model utilizes biophysical data, licensing information, field data, censuses, atlases, and per capita rates to calculate the total loads that can impact the water body. The research results provide insights into load quantities per unit of analysis, contributing to action prioritization and identification of primary pollution sources and pathways. Furthermore, the results have been processed and presented in a WEB-GIS system, allowing for the evaluation of different intervention scenarios and providing a more precise understanding for decision-makers and governmental institutions. Therefore, the primary objective of this research was to develop a model to estimate pollutant loads, enabling the identification of diffuse and point sources. This model can serve as a crucial tool in defining and monitoring compliance goals, as well as in prioritizing actions necessary to maintain or achieve the desired quality in each segment of the water body.

Keywords: Water Quality Framework; Paranapanema Basin; Diffuse and Point Loads; Regionalized Emissions Modeling (MoRE); WEB-GIS; Decision Support System.

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LIST OF ACRONYMS

AGNPS	Agricultural Non-Point Source Pollution Model
ANA	National Water Agency (*Agência Nacional de Águas)*
APEX	Agricultural Policy/Environmental eXtender Model
CNRH	National Water Resources Council (*Conselho Nacional de Recursos Hídricos*)
Conama	National Council for the Environment (*Conselho Nacional do Meio Ambiente*)
CPRM	Geological Survey of Brazil (*Companhia de Pesquisa de Recursos Minerais*)
DAEE	Department of Water and Electric Energy (*Departamento de Águas e Energia Elétrica*)
DEM	Digital Elevation Model
EAA	The European Environmental Agency
EPA	Environmental Protection Agency
ETE	Wastewater Treatment Plant (*Estação de tratamento de Esgoto*)
FAO	Food and Agriculture Organization
GEE	Google Engine
GIA	Integrated Aquaculture and Environmental Studies Group (*Grupo Integrado de Aquicultura e Estudos Ambientais*)
GSSHA	Gridded Surface Subsurface Hydrologic Analysis
HSPF	Hydrological Simulation Program – Fortran
IAT	Water and Land Institute (Instituto Água e Terra)
InVEST	Integrated Valuation of Environmental Services and Tradeoffs
IWRM	Integrated Water Resources Management
LSPC	Loading Simulation Program in C++
LULC	Land Use Land Cover
MCDA	Multi-Criteria Decision Analysis
MDE	Modelo Digital de Elevação Digital
MoRE	Modeling of Regionalized Emissions
NPS	Non-Point Source Pollution
PIRH	Integrated Water Resources Management Plan (*Plano Integrado de Recursos Hídricos*)
PLOAD	Pollutant Loading Application Overview
PNRH	National Water Resources Policy (*Política Nacional de Recursos Hídricos*)
RIMAS	Rede Integrada de Monitoramento das Águas Subterrâneas
ROI	Return Of Investment
SCS	Soil Conservation Service
SDR	Sediment Delivery Ratio
SNGRH	National Water Resources Management System (*Sistema Nacional de Gerenciamento de Recursos Hídricos*)
SPARROW	Spatially Referenced Regressions On Watershed attributes

SRTM	Shuttle Radar Topography Mission
STORM	Storage, Treatment, Overflow, Runoff Model
SWAT	Soil & Water Assessment Tool
SWIM	Soil and Water Integrated Model
SWMM	Storm Water Management Model
UGRH	Water Resources Management Unit (*Unidade de Gestão de Recursos Hídricos*)
UNESCO	United Nations Educational, Scientific and Cultural Organization
USA	United States of America
USDA	United States Department of Agriculture
USEPA	United States Environmental Protection Agency
USLE	Universal Soil Loss Equation ou Equação Universal de Perda de Solo
WARMF	Watershed Analysis Risk Management Framework
Web-GIS	Web Geographic Information Systems
WEEP	Water Erosion Prediction Project
WHO	World Health Organization
WQS	Water Quality Standards
WWTP	Wastewater Treatment Plant

LIST OF ABBREVIATIONS AND SYMBOLS

BOD / DBO	Biological Oxygen Demand / *Demanda Biológica de Oxigênio*
g	grams
ID	Unique Identifier
kg/dia	Kilogram per day (*Quilograma por dia*)
Kg/km^2/day	Kilogram per day per square kilometer (*Quilograma por dia por quilômetro quadrado*)
km^2	Square kilometers
m^3/s	Cubic meter by second
mg/kg	Milgram by kilogram
mg/L	Milligrams by liter
MJ·mm/(ha·h)· year)	Megajoules by millimeter in a hectare per year by year
TN /NT	Total Nitrogen / *Nitrogênio Total*
TP / PT	Total Phosphorus / *Fósforo Total*
t/ year	Tons by year
t/(ha·year) / t/(ha·ano)	Tons by hectare by year / Toneladas por hectare por ano
t·h/(MJ·mm)	Tons by hour by megajoules by millimeter

SUMMARY

1 INTRODUCTION

The anthropogenic uses and occupation of the river basin result in perturbations in the freshwater natural equilibrium manifesting in various ways, such as, accelerated erosive processes, water pollution (Von Sperling, 1996), alterations in the fluvial regime (Gomes et al., 2021), groundwater depletion (Marques et al., 2020), and loss habitat for freshwater biodiversity (Pereira Lima-Junior et al., preprint).

The problems related to water scarcity and quality are concerns for Brazil particularly in semi-arid regions where exist a natural scarcity and in localities with high-water demand like cities or irrigated areas. These problems could be related to natural availability but also to modifications in the climate patterns, like a severe drought that extended from 2012 to 2017, and in 2020 in a large part of Brazil (ANA, 2021; Grimm et al., 2020). Also, in places with high demand the problem is related to a sum of factors that also encompasses an effective response from authorities to crisis, effective governance, control and consequently quick and clear access to information (Nobre et al., 2016; Beard et al., 2022).

The water availability is the result of the characteristics of the river basin and also could be affected by pollution (ANA, 2021). Over time it is possible to observe emerging issues related to water quality. In 2020, the contamination of the Guandu river (principal supply system for Rio de Janeiro) was attributed to high levels of geosmin resulting from sediments runoff due to land use and land cover (LULC) changes upstream (Bacha et al., 2023). Another example is the Piracicaba River in the State of São Paulo where water pollution arises from urbanization, agriculture, and industrial activities (Madeira et al., 2023). The mining industries also represents a big problem as seen in the Paraopeba river where a tailings dam collapsed in 2019 led to pollution (Parente et al., 2021), and in 2023 the potable water taken from Paraopeba to supply Congonhas municipality was polluted with iron (FE), also for mining waste (Calisto et al., 2023). Additionally, the collapse of another tailings dam in Mariana in 2015 had contaminated about 660 kilometers in the Rio Doce basin, and its adjacent estuarine area (Calisto et al., 2023).

Despite the existence of clear rules and laws regarding water, such as the Water Code and the Water Resources Law, there is a lack of effective implementation. There remains the necessity to generate information to recognize the processes of pollution and the intrinsic vulnerabilities of the system. The appropriate transfer of information to the decision makers about the processes involved in river pollution, including sources, transportation, and the interaction of contaminants with river systems allow a more rational and sustainable strategy for the management of river basins (Kan *et al.*, 2019; Uusitalo *et al.*, 2015; Vrugt *et al.*, 2005). Authorities responsible for managing and using the basin's resources have the task of analyzing different possible situations and assessing the likely consequences of proposed strategies for control measures, as well as land use and occupation.

To attend the complexity inherent to water quality, mathematical models are often employed to assist in decision-making processes. These models allow to simulate process, predict and assessment various scenarios to analyze the impacts of LULC modifications in the basin, actions implemented and sometimes the river assimilative capacity. Advances in computing and technology allow for the development of increasingly complex deterministic and distributed models that consider both spatial and temporal variability. (Uusitalo *et al.*, 2015; Tucci, 2005).

However, the models are simplified representations of reality (Chapra, 2003), and their application may be constrained by computational capacity, data availability and uncertainty related to equations modeling process or errors in input data. A complete and comprehensive model would require an immense amount of data and would become impractical to apply. This is observed in practice in two ways: In many situations, there is a lack of measured data series that are sufficiently and simultaneously collected to estimate loads; and another way there are a lot of processes that occur at a landscape or ground level that is not possible to have accurately.

It's not surprising, given these limitations, that there are different models for the same phenomenon, varying both in their formulation and input data. Each model may have the same objective, but it must deal with different levels of uncertainty associated with the input data and the simplifications introduced in the model. Any errors or lack of input data combine within the modeling steps, leading to the propagation of uncertainty throughout the model. As a result, the degree of uncertainty in the outcome is increased (Wang and Solomatine, 2019; Uusitalo *et al.*, 2015).

Within the process of managing a basin, it is expected that models provide a response with the least possible uncertainty, or that the manager is aware of the inherent degree of uncertainty, to support decision-making and enable the best possible solution to the problem. This would prevent the decision from leading to errors or introducing new potential risks or causing further harm (Uusitalo *et al*., 2015; Bremer *et al*., 2016; Vogl *et al*., 2017; Klein *et al*., 2016; Coelho *et al*., 2019).

There is indeed a real problem associated with the use of models. On one hand, effective basin management requires agile and sufficiently reliable modeling to justify decisions. On the other hand, engineers face limitations in data and intrinsic simplifications or assumptions of the model, which introduce uncertainty in the result.

1.1 Research problem:

Despite the existence of many models for estimating and quantifying loads, there are still significant challenges in understanding the results, uncertainty, and their utilization in defining load allocation goals in rivers. There is a lack of defining a model that encompasses all potential sources of pollutants in the local reality. Difficulty arises in accurately quantifying both point and diffuse sources of pollutant loads reaching water bodies, complicating effective management strategies. The issue lies not only in estimation methods, but also in obtaining an accessible and reliable database that can encompass all potential sources within the basin and integrate them into a single model that addresses the demands of basin management, within the necessary temporal and spatial scales. Most models were developed to estimate pollutants carried in surface runoff from agricultural or vegetative areas, and they do not have routines to assess emitted loads and identify which basins have the highest pollutant production and what the sources of this pollution are - an important demand of management. Existing models are either complex or do not cover all specific sources in the study area. However, it is increasingly important to assess all current and future uses of the basin, incorporating estimates of potential inputs from clandestine sewage, mining, fish farming, or even the efficiency of wastewater treatment plants, which are often not identified when defining compliance goals or in the definitions of actions to improve water quality, or even in the prioritization of watershed restoration actions, for example.

1.2 Objectives

1.2.1 General Objective

The purpose of the research is to enhance a pollutant load basin model, to estimate the amount and spatial distribution exportation of pollutants (diffuse and point source loads). The model result will serve as a tool for setting and monitoring Water Quality

Goals. It could help in decision-making processes, facilitating the prioritizing of actions to maintain or achieve the defined quality standards for each section of the water body.

1.2.2 Specific Objectives

•To determine an approach for diagnosing the main pathways of pollution, both point and diffuse, in Paranapanema river basin, overcoming the limitation of data availability while meeting management objectives.

•To produce an intrinsic characterization of the basins that allows decision-makers to have knowledge of the sub watershed with most contribution.

•To evaluate the potential of actions and the contribution of load modeling to basin management through the creation of Geographic Information System (GIS) implemented routines for Modeling of Regionalized Emissions (MoRE) to prioritize the basins and actions to be taken to assist in the definition of river segments within the study area.

•To develop a Web-GIS for decision making support, that facilitated the identifying the primary sources and pathways of pollution, prioritizing basins with the highest load production, and determining realistic possibilities of load reduction through effective measures.

2 THEORETICAL FRAMEWORK

2.1 Integrated Water Resources Management

The Integrated Water Resources Management (IWRM) was described as “a process that promotes the coordinated development and management of the water, land and related resources to maximize economic and social welfare in an equitable and sustainable manner” UN-Environment (2018).

While water management has ancient roots, it was primarily focused on storage, flood control, and irrigation in early civilizations (UNESCO, 2011), its evolution is marked by the incorporation of novel concepts or aspects in response to escalating needs. For example, with the hydroelectric demand and industrialization news regulations and agencies were necessary to control the resource (UNESCO, 2011). In the 1980's it was started to understand that water management needed to be “integrated”, including the delimitation by watershed, the integrations of all purposes, although the participations of relevant users and agencies (Irvine et al., 2010). In 1992, in the United Nations Conference on Environment and Development in Rio de Janeiro was highlighted the importance of be “sustainable”, based in the perception of water as an integral part of the ecosystem (United Nations, 1993). In the 20’s institutions World Bank, UNESCO, and the Food and Agriculture Organization (FAO) promoted IWRM in their water-related programs and projects (Savenije & Zaag, 2008).

However, is relevant to mention the necessity to keep the holistic view of IWRM not only qualitative and quantitative, demand and supply but also include: all the forms of water, the different water uses, and the scales temporal and spatial (Savenije & Zaag, 2008; Agarwal et al., 2000). The holistic view requires incorporating water in all its forms of occurrence, including saltwater, groundwater, fossil water, and so forward. Additionally, all the water uses, including economic, natural regulation, to sustain sociobiodiversity[1], river functions, cultural and recreational. Also, when Savenije & Zaag (2008) mention spatial refers to water resources issues at different political levels (federal, municipal, international level, etc) and the temporal scales refers to the hydrologic regime including floods, droughts, peak demands ecological patterns, etc. At the same time, Higgins et al., (2021) mentions the necessary to guarantee the components of integrity of

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[1] Sociobiodiversity: The concept refers to an integrated system of nature and communities, including, in a broader perspective, efforts in order to raise awareness about the use of natural resources and equal distribution to all beneficiaries in a territory (link).

systems (hydrologic regime, quality, biodiversity, habitat and connectivity of the river) to maintain the good ecological status of resources.

Unfortunately, future projections only increase the list of places facing water crisis. It is anticipated that by 2025, more than half of the population may experience water stress, whether due to availability, lack of potable water, or increased demand (World Health Organization - WHO, 2017; Crawford, 2017). At the 2023 UN Water Conference in New York, it was already appointed that more than 50 per cent of the world's cities and 75 per cent of all irrigated areas are experiencing recurring water shortages (United Nations, 2023).

In the Brazilian context, problems related to water resources have intensified due to climate change and increased consumptive demands (ANA, 2019), triggering water supply crisis in major cities (Grimm et al., 2020) and conflicts over usage (McGrane, 2016). Examples in Brazil are São Paulo's water shortage from 2015-2016 (Millington, 2018) and the Federal District crisis in 2016-2019, resulting in conflicts between urban residents and irrigators, impacting both water supply and energy generation (Diniz, 2019). In 2020, Curitiba's metropolitan region was affected by the reduction of water resources, prompting the Paraná Sanitation Company to implement a rotational water supply system, leading the Government of Paraná to declare a state of water emergency (Carvalho et al., 2022).

Given the evidence of the decrease in water availability, mainly resulting from environmental pollution and population growth demand, mechanisms and guidelines are needed to regulate water usage, including all ecological processes and systems that depend on it.

However, in 2015, the United Nations (2015) defined the 2030 Agenda for Sustainable Development 17 Sustainable Development Goals and 169 targets. The Goal 6: Ensure availability and sustainable management of water and sanitation, and other that depend on IWRM to be able to reach. In 2023 at UN Water Conference New York, still observed the necessity of give more attention to IWRM to reach the Sustainable Development Goal targets that including sustainable water (Goal 6 and Goals 2,8,9,11 and 12) (United Nations, 2023; United Nations, 2023b). The current challenge is to try to maintain or improve the availability of water resources, focusing not only on preserving the volume but also on improving the quality of degraded water bodies and ensuring the resource for the future.

2.1.1 Legal and Institutional Frameworks

Effective IWRM is guided by a set of fundamental principles, including equitable access, ecosystem protection, and integrated planning. These principles provide a framework for sustainable water use and allocation. The concern to establish management mechanisms began around 1850 due to the degradation issues of water bodies caused by the peak of the Industrial Revolution in Europe. Later, the United States and Canada joined this initiative, establishing classification criteria based on the physical, chemical, and biological variables of water bodies (Newman et al., 1994 apud LACTEC; FINEP, 2007).

All the countries have different strategies and concerts about water resources. In the USA the principal instruments are the Clean Water Act of 1972 (United States Congress, 2018) and Safe Drinking Water Act of 1974 (United States Congress, 1996) achieved to restore and maintain the chemical, physical, and ecological integrity of the Nation’s waters (Brown, 2019). The Environmental Protection Agency (EPA) supervises the implementation of these laws and standards for water quality.

In Europe's the Water Framework Directive (2000/60/EC) was adopted as a pioneering approach to protecting water based on the river basins (EUROPEAN UNION, 2000). The framework aimed at achieving "good ecological status" for all water bodies within the European Union, including the ecological status, the chemical for surface water, the chemical for groundwater and the quantitative status of groundwater (European Environment Agency, 2018). The European Environmental Agency (EAA) is who is supporting policy development and key global processes providing and maintaining an efficient reporting infrastructure for national and international data flows.

While both the United States of America (USA) and Europe share the objective of achieving sustainable water management, they differ significantly in their approaches. The USA employs a regulatory-centric model, focusing on pollution control and compliance, and Europe adopts an ecosystem-based approach, emphasizing holistic management and stakeholder participation.

In Brazil, a concern for water resource management dates back to 1934 with the increased use of hydroelectric energy for industries, which prompted the creation of the so-called Water Code (Decreto Nº24.643,1934). This code addressed primarily economic and the rational use of water resources. In the subsequent years, the development patterns of countries and the increase in population added to the national and international discourse, themes regarding the importance of ensuring water availability with quality for the future. It was then defined that it is crucial to assess basins, taking into consideration both groundwater and surface water, multiple uses, food security, health, and the balance of ecosystems.

According to the National Water Agency – ANA (2002), the process evolved through a series of discussions and statements from various institutions that recognized the need for the creation of a national water resources system and the improvement of relevant legislation. Each state had started a management process, but during the evolution of the process, the need for integration in large basins such as the Paraíba do Sul and the Amazonas became evident, as the basin boundaries extended beyond state borders.

Efforts to have a legal instrument that ensured the availability of water in suitable conditions were realized when the National Water Resources Policy was defined, along with the establishment of the National Water Resources Management System through Law No. 9,433 (Brazil, 1997).

The Law No. 9,443 also already provides instruments that allow the establishment of parameters and indicators to monitor and control the quality of rivers:

> *"i) Water Resources Plans; ii) the categorization of water bodies into classes, according to their predominant uses; ii) Authorization of water resource use rights; iv) Charge for the use of water resources; v) Compensation to municipalities and vi) Water Resources Information System" (Brazil, 1997).*

Brazil also employs a decentralized approach, involving state and local agencies in water management.

2.1.2 Water Quality Framework: The classification of water bodies into classes

Water Quality Framework typically refers to a structured approach or set of guidelines used to assess, monitor, and manage the quality of water in a particular area or for a specific purpose. This framework often includes elements such as defining quality parameters, setting water quality standards or goals, establishing monitoring programs, implementing management practices, and responding to any deviations from desired quality levels.

In Brazil the legislation already accounts for this, considering the classification of water bodies into classes of predominant uses as one of the instruments for implementing the National Water Resources Policy. This establishes quality levels to be achieved or maintained in water bodies over time. The law establishes the classification of water bodies into classes of predominant uses aims to:

> *"i) Ensure that the water quality is compatible with the most demanding uses to which it is destined and ii) Reduce the costs of combating water pollution through permanent preventive actions" (Brazil, 1997)*

At the same time, Resolution Conama 357 (2005) stipulates that classification should be based not necessarily on their current state, but on the desired quality levels to meet the community's needs.

To establish classification goals, decision-makers need tools that help them understand the intrinsic characteristics of the area and the hazards that threaten the established water quality goals, or to analyze the changes to be made to achieve the established goals (Sun et al., 2021). Within this process, a typical course of action is usually established, starting with the definition of a diagnosis, followed by a prognosis, and finally, the goals and strategies. In Brazil, the classification of water bodies is divided into four main stages: i) basin diagnosis, ii) basin prognosis, iii) development of a classification proposal, and finally iv) analysis and deliberation by the basin committee and the Water Resources Council (ANA, 2009).

The basin diagnosis, which implies the understanding of the current conditions, characteristics and challenges of the basin is one of the most complex stages, mainly due to the lack of updated databases. The systematization of information about pollutant loads becomes a challenge due to the scarcity of monitoring data and measurements of diffuse pollution in the field.

The basin prognosis that refers to the assessment and projection of future conditions, trends, and scenarios for a river basin or watershed.

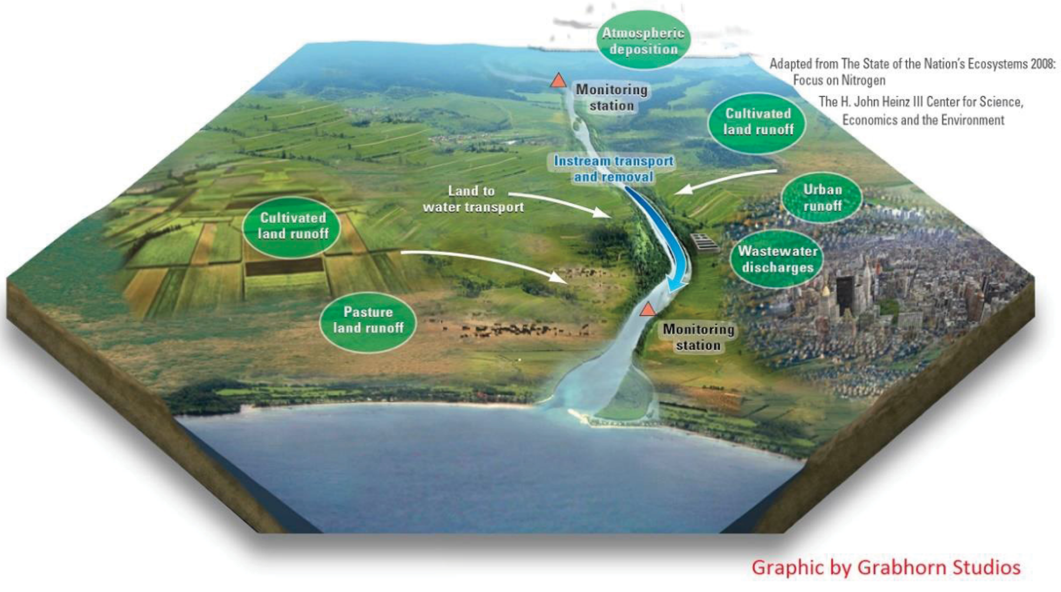
The classification of water bodies, according to their predominant water uses and the Water Resources Information System, is directly related to this research. The classification was based on two federal resolutions: CONAMA Resolution No. 357/05 and CNRH Resolution No. 91/08. CONAMA Resolution No. 357/05 assigns classes from 1 to 4 (from better to worse quality, respectively) to identify the environmental quality of rivers according to their predominant uses and establishes limits for various parameters (Brazil, 2005).

The National Water Resources Council Resolution CNRH No. 91/08 outlines the steps to be followed in a classification study. Classification should be based on the quality required by the demanded water uses (current and future) and should not be based on the current quality presented by the river (Brazil, 2008). Therefore, this instrument should ensure that water quality is compatible with the most demanding use located in the basin, thus guaranteeing pollution reductions according to the needs established by society (Machado et al., 2019).

2.2 Water Pollution and pathways

Water pollution is a term associated with the physical, chemical, and biological characteristics of water, and it is linked to a quality standard established for ecological or human use purposes. Since water is a vital resource for life and the economy, and serves as the recipient of all emissions, whether natural or not, water bodies are at great risk of pollution and scarcity. Management is the key to their protection.

FIGURE 1 – PATHWAYS AND SOURCES OF POLLUTION



SOURCE: USGS (2017)

The impacts of human activities on water resources begin because of the overexploitation of the resource, as naturally, water body have the capacity for self-purification. The water body is regulated by various processes such as dilution, sedimentation, atmospheric aeration, oxidation, and decomposition (Von Sperling, 1996; Andrade, 2010).

Pollution occurs when an imbalance is caused by the entry of pollutant loads that exceed the water body's capacity to recover, resulting in damage to natural resources, aquatic organisms, and hindrance to economic activities. However, it can also be caused not only by the introduction of substances but also by excessive extraction of water volume from the water body, leading to an increase in pollutant concentrations (Carapeto, 1999).

The increase in concentrations of substances creates a disturbance that disrupts the physical and biological processes of rivers and reservoirs, potentially causing short, medium, or long-term effects on organisms. These pollutants also have consequences on water bodies, altering oxygen levels, increasing turbidity, leading to eutrophication due to nutrient enrichment, causing mortality in biotic communities, and promoting the proliferation of macrophytes and other effects (Esteves, 2011; Horne, 1994).

Since the concentration behaves differently over time and space within the water body, reaching critical concentrations will depend on the rate of occurrence of these processes. Environmental conditions, especially external loads entering the water column, or even internal ones, such as contaminated sediment in riverbeds, which under certain conditions may return to the water column, can also become a significant source of water pollution.

The inclusion of a characterization and recognition of pollution sources, both point and diffuse, can be an alternative to establish a spectrum of degradation (Pizella and Souza, 2007). Furthermore, it provides support for defining source control measures.

Point source loads are defined as pollutant discharges that are directly released into the water body, usually through a pipe or channel, with identifiable spatial location. Currently, the main point sources are discharges from sewage treatment plants, industrial effluents, and urban stormwater drainage systems (Thomann e Mueller, 1987; Sperling, 1996).

Diffuse loads refer to the type of contamination that does not have a specific point of discharge into the water body, originating from sources that cannot be easily located or verified, generated in a distributed manner across the surface. They generally reach the water body through surface runoff or movement of groundwater and atmospheric deposition (Eiger *et al*., 1999; Pizella e Souza, 2007).

Non-Point Source Pollution (NPS) from agriculture is one of the main causes of deterioration in rivers and streams in Brazil. Although diffuse loads have been the subject of intensive research, several models have been developed throughout Brazil. Results without source identification do not provide a conceptual understanding for managers and those responsible for water quality management planning. This is particularly crucial for large basins where it is necessary to allocate and define mitigation activities.

2.3 Estimating diffuse and point source pollutant loads and the sources

There are several models available to determine pollutant loads. The widely used models are those that estimate diffuse loads in agricultural areas, like Water Erosion Prediction Project (WEEP) by USDA (1995), the Soil and Water Integrated Model (SWIM) detailed by Krysanova et al. (2022), the Pollutant Loading Application Overview (PLOAD) as described by United States Environmental Protection Agency (USEPA, 2001), Agricultural Non-Point Source Pollution Model (AGNPS) by Finn et al. (2003), and the Agricultural Policy/Environmental eXtender Model (APEX) described by Waidler et al. (2011). Other models can incorporate estimations also for natural area like the Integrated Valuation of Environmental Services and Tradeoffs (InVEST) developed by Sharp et al. (2016), and the Gridded Surface Subsurface Hydrologic Analysis (GSSHA) by Downer et al. (2008).

However, the increase in industrial activities, rapid urbanization, lack of domestic effluent treatment, and intensification of agriculture, demand models that could predict the loads also from point sources. Some models like the Storm Water Management Model (SWMM) by Rossman (2015) and the Storage, Treatment, Overflow, Runoff Model (STORM) developed by US Army Corps of Engineers (1977) are often used for determining pollution in urban areas.

Nevertheless, Pizella and Souza (2007) emphasizes the importance of recognizing the contribution to water quality issues not only from point but also for diffuse sources. Currently, there is a growing effort to develop models that encompass the estimation of loads from various sources. Some models include the possibility to estimate both, diffuse and point loads, like Soil & Water Assessment Tool (SWAT) by Neitsch et al. (2011), Modeling of Regionalized Emissions (MoRE) by Fuchs et al. (2012), the Hydrological Simulation Program – Fortran (HSPF) developed by Johanson et al. (1984) and Loading Simulation Program in C++ (LSPC) by Tetra Tech (2017).

Finally, models such as the SPAtially Referenced Regressions On Watershed attributes (SPARROW), developed by Schwarz et al. (2006), utilize statistical techniques to estimate pollutant from point and nonpoint sources on land to through the stream and river network, from the watershed characteristics and monitoring data non-linear regression.

Hydrological models are one of the tools that science has developed to better understand and represent the behavior of a watershed and to predict conditions different from those observed (Tucci, 2005, Pinto, 2011). Models are tools that can be valuable in decision-making and analyzing the objectives of water resources management plans (Cho et al., 2019; Hamel et al., 2020; Dinar & Quinn, 2022). Although the choice between different models depends on our objectives, ranging from calculating about daily pollution loads predictions, estimation of ecosystem services, definition of priorities, and trade-offs (Dennedy-Frank et al., 2016; Cong et al., 2020), and also for calculation the effect of modification in LULC (Liu et al., 2022; Rao et al., 2007; Baker, 2014).

In a study by Vogl et al. (2017) InVest model was employed to map the production of sediments until they reach the water body to assess the benefits of its implementation Natural based Solutions (NbS). The study demonstrates how modeling can effectively identify erosion areas and prioritize actions in sub-watersheds to improve the water quality. Additionally, Fisher et al. (2018) presented an example where SWAT was used in the Camboriú watershed in south of Brazil, to evaluate the impact of LULC classification and resolution in the sediment loads prediction. The study also shows how modeling could be used to influence decision makers especially in terms to show them which is the return of investment (ROI) for water treatment in the municipality (Fisher et al., 2018; Kroeger et al., 2019). Similar studies were carried with SWAT for other authors (e.g., Blainski et al., 2017; Dos Santos et al., 2010; Acosta et al., 2023).

However, hydrological models are simulations of a complex reality that have many uncertainties, and in some cases, it is necessary to work very hard in flow calibration to understand the model limitations. In a Study by Chen et al. (2019) SWAT and HSPF were compared to predict the impact and uncertainty of expansion of urban areas and reduction of cropland and on the runoff in three scenarios (1985, 2002, 2014). The study indicated increases in annual and monthly discharges due to urbanization and decrease in annual 7-day minimum discharge consistent with other studies (e.g., Liu et al., 2023; Acosta et al., 2023). In most of them they don't evaluate the effect in quality despite it's possible once the water component is calibrated.

While it is true that, to have a load estimation, it is necessary first to calibrate the hydrological components in year, monthly, daily our hourly basis, sometimes is important to obtain a deep understanding of the requirements of decision-makers prior to model selection. This ensures alignment of the main purpose with the model complexity optimizing effort, time, and cost (Hamel, et al., (2020), Vogl et al. (2017) and Cho et al. (2023). Often, they require the production of the minimum viable scientific product to take the best decision (Hamel, et al., 2020). This information was corroborated by Cong et al. (2020) in their comparative study between InVEST and SWAT. Both models provided similar spatial pattern estimates, hot spot distributions and trade-off relations for determining hydrological ecosystem service, although INVEST is simpler than SWAT.

One of the questions of this research was understanding the importance of all the sources of pollution and the spatial distribution of the basin. In a study carried by Robertson et al. (2019), SPARROW Watershed Models was implemented to estimate the Phosphorus (P) and Nitrogen (N) transport and spatial distribution for the Great Lakes contribution basins. The results show where and from what sources the nutrients originate, showing for example that the importance of Wastewater Treatment Plant (WWTP) effluent, urban and open areas, manure atmospheric deposition and agriculture Contributions for the lakes contamination. Similar studies were carried also by Acosta P et al. (2016) with MoRE for Alto Iguaçu River showing the importance in contribution of phosphorus is about 50% from urban and open areas and form WWTP effluent, and corroborate by Sotiri et al. (2022) in a study more specific about phosphorus input from urban areas. The two models were used by the national agencies to influence decisions about water quality. In the U.S. Geological Survey report by Saad et al. (2019), is estimated the Nutrient and Suspended-Sediment Loads for United States, and in the German Environment Agency report by (Fuchs & Brecht, 2022) is explain the principal results from MoRe phosphorus estimative.

As stated by Pinto (2011), modeling can also simulate future scenarios of land use and occupation, which can provide support for implementing conservation practices for sustainable development. In the Table 1, there is a summary about the different models mentioned showing a comparative between input and output data, application area and resolution temporal and Spatial.

TABLE 1 – LIST OF COMMON MODELS USED FOR POLLUTANT WATERSHED MODELING

Description /	Model or framework	InVest[1]	SWAT[2]	PLOAD[3]	MoRE[4]	SPARROW[5]	HSPF[6]	SWMM[7]	AGNPS[8]	STORM[9]	LSPC[10]	GSSHA[11]	WEPP[12]	SWIM[13]	APEX[14]
Input Data	Digital Elevation Model (DEM)	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		✓	✓	✓
	Land Use and Cover Data	✓	✓	✓	✓	✓		✓	✓	✓		✓	✓	✓	
	runoff coefficients	✓	✓				✓	✓	✓				✓		✓
	Leaf area index and root depth		✓									✓	✓	✓	
	Soil Data or/and Soil Map	✓	✓	✓	✓	✓	✓			✓	✓	✓	✓	✓	✓
	Climate Data/Precipitation/IDF	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
	Historical streamflow data		✓	✓	✓	✓		✓	✓	✓	✓	✓			
	Historical quality data, parameters		✓			✓	✓			✓	✓				
	Reservoir Data		✓			✓	✓				✓	✓		✓	✓
	Best Management Practices	✓	✓	✓	✓		✓		✓		✓		✓	✓	✓
	Crop Parameters														✓
	Livestock and Animal Waste														✓
	Phosphorus Loading Coefficients			✓											
	Pest and Disease Data														✓
	Sediment/Nutrient Retention Coefficients	✓													
	Point and Diffuse Source pollutants		✓		✓		✓	✓	✓	✓	✓		✓		
	Population and Demographic Data				✓										
	Calibration and Validation Data	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
	Stream Network Data					✓	✓	✓						✓	
	Travel Time Data					✓									
	Groundwater data, infiltration				✓		✓					✓		✓	
	Hydraulic Data, Channel data							✓		✓	✓	✓	✓	✓	✓
	Stormwater Management Practices									✓					
	Attenuation Coefficients					✓									
Area of Application	Urban areas		✓		✓		✓	✓		✓	✓				
	Natural areas	✓	✓		✓		✓				✓	✓			
	Agricultural areas	✓	✓	✓	✓		✓		✓		✓	✓	✓	✓	✓
	Watersheds scale		✓	✓	✓	✓								✓	✓
outputs	Transport of pollutants in water		✓			✓	✓	✓			✓	✓			✓
	Pollutants subsurface flow											✓			
	Quantity of stormwater runoff							✓		✓					

	Description / Model or framework	InVest[1]	SWAT[2]	PLOAD[3]	MoRE[4]	SPARROW[5]	HSPF[6]	SWMM[7]	AGNPS[8]	STORM[9]	LSPC[10]	GSSHA[11]	WEPP[12]	SWIM[13]	APEX[14]
	Quality on runoff / pullotographs							✓		✓					
	Point source pollutants loads		✓		✓		✓	✓	✓		✓			✓	✓
	Diffuse source pollutants load	✓	✓		✓	✓	✓	✓	✓		✓		✓		
	Scenarios	✓	✓		✓	✓							✓	✓	✓
	Nutrients	✓	✓	✓*	✓	✓	✓		✓		✓	✓			✓
	Pesticides		✓		✓		✓		✓						✓
	Sediments	✓	✓			✓	✓		✓				✓		✓
	Soil erosion	✓	✓				✓		✓				✓		
	Streamflow		✓			✓	✓	✓	✓			✓			✓
	Best Management Practices impact	✓	✓		✓		✓		✓		✓				✓
Resolution (spatial and temporal)	Daily or sub daily time step	▪	✓	✓		▪	✓	✓	✓	✓	✓	✓	✓	✓	✓
	Monthly time step or seasonal		✓	✓	✓				✓		✓		✓		
	Annual or annual average	✓	✓	✓	✓	✓			✓		✓		✓		
	Regional/ Large River basin		✓	✓	✓	✓	✓	✓				✓	✓		
	Local/ or small watershed		✓	✓	✓		✓	✓	✓	✓	✓	✓	✓	✓	✓
	Grided											✓			

*Just phosphorus

Source: Compiled by the author from [1]Sharp et al. (2016); [2]Neitsch et al. (2011); Arnold et al. (2012); [3]USEPA (2001); [4]Fuchs et al. (2012); [5]Schwarz et al. (2006); [6]Johanson et al. (1984); [7]Rossman (2015); [8] Finn et al. (2003); [9]US Army Corps of Engineers (1977); [10]Tetra Tech (2017); [11]Downer et al. (2008); [12]USDA (1995); [13]Krysanova et al. (2022); [14]Waidler et al. (2011)

All the models have their limitations often lie in the absence and use of simplifications for complex processes, such as nutrient retention, transport, sedimentation, groundwater recharge, among others (Kovacs e Honti, 2008). For example, InVest is capable of estimating nutrients and sediment exportation in the pixel, transport overland but doesn't estimate point sources loads from urban areas, industries (Vogl et al., 2015). Same as APEX, SWIM and WEEP.

Also, in Table 1 is presented how, MoRE, PLAD, InVest, STORM, LSPC, WEEP and SWIM lack a water routing algorithm. The SWAT has uncertainty in parameterization and complicated calibration, also estimation problems in areas with high slopes. Additionally, SWAT and MoRE requires a large amount of data (Fuchs et al., 2017).

However, despite of limitations SPARROW and MoRE are models designed to be used in decision-making and which allows us to offer guidelines to achieve a good ecological status of surface water bodies so that they meet defined quality standards results in a variety of scales (Fuchs *et al*., 2012; Schwarz et al., 2006). SPARROW requires a detailed network of stations with historical series for performing the regression that is not a reality for Brazil, and MoRE is an open source where the algorithms could be adapted to local reality (Schwarz et al., 2006).

2.4 Web-GIS for support decision

Currently, one of the biggest challenges in management is the lack of access to information in an agile, easy to interpret and interactive manner. Therefore, decision makers need computational tools where they can test alternative scenarios and such information supports the appropriate decision on defining framing goals (Machado et al., 2019; Quinn et al., 2022).

Numerous studies have documented the importance and benefits of integrating results into decision support tools (Rao et al., 2007; Kourgialas et al., 2022; Botha et al., 2023; Dinar & Quinn, 2022). The primary purpose of using a Web-GIS for decision support is to present information to the decision maker in an easy-to-use -understand way. The Web-GIS tools can help users visualize and analyze water quality standards, making it easier to understand and manage water quality data.

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3 METHODS

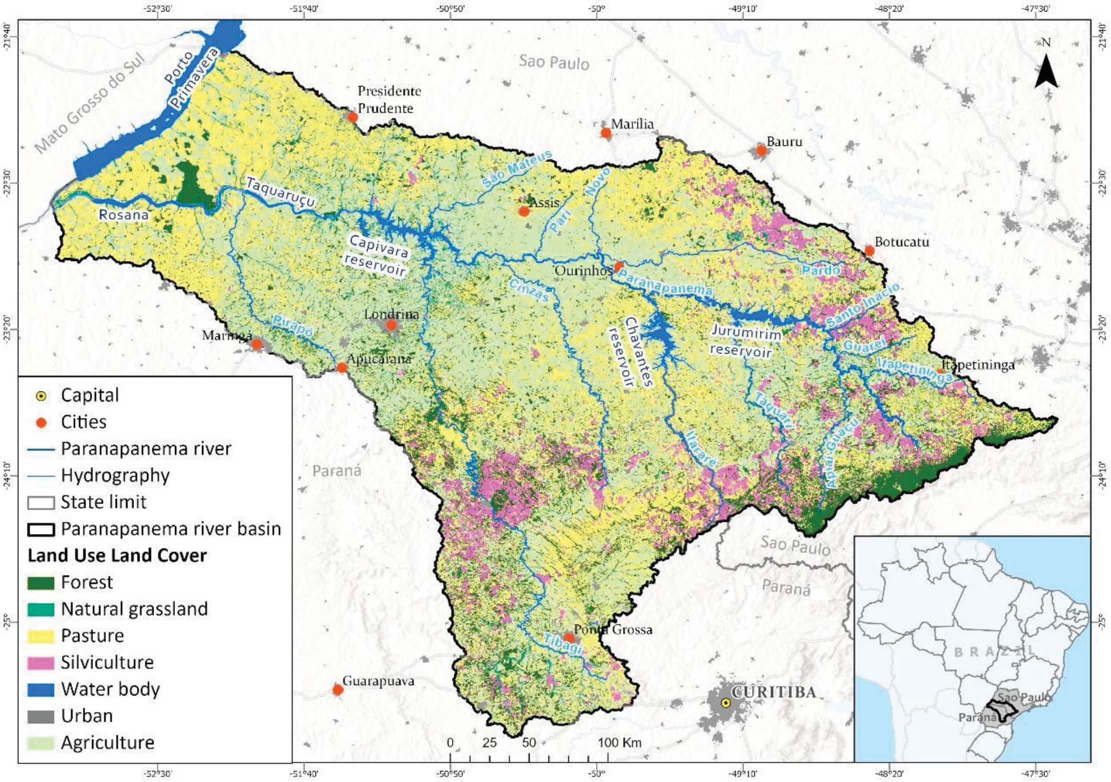
The research was structured in four phases. In the first phase, a model was implemented, aimed at the primary objective of estimating pollutant loads within the sub-basins. The modeling framework employed equations derived from the Model Regionalized emissions (MoRE) Fuchs (2012) and was adapted to the specific context of Brazil for Paranapanema river basin (Acosta et al. 2021; Rieke et al. 2021). In the second phase, a routine was developed within a Geographic Information System (GIS), using the MoRE algorithms adapted to Brazil. This routine was designed to streamline the processing of spatial data and calculations, enhancing overall efficiency. The third one was based on strategies and alternatives which were identified to encompass the classification of water bodies and the pollutant reductions. Finally, Web-GIS as a tool to present and consolidate the outcomes of the modeling results aiding in decision-making for defining framework goals (Acosta et al. 2023).

3.1 Study area

The study area is the Paranapanema River basin (Figure 2), which extends over approximately 900 kilometers in length, with a drainage area of about 100,800 square kilometers (ANA, 2016). It is an interstate basin of significant economic importance for two Brazilian states, São Paulo and Paraná. It is home to nearly 4.7 million inhabitants, primarily concentrated in urban areas. The primary economic activities are agriculture and livestock farming (occupying nearly 70% of the basin) and forestry plantation (8% of the basin). Natural areas consist of 14% native forest cover and 4% native pastures. The remaining territory, amounting to 4%, includes other activities such as industries, urban areas, and water bodies.

The Paranapanema Basin is an integral part of Brazil's interconnected electric power production and transmission system, contributing to approximately 6% of the capacity of the southeast/central-west subsystem (ONS, 2022). Three large reservoirs with multipurpose hydroelectric plants have been established, namely Jurumirim, Chavantes, and Capivara, which have altered the river's flow and, in conjunction with human activities, demand effective basin management to ensure water quality for all users.

FIGURE 2 – STUDY AREA



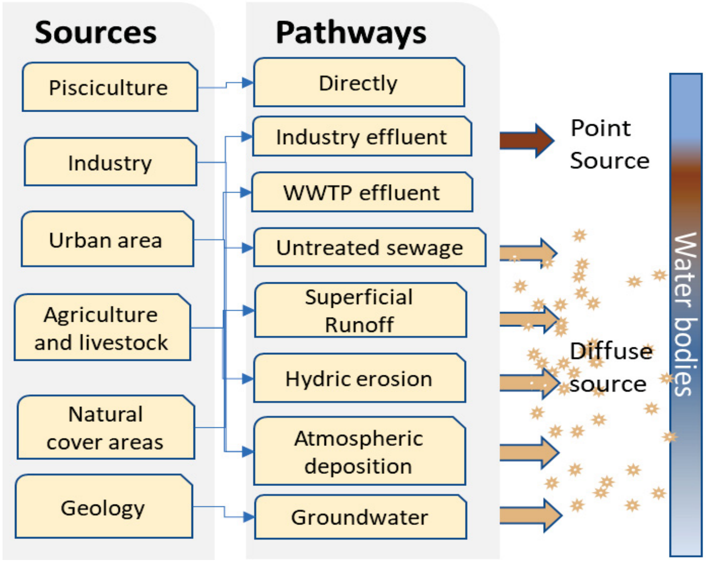
SOURCE: ACOSTA ET AL. (2023)

3.2 Loads estimative approach

For the configuration of the pollutant load estimation model in the selected basin, a thorough analysis of the primary sources of pollutants was conducted. This analysis was further discussed in meetings within the research team of the project – “Elaboration of Study of Implementation and Application of Hydrodynamic and Quality Models of Surface Waters of Federal Domain as support for Decision Making in Framework Proposal carried out by UFPR and National Water Agency” ANA (2022a). Based on this research and the availability of input data, a modified model was implemented to identify the predominant pollution pathways and accurately reflect the Brazilian context.

In total, eight calculation substances pathways (algorithms modules) were selected for the Paranapanema Basin, comprising three modules for point sources (pisciculture, wastewater from WWTPs and industrial wastewater) and five modules for diffuse sources (untreated sewage; erosion and surface runoff from Land Use, Land Cover (LULC); atmospheric deposition and groundwater), as depicted in Figure 3.

FIGURE 3– DIAGRAM OF POLLUTION SOURCES AND PATHWAYS CONSIDERED IN THE MORE MODEL FOR PARANAPANEMA BASIN



SOURCE: ANA (2022); ADAPTED BY THE AUTHOR (2023).

During this methodological step, MoRE's approaches were reviewed to adapt the algorithms to the Brazilian reality and data availability (Rieke et al., 2021; Acosta et al., 2022). The MoRE model predominantly takes a tabular form, where all attributes are linked to a unique identifier (ID), and the algorithms are coded within a calculation engine housed in an open-access processor. These processes include the algorithms derived from MoRE, which were defined and customized. Each individual module will be detailed explained in the following sections.

3.2.1 Pisciculture

In the Paranapanema region, aquaculture, specifically pisciculture, holds significance land use. This is noteworthy due to the substantial presence of fish farming activities conducted within the reservoirs (GIA, 2013).

The major environmental impact associated with these activities is related to fish feeding using manufactured feeds. The GIA project estimated the nutrient input into the Paranapanema River reservoirs through a comprehensive approach that included literature information and on-site research. This research covered various aspects such as feed composition, zootechnical performance, body composition, effective consumption, and losses (GIA, 2013; Rieke et al., 2021). To estimate the loads, Equation 1 was employed:

$$Ps_{P;N} = P_{SC_{P;N}} \cdot Aq_a$$ Equation 1

Where:

$P_{S_{P;N}}$ – Substance loads by pisciculture

$P_{SC_{P;N}}$ – Quantity of substance input into the water body (kgP/ha/ano)

Aq_a – Area of the aquaculture site (ha)

3.2.2 Industrial Load

Given the unavailability of data on effluents from each industry, the approach used in this study involved utilizing the maximum flow rate and concentration allowed by the permitting process. The maximum concentration acceptable in water from the World Bank's Pollution Prevention and Reduction Manual (Ackermann et al., 1999) was used based on the type of industry. Flow rate effluent licensed information from concessions was obtained by consulting the data from the Water and Land Institute (Instituto Água e Terra - IAT), Department of Water and Electric Energy (DAEE) and national water grants from the National Water Agency (Agência Nacional das Águas - ANA). An approach involving the pollutant load declarations required during the environmental licensing of industries could significantly reduce uncertainties in estimating this module. However, limitations in accessing information prevented the use of this more accurate approach (Fuchs, 2017; Rieke, 2021).

To estimate emissions from each industry, Equation 2 was employed:

$$ID_{E_P} = Q_{out} \cdot C_{subs} \cdot Coef_{unid}$$ Equation 2

Where:

ID_{E_P} – Substance exportation via industrial discharge (t/ year);

Q_{out}– Licensed flow rate (m^3/s);

C_{subs}– Concentration of the substance in industrial effluent (mg/L);

$Coef_{unid}$ – Unit conversion coefficient ($t \cdot s \cdot L/(mg \cdot year \cdot m^3)$).

3.2.3 Waste Water Treatment Plant (WWTP) loads

While Waste Water Treatment Plants (WWTPs) signify a significant advancement in sanitation, treating wastewater does not ensure the complete removal of all substances and nutrients present in sewage. Consequently, the discharge of treated wastewater into bodies of water introduces an aggregated pollutant load that can exceed the self-purification capacity. The implemented treatment plant efficiencies range from 65% to 80% (ANA, 2017). For estimating emissions, secondary data from WWTPs compiled for the Paranapanema Integrated Water Resources Plan (ANA, 2016), along with tables and georeferenced information layers from the Sewer Atlas, were considered.

To estimate exportation from each industry, Equation 3 was employed:

$$WWTP_{E_P} = Q_{ef} \cdot C_{wwtp} \cdot Coef_{unid} \qquad \text{Equation 3}$$

Where:

$WWTP_{E_P}$ – Substance exportation via WWTP (t/year);

Q_{ef}– Effluent flow rate from WWTPs (m³/s);

C_{subs}– Concentration of the pollutant in WWTP effluents (mg/L);

$Coef_{unid}$ – Unit conversion coefficient (t·s·L/(mg· year ·m³)).

3.2.4 Erosion-based loads

The erosion module assesses the potential rate of sediment export across a range of land use and land cover (LULC) types. This estimation employs the empirical Universal Soil Loss Equation Revised (RUSLE), a widely adopted method to comprehend the erosive hydraulic potential of diverse areas by considering soil, slope, and vegetation characteristics. The applied approach follows the equation established by Wischmeier e Smith (1978), as expressed by Equation 4.

$$RUSLE = R \cdot K \cdot C \cdot P \cdot LS \qquad \text{Equation 4}$$

Where:

$USLE$– Historical average soil loss per unit of area and time (t/(ha·year);

R– Rainfall erosivity (MJ·mm/(ha·h· year));

K – Soil erodibility (t·h/(MJ·mm));

C– Land use and land cover;

P– Management, and conservation practices;

LS–Slope length and average gradient.

To obtain the soil loss map, a custom code was formulated within the Google

Earth Engine (GEE) framework for the Paranapanema region (Appendix 1). The C-factor was computed for the year 2020, employing the methodology outlined by Islam (2022) and Pontes et al. (2022) and drawing data from the Sentinel-2 platform. The LS-factor was determined following the approach of Schmidt et al. (2021); Desmet & Grovers (1996) while the K-factor was derived from the methodology established by Islam (2002); Wischmeier e Smith (1978), with data sourced from Hengl (2018a); Hengl (2018b); Hengl & Wheeler (2018). Finally, the rain erosivity (R) was derived from monthly precipitation in mm at 1 km resolution Hengl & Parente (2022).

To obtain the specific soil loss in the areas of cultivation in the modeling year (2012), a correction factor is applied based on the annual sum of the precipitation of the analyzed year (P) between the historical average of the annual precipitation (P) Equation 5 (Fuchs et al., 2017; Acosta et al., 2021). This correction factor allows adjusting the historical average erosion for the year of study.

$$ER_{SD_{corr}} = \Big(\big(ER_{AL_{sl}} \cdot IM_{AL_{total}} \cdot\big) + \big(BI_{GL_A} \cdot BI_{GL_{SL}}\big) + \big(BI_{SIL_{SL}} \cdot BI_{SIL_A}\big) + \big(ER_{NAT_{sl}} \cdot BI_{NAT_A} \cdot\big) + \big(BI_{CAM_A} \cdot BI_{CAM_{SL}}\big)\Big) \cdot 100 \cdot ER_{PREC_{corr}} \qquad \text{Equation 5}$$

Where:

$ER_{SD_{corr}}$ – Corrected erosion loss (t/ha);

$ER_{AL_{sl}}$ – Average erosion rate for each crop according to slope (t/ha/year);

$IM_{AL_{total}}$ – Areas within the analysis unit with agriculture (km^2);

BI_{GL_A}– Areas within the analysis unit with pasture (km^2);

$BI_{GL_{SL}}$– average erosion rate for pasture (t/ha/year);

$BI_{SIL_{SL}}$– Average erosion rate for each forestry according to slope (t/ha/ year);

BI_{SIL_A}– Areas within the analysis unit with forestry (km^2);

$ER_{NAT_{sl}}$ – Average erosion rate for native forest cover (t/ha/ year);

BI_{NAT_A}. – Areas within the analysis unit with native forest cover (km^2);

BI_{CAM_A}– Areas within the analysis unit with natural grassland cover (km^2);

$BI_{CAM_{SL}}$–Average erosion rate for natural grassland areas (t/ha/year).

$ER_{PREC_{corr}}$– Correction factor based on annual precipitation (annual precipitation /long term precipitation (mm/year)).

After calculating the overall soil loss due to total erosion, adjusted for the various types of land use present in the basin, only a portion of the eroded sediments from the basin can be carried in runoff to reach the water body. The connection between this portion and the erosion loss establishes the concept referred to as the sediment input rate (Equation 6).

$$ER_{SDR} = CE1 \cdot \left(BL_{slope} + CE4\right)^{CE2} \cdot (A_{al})^{CE3}$$ Equation 6

Where:

ER_{SDR} – Sediment delivery rate (%);

BL_{slope} – Average slope of the analysis unit (%);

A_{al} –Percentage of agricultural soil within the Analysis Unit (%);

CE_x – Model constants, CE1=0,00668; CE2=0,3; CE3=1,5; CE4= -0,25.

To obtain the total sediment yield, Equation 7 was used, which determines the portion of erosion that could reach water bodies.

$$ER_{SDR_{in}} = ER_{SD_{corr}} \cdot ER_{SDR}$$ Equation 7

Where:

$ER_{SDR_{in}}$ – Sediment exportation (t/year);

$ER_{SD_{corr}}$ – Corrected erosion loss (t/ha);

ER_{SDR} – Sediment delivery rate (%);

The transfer rate (ER_{ENR}) represents the enrichment process that particles can undergo during the process, defined as a relationship between sediment emissions and the area of the analysis unit. If this relationship is less than 1, a constant rate (CE_7); is considered; if the relationship is greater than 1, the rate is calculated using Equation 8.

$$ER_{ENR} = CE_7 \cdot \left(\frac{ER_{SDR}}{BI_{AU_A}}\right)^{CE_9}$$ Equation 8

Where:

ER_{ENR} – Transfer rate;

$ER_{SDR_{in}}$ – Sediment exportation (t/year);

BI_{AU_A} – Analysis unit area (km^2);

CE_7 – Enrichment factor for phosphorus (18);

CE_9 – Default value -0.47

Finally, the pollutant loads of total nitrogen and total phosphorus for each analysis unit were estimated using Equations 9 and 10

Equation 9

$$ER_{E_P} = \frac{ER_{CONT_{topsoil_P}}}{10^6} \cdot \left(ER_{SED_{in}} - ER_{NATCOV_{SL}}\right) \cdot ER_{ENR} + \frac{ER_{CONT_{geo_P}}}{10^6} \cdot ER_{NATCOV_{SL}}$$

Where:

ER_{E_P} – Phosphorus emissions via soil loss on agriculture areas (t/ year);

$ER_{CONT_{topsoil_P}}$– Phosphorus content in topsoil (mg/kg);

$ER_{SED_{in}}$– Sediment exportation rate (t/year);

$ER_{NATCOV_{SL}}$– Soil loss in natural cover areas (t/ year);

ER_{ENR_P}– Phosphorus enrichment rate (dimensionless);

$R_{CONT_{geo_P}}$– Phosphorus content in soil (geology) (mg/kg);

Equation 10

$$ER_{E_N} = \left(\frac{ER_{CONT_{topsoil_N}}}{10^6} \cdot ER_{AGRL_{SL}} \cdot SR_{SDR} \cdot ER_{ENR}\right) + \left(ER_{NATCOV_{SL}} \cdot \frac{ER_{CONT_{geo_N}}}{10^6}\right)$$

Where:

ER_{E_N} – Nitrogen emissions via erosion (t/a);

$ER_{CONT_{topsoil_N}}$– Nitrogen content in topsoil (mg/kg);

$ER_{SED_{in}}$– Sediment exportation (t/year);

$ER_{NATCOV_{SL}}$– Soil loss in natural cover areas (t/ year);

$ER_{AGRL_{SL}}$– Soil loss in agricultural areas (t/ year);

ER_{ENR_N}– Enrichment rate (dimensionless);

$R_{CONT_{geo_N}}$– Nitrogen content in soil (geology) (mg/kg);

3.2.5 Untreated Domestic Effluent

To estimate diffuse loads originating from regions where sewage treatment plants and sewer systems lack complete coverage, data were gathered through a survey of the IBGE (2010) census and information from the Sewer Atlas (ANA, 2017). This portion delineates the quantity of wastewater that can reach the water body without proper treatment.

Firstly, an estimation was made for the portion of the load that could enter the water body from the population utilizing individual sanitation solutions ($US_{SI_{P;N}}$). It was assumed that these individual treatments have an average efficiency of 30% for the removal of Total Phosphorus (PT) and Total Nitrogen (NT) (Sperling, 2017). The per capita load was estimated per inhabitant and then multiplied by the efficiency and the population count associated with this type of solution.

To estimate the amount of substances that could directly reach the water body through the collection network lacking sewage treatment, the index of the population reporting collection systems but without access to a treatment facility ($US_{Rede_{P;N}}$) was utilized.

Finally, to estimate the amount of substances that could reach the water body from the portion of the population lacking basic sanitation, the index of the population without basic sanitation facilities (US_{Sem_p}) was used.

Consequently, the diffuse sewage loads were calculated as the sum of these three portions (Rieke et al., 2021), in accordance with Equation 11.

$$US_{E_{P;N}} = \left(US_{SI_{P;N}} \cdot C_{P;N} + US_{Rede_{P;N}} \cdot c_{P;N} + US_{Sem_{P;N}}\right) \qquad \text{Equation 11}$$

Where:

$US_{E_{P;N}}$– Loads of untreated sewage entering the system (not treated by WWTP) (t/year).

$C_{P;N}$ – Average load per capita (g)

US_{SI_p}– Index of population with individual sanitation solutions

US_{Sem_p}– Index of population without access

US_{Rede_p}– Index of population with collection systems but without treatment

3.2.6 Surface runoff from natural areas with vegetation

To estimate the amount of substance in superficial runoff of different LULC, the runoff was estimated with the curve number from Soil Conservation Service (SCS) model or we used the estimative by Linke et al. (2019) in each watershed. When calculating nutrient emissions from surface runoff, only the portion of dissolved nutrients is considered Fuchs (2010). The nutrient concentration in surface runoff is calculated as the average concentration weighted by the land use area:

Equation 12

$$Q_{E_{P;N}} = \left(SR_{Q_{P;N}} \cdot SRC_{P;N}\right)$$

Where:

$Q_{E_{P;N}}$– Substance loads in superficial runoff of different LULC

$SRC_{P;N}$ – Substance concentration in runoff from vegetation-covered surfaces (mg/l)

$SR_{Q_{P;N}}$– Surface runoff flow (m^3/s)

3.2.7 Atmospheric Deposition

The process of quantifying emissions through atmospheric deposition involves utilizing the water surface area and a specific deposition rate for the given substance, as outlined in Equation 13. The substance deposition rate is typically sourced from country-specific data collected through air emissions monitoring.

Equation 13

$$AD_{E_{P;N}} = \left(AD_{r_{P;N}} \cdot IM_{ws}\right)$$

Where:

$AD_{E_{P;N}}$– Substance input via atmospheric deposition (t/a)

$AD_{r_{P;N}}$ – Substance deposition rate country-specific (mg/m^2)

IM_{ws} – Water Surface Area, Total (km^2)

3.2.8 Groundwater Flow

To estimate the substance concentration in groundwater contribution, an approximation was used using data of concentration from piezometric well monitoring data of the RIMAS (Rede Integrada de Monitoramento das Águas Subterrâneas) from Brazilian Geological Service (SGB). As there is no data available for the entire region, representative wells from the outcropping aquifer layer were assumed. Also, an estimated baseflow for each sub-basin from (ANA) was used as a parcel of contribution. Equation 14, is employed to compute loads via groundwater.

Equation 14

$$GW_{E_{P;N}} = \left(C_{well_{P;N}} \cdot Bf\right)$$

Where:

$GW_{E_{P;N}}$ – Substance entering by groundwater way (t/year).

$C_{well_{P;N}}$– Substance concentration in the base flow by outcropping aquifer layer (mg/l)

Bf– baseflow for each sub-basin (m^3/s)

3.3 Database for loads modeling

The spatial data (Table 2) was obtained from the Integrated Water Resources Management Plan for the Paranapanema River Basin (PIRH Paranapanema) (ANA, 2016). There is certain data that is accessible but with some limitations. In certain approaches, there has been recognition of the availability of more representative load data, which, however, remains inaccessible. This is particularly evident in cases such as the declaration of pollutant loads from self-monitoring.

TABLE 2 – INPUT DATA FOR THE MORE MODEL IN THE PARANAPANEMA RIVER BASIN

	Pathway	Input data	Source	Descriptions
1	Pisciculture	Concentration of TP and NT	GIA, 2013	Local study in the Paranapanema basin
2	Industry	Outflow rate	IAT, DAEE, and ANA	The discharged effluent was not accessible, the water concessions for discharge was used
		Concentration	IAT	Literature data for discharge limits by industrial type and effluent discharge limits permitted by legislation
3	WWTP	Population served;	ANA	Sewer atlas: Treatment efficiency for TP and TN based on literature and removal technology information for each WWTP
		Per capita load		
		Treatment efficiency		
4	Soil erosion	Digital Elevation Model (DEM)	SRTM	Shuttle Radar Topography Mission: Data derived from the 30-meter base of the mission with void correction.
		Land use and land cover map (LULC)	PIRH Paranapanema	LULC, generated by classification of imagens LANDSAT 8, year 2014.
		Soil type	PIRH Paranapanema	Integrated Water Resources Plan of the Paranapanema Water Resources Management Unit (PIRH Paranapanema)
		Precipitation	SNIRH e DAEE	Precipitation from 25 monitoring stations
5	Untreated Domestic Effluent	Population without WWTP service	ANA	Sewer atlas: Population without sewage collection and Population with sewage collection and treatment and Population served with individual sewage solution.
		Per capita load		
		Treatment average efficiency		

6	Surface runoff from natural areas with vegetation	Precipitation LULC	SCS, 1957	Estimated using the Runoff curve number from Soil Conservation Service (SCS) model f in each sub-basin
7	Atmospheric Deposition	Atmospheric deposition rate of the substance		Literature from different studies
		Surface area of water bodies	PIRH Paranapanema	
8	Groundwater Flow	Substance concentration	CPRM	Well readings data from Integrated Underground Water Monitoring Network - RIMAS
		Outcropping aquifers layer	PIRH Paranapanema	
		Low rate fow (Q_{95})	ANA	

SOURCE: ANA (2021)

3.3.1 Monitoring Data for Calibration/Validation

One hundred and fifty-nine stations available within the National System of Water Resources Information (SNIRH), Department of Water and Electrical Energy (DAEE) and Water and Land Institute (IAT) were chosen for the study's geographical scope. Among these, a total of 64 stations where data on phosphorus concentration could be found, 49 stations with total nitrogen concentration, and 81 with biochemical oxygen demand (BOD) data where it's possible to pair with flow data (FIGURE 8). This process ended in the identification of stations that yielded synchronous datasets encompassing Nitrogen and phosphorus measurements and flow rates at the same stations (Table 3).

TABLE 3 – SELECTED STATIONS FOR MODEL EVALUATION

Sub watershed	Station ID	River name	Lat	Lon.	BOD	TN	TP	Flow
			---decimal----		-----average mg/l-----			m^3/s
4	PARP02900	Rio Paranapanema	-22.597	-52.874	2.50		0.02	
47	PIZI02900	Rio Pirapozinho	-22.524	-52.018	2.00		0.03	
49	64560000	Ribeirão Pirapó	-22.611	-52.002	1.20			66.1
63	64550000	Ribeirão Pirapó	-22.857	-52.078	2.73	0.94	0.09	70.1
72	64549000	Rio Bandeirantes Do Norte	-22.891	-52.027	1.25			
91	64515000	Rio Paranapanema	-22.656	-51.365				981.2
91	64516080	Rio Paranapanema	-22.663	-51.359				1204.2
91	64516900	Rio Paranapanema	-22.661	-51.388	2.30		0.03	
91	64517000	Rio Paranapanema	-22.667	-51.400	1.74	0.43	0.03	1356.7
91	PARN02750	Rio Paranapanema	-22.660	-51.377	2.19		0.03	
91	PARP02750	Rio Paranapanema	-22.661	-51.388	2.07			
94	64547000	Rio Bandeirantes Do Norte	-22.983	-51.817	1.25			16.5
99	64544000	Rio Porecatu	-23.186	-52.150	73.67	0.69	0.21	1.0

Sub watershed	Station ID	River name	Lat	Lon.	BOD	TN	TP	Flow
			---decimal----		-----average mg/l-----			m^3/s
100	64543000	Ribeirão Pirapó	-23.117	-52.000	1.50			47.0
131	64540000	Ribeirão Pirapó	-23.314	-51.847	2.50			
137	64545700	Rio Bandeirantes Do Norte	-23.300	-51.417	1.00			1.5
142	64541000	Ribeirão Pirapó	-23.326	-51.845	5.17	0.70	0.16	16.7
149	64515900	Ribeirão Guarazinho	-23.036	-51.232	3.29	0.50	0.05	0.4
162	64346000	Ribeirão Capivari	-22.533	-50.917				7.8
162	7D-012	Ribeirão Capivari	-22.532	-50.908				7.9
162	PIVI02850	Ribeirão Capivari	-22.532	-50.908	2.00		0.08	
173	64395000	Rio Da Capivara	-22.617	-50.683				20.4
173	7D-008	Rio Da Capivara	-22.623	-50.691				15.1
173	PIVR02700	Rio Da Capivara	-22.622	-50.684	2.53		0.05	
181	64529900	Ribeirão Caviuna	-23.500	-51.472	2.48	0.44	0.04	0.9
186	64508500	Rio Congonhas	-23.170	-50.788	2.18	0.81	0.16	16.3
196	64508020	Rio Congonhas	-23.232	-50.733	2.58	0.69	0.06	13.8
206	64507100	Ribeirão Jacutinga	-23.249	-51.068	2.56	0.60	0.04	2.1
211	64504600	Ribeirão Três Bocas	-23.356	-51.016	1.00			
211	64504700	Rio Tibagi	-23.352	-51.007				493.2
211	64506000	Rio Tibagi	-23.312	-50.995	3.29	2.24	0.05	442.6
211	64506500	Rio Tibagi	-23.267	-50.983	3.00			464.9
211	64507000	Rio Tibagi	-23.250	-50.984	3.15	0.60		369.8
222	64390000	Rio Laranjinha	-23.123	-50.450	2.54	0.81	0.06	45.4
223	64345000	Rio do Pari	-22.800	-50.300				13.0
223	7D-006	Rio do Pari / Veado.	-22.816	-50.316				13.0
223	PARI02700	Rio Do Pari	-22.817	-50.316	2.63		0.11	
233	64370000	Rio Das Cinzas	-23.086	-50.285	2.35	0.60	0.03	64.0
236	64389900	Rio Araras	-23.160	-50.525	2.00			
244	64504581	Ribeirão Do Cafezal	-23.345	-51.297	2.75	0.58	0.06	0.8
244	64504591	Ribeirão Do Cafezal	-23.354	-51.196	2.67	0.68	0.05	2.7
251	64504100	Ribeirão Jataizinho	-23.439	-50.824	4.27	0.86	0.20	0.5
253	64502000	Rio Taquara	-23.561	-51.030	2.86	0.67	0.07	38.0
255	64501950	Rio São Jerônimo	-23.546	-50.883	4.67	1.44		9.4
259	64504210	Rio Tibagi	-23.465	-51.309				417.3
259	64504450	Ribeirão Dos Apertados	-23.465	-51.309	4.08	0.70	0.09	118.5
259	64504500	Ribeirão Dos Apertados	-23.466	-51.311				10.1
260	64332080	Rio Paranapanema	-22.905	-50.001				497.2
260	64335000	Rio Paranapanema	-22.900	-50.033	2.67			
260	64335100	Rio Paranapanema	-22.900	-50.017	1.33			390.4
268	64501000	Rio Tibagi	-23.637	-50.923	2.37	0.68	0.07	374.9
273	64280000	Rio Paranapanema	-23.017	-49.900				336.5
273	64326000	Rio Paranapanema	-22.998	-49.908	2.45		0.03	
273	PARP02500	Rio Paranapanema	-22.998	-49.908	2.30			
274	64382000	Rio Laranjinha	-23.400	-50.450	2.35	0.75	0.05	40.9

Sub watershed	Station ID	River name	Lat	Lon.	BOD	TN	TP	Flow
			---decimal----		-----average mg/l-----			m^3/s
276	64385000	Rio Laranjinha	-23.414	-50.452				27.5
281	64498550	Rio Tibagi	-23.700	-50.917				376.4
282	64500000	Rio Do Tigre	-23.719	-50.775	3.00	0.63	0.11	3.8
283	64325000	Rio Pardo	-22.954	-49.867	2.51		0.07	
283	PADO02600	Rio Pardo	-22.954	-49.867	2.18			
285	64366500	Rio Jacarézinho	-23.215	-50.009	3.20	0.37	0.16	7.0
298	64278080	Rio Paranapanema	-23.068	-49.838	3.24	0.65	0.11	354.1
298	64278500	Rio Paranapanema	-23.071	-49.846				496.0
300	64362000	Rio Das Cinzas	-23.342	-50.163	2.20	1.00	0.08	61.6
319	64270000	Rio Paranapanema	-23.129	-49.727	1.00			
319	64270050	Rio Paranapanema	-23.121	-49.728	4.19			
319	64270080	Rio Paranapanema	-23.128	-49.732				374.9
319	64273000	Rio Paranapanema	-23.098	-49.740				285.6
319	64275000	Rio Paranapanema	-23.100	-49.750				332.6
319	6E_001	Rio Paranapanema	-23.098	-49.744				285.6
342	64320000	Rio Pardo	-22.900	-49.617	3.00			46.9
342	64320010	Rio Pardo	-22.907	-49.625				56.0
342	64323000	Rio Pardo	-22.900	-49.617				46.1
342	64324000	Rio Pardo	-22.904	-49.619	2.43		0.08	
342	6D_001	Rio Pardo	-22.906	-49.623				46.9
342	PADO02500	Rio Pardo	-22.904	-49.619	2.23			
353	64380000	Rio Laranjinha	-23.850	-50.391				15.9
356	64365800	Rio Lajeado	-23.579	-49.870	3.20	0.55	0.07	0.4
356	64365850	Rio Jacarézinho	-23.497	-49.887	3.19	0.70	0.10	1.3
373	64491000	Rio Tibagi	-24.032	-50.693	1.81	0.60		236.4
396	64360100	Ribeirão Jabuticabal	-23.741	-50.081	2.89	0.66	0.04	7.7
398	64315000	Rio Pardo	-22.879	-49.238				42.1
398	6D_002	Rio Pardo	-22.879	-49.240				42.0
398	PADO02400	Rio Pardo	-22.879	-49.240	2.00		0.07	
403	64219000	Rio Paranapanema	-23.160	-49.368	3.44	0.70	0.07	
403	64219080	Rio Paranapanema	-23.154	-49.380				258.7
403	64219200	Rio Paranapanema	-23.160	-49.379				396.6
403	64220000	Rio Paranapanema	-23.183	-49.383				210.8
403	64220050	Rio Paranapanema	-23.179	-49.392				275.8
409	64250000	Rio Verde	-23.700	-49.467				15.8
409	VERD02750	Rio Verde	-23.707	-49.471	2.16		0.08	
427	64360000	Rio Das Cinzas	-23.767	-49.950	2.42	0.86	0.06	29.4
432	64215080	Rio Paranapanema	-23.210	-49.229				246.7
450	64245000	Rio Itararé	-23.717	-49.550	2.00			65.1
450	64245200	Rio Itararé	-23.726	-49.553	2.75		0.09	
450	64247000	Rio Itararé	-23.723	-49.556	4.53			60.2
450	ITAR02500	Rio Itararé	-23.726	-49.553	2.84			
452	64359950	Ribeirão Da Natureza	-23.922	-49.838	2.56	0.69	0.03	

Sub watershed	Station ID	River name	Lat	Lon.	BOD	TN	TP	Flow
			---decimal----		-----average mg/l-----			m^3/s
472	64250010	Rio Verde	-23.733	-49.430				19.2
477	64214000	Rio Paranapanema	-23.261	-49.001	2.13		0.03	
477	JURU02500	Reservatorio Rio Jurumirim	-23.261	-49.001	2.13			
478	62716000	Rio Novo	-22.998	-48.840	3.07		0.05	
478	NOVO02450	Rio Novo	-22.998	-48.840	2.51			
486	64482000	Rio Tibagi	-24.360	-50.594	2.02	0.50	0.06	308.8
496	64242200	Rio Da Pescaria	-23.928	-49.660	3.15	0.55	0.06	6.9
514	64242000	Rio Jaguariaíva	-23.977	-49.596	2.35	1.15	0.04	31.8
534	64231000	Rio Itararé	-24.033	-49.461	2.83	0.67	0.06	25.9
543	64465000	Rio Tibagi	-24.509	-50.410	2.17	0.54	0.05	166.8
549	BOIB02950	Córrego Boi Branco	-23.489	-48.905	2.00		0.16	
556	64230500	Rio Jaguaricatu	-24.100	-49.467	7.33	0.74		20.5
580	64460000	Rio Capivari	-24.705	-50.493	1.96	0.71	0.04	12.0
586	64198000	Rio Taquari	-23.786	-49.056	3.61			22.3
596	64447500	Rio Tibagi	-24.850	-50.300	1.80			189.0
596	64453000	Rio Pitangui	-24.856	-50.294	2.67	1.93		25.7
608	64477000	Rio Iapó	-24.751	-50.088				0.2
608	64477600	Rio Iapó	-24.750	-50.089	2.11	0.84	0.10	36.9
625	64135000	Rio Guarei	-23.474	-48.435				10.7
625	GREI02750	Rio Guarei	-23.486	-48.454			0.13	
625	GREI02750	Rio Guarei	-23.486	-48.454	2.86			
626	64476000	Rio Iapó	-24.767	-50.067	1.00	0.02		23.5
628	64185000	Rio Taquari	-23.961	-48.950				9.5
628	64190000	Rio Taquari	-23.983	-48.917				10.0
628	64190800	Rio Taquari	-23.974	-48.917	3.73		0.53	
628	5E_002	Taquari	-23.961	-48.950				10.2
628	TAQR02400	Rio Taquari	-23.974	-48.917	4.63			
633	64080000	Rio Paranapanema	-23.593	-48.491	4.79			75.2
633	64081000	Rio Paranapanema	-23.591	-48.494	2.64		0.46	
633	PARP02100	Rio Paranapanema	-23.591	-48.494	2.66			
644	64075100	Rio Guarei	-23.464	-48.421	2.95		0.08	
644	GREI02700	Rio Guarei	-23.465	-48.422	3.02			
644	5E_013	Rio Guarei	-23.466	-48.420				7.6
655	64447000	Rio Tibagi	-24.947	-50.391	1.90	0.63	0.07	117.5
662	64074800	Rio Itapetininga	-23.557	-48.372	2.41		0.08	
662	64075000	Rio Itapetininga	-23.564	-48.390	3.92		0.00	31.2
662	64082000	Rio Paranapanema	-23.600	-48.483	2.25			82.4
662	ITAP02800	Rio Itapetininga	-23.557	-48.372	2.46			
665	64450002	Rio Pitangui	-25.033	-50.083	1.80	0.58		6.4
674	64444000	Rio Tibagi	-25.076	-50.389	1.67	1.07	0.16	273.7
683	64449500	Rio Pitangui	-24.960	-49.942	3.13	0.34	0.05	10.0
684	64449570	Rio Paranapanema	-24.966	-49.980				4.1
698	64095000	Rio Apiai-Guaçu	-23.924	-48.659				13.2

Sub watershed	Station ID	River name	Lat	Lon.	BOD	TN	TP	Flow
			---decimal----		-----average mg/l-----			m^3/s
698	5E_001	Rio Apiai-Guacu	-23.924	-48.659				12.4
698	APIA02600	Rio Apiai-Guacu	-23.928	-48.656	2.00		0.04	
715	64065000	Rio Itapetininga	-23.625	-48.105				18.9
715	64066000	Ribeirão Ponte Alta	-23.601	-48.125	7.31		0.22	
715	5E_006	Rio Itapetininga	-23.626	-48.105				20.1
715	PALT04970	Ribeirão Ponte Alta	-23.601	-48.125	8.07			
717	64442800	Rio Imbituva	-25.199	-50.525	2.67	1.37		28.3
721	64015000	Rio Turvo	-23.851	-48.211		0.00		12.9
721	TURR02800	Rio Turvo	-23.850	-48.211	2.00		0.07	
726	64440000	Rio Tibagi	-25.200	-50.150	3.58	1.15	0.20	21.6
751	64442300	Rio Barreiro	-25.248	-50.633	2.00	0.25	0.07	10.9
761	64012500	Rio São Miguel Arcanjo	-23.870	-48.029	2.00		0.06	
761	64013000	Rio São Miguel Arcanjo	-23.888	-48.026	5.06		0.16	
761	GAPE02900	Lagoa Do Guapé	-23.881	-48.003			0.11	
761	SMIG02800	Rio São Miguel Arcanjo	-23.888	-48.026	5.15			
762	64430200	Rio Tibagi	-25.317	-49.983	1.11	0.89	0.04	7.7
763	64429000	Rio Pugas	-25.426	-49.978	3.50	0.53	0.11	0.6
768	64441020	Rio Imbituva	-25.464	-50.533	3.22	0.96	0.05	4.3

SOURCE: SINRH (2021). COMPILED BY THE AUTHOR (2023)

To calculate observed loads, flow duration curves were developed to estimate flow indicators such as Q_{50} for median flows, Q_{90} for low flows, and Q_{10} for high pulses. Regarding concentration, data from quartiles were utilized. Consequently, by multiplying concentration with flow, an approximation of observed pollutant loads was derived for each station.

3.4 Routines and algorithms in the GIS environment

The MoRE model operates primarily through tables, where each attribute is linked to a unique identifier processed by algorithms within an open-access platform. Managing and preparing a large volume of data is a challenging task that can impact modeling efficiency. To address this, data processing routines were created using the 'ModelBuilder' tool in ArcGIS, with some methodologies also integrated into Google Earth Engine (GEE). The description of these is in the paper II (item 4.2) and the Appendix 1.

3.5 Web-GIS development for water framework decision-making

The methodology about this topic was explained by Acosta et al (2023) and is included in paper II (item 4.2). The Web-GIS was developed as part of the project called "Modeling of Water Quality in the Paranapanema Basin: Base for the water quality standards", between ANA and UFPR (ANA, 2022), and it was created with the aim of harmonizing and visualizing the results of the modeling of the basin load emission estimates, hydrodynamic modeling of rivers, and substance concentration estimates in the reservoirs. Acosta et al (2023), presents a brief description of the previous stages, data preparation and modeling, and the development of the Web-GIS platform to support decision-making. The Web-GIS is available at the link <https://bit.ly/paranapanema_modelagem>

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4 RESULTS

The principal results are present trough tree papers:

The first paper, "Total Phosphorus Estimative for the Tibagi River Water Basin Management," refers results about the estimation of total phosphorus loads, for effective management of the Tibagi River water basin.

The second one "Evaluating diffuse and point sources in dub-Watersheds using a GIS-Based pollutant loads estimative," focus in assessing both diffuse and point sources of pollutants in sub-watersheds. This paper employs a Geographic Information System (GIS) to estimate pollutant loads, providing a comprehensive approach to understanding the dynamics of water quality.

Finally, the third paper, "A Web-GIS for Decision Making to Achieve Water Quality Standards of Water Bodies Through Collaborative Watershed Modeling," explores the integration of web-based GIS tools to facilitate collaborative watershed modeling, with the goal of achieving and maintaining water quality standards in various water bodies.

Together, these papers represent the principal results about the evaluation on water quality assessment and management, showcasing innovative approaches that can significantly contribute to sustainable water resource practices.

4.1 Paper I –Total phosphorus estimative for the Tibagi river water basin management

HIGHLIGHTS:

This part of the research refers to the article submitted to the "*XXIV SBRH - Simpósio Brasileiro de Recursos Hídricos conference 2021*" that focuses on a case study applied to estimate phosphorus pollutant loads in the Tibagi basin and summarizes some of the modeling results.

Data: 21/11/2021 - 26/11/2021
Local: BELO HORIZONTE - MG
ISSN: 2318-0358

Available in Portuguese in: https://anais.abrhidro.org.br/job.php?job=13605

XXIV SIMPÓSIO BRASILEIRO DE RECURSOS HÍDRICOS

CARGA DE FÓSFORO TOTAL. ESTIMATIVA PARA A GESTÃO DA BACIA HIDROGRÁFICA DO RIO TIBAGI

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Resumo

O entendimento das vias e fontes da poluição tanto pontual como difusa tem sido um desafio na elaboração de planos de bacias que visam a equilibrar a demanda e oferta de água de qualidade para o bem-estar da população. Muitas pesquisas têm se desenvolvido nesta área, mas, apesar do esforço, ainda importantes desafios continuam se impondo ante às comunidades científicas, não apenas na modelagem, mas também na geração de metodologias mais apuradas. Os gestores exigem métodos que garantam que o investimento do recurso seja atribuído a ações que garantam um ambiente ecologicamente

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saudável. Para estimar as cargas segundo via de poluição, foi utilizada uma estrutura de modelagem de complexidade reduzida baseada no *Modeling of Regionalized Emissions* (MoRE). Os resultados da simulação do modelo mostram as quantidades de cargas por unidade de análise, ajudando a estabelecer um ranking de priorização de bacias, que a sua vez permite diagnosticar as principais fontes difusas e pontuais de contribuição. Neste artigo, se apresenta um estudo de caso em que se estimam as cargas de fósforo total para a bacia hidrográfica de Tibagi. Sendo também parte de um estudo maior com objetivo de estimar as cargas poluentes (Nitrogênio, Fósforo e DBO) para fins de enquadramento da bacia de Paranapanema.

Palavras-Chave: Bacia Tibagi; Cargas difusas e pontuais; Modelo MoRE.

4.1.1 Introdução

O uso e ocupação da bacia pelo homem tem como consequência o desequilíbrio natural e origina problemas ambientais como a aceleração de processos erosivos, poluição da água e alterações do regime fluviométrico, cuja mitigação demanda a compreensão dos fenômenos envolvidos (Kan et al., 2019). O entendimento dos processos e das vulnerabilidades intrínsecas do meio permitem uma estratégia mais racional e sustentável do desenvolvimento das bacias hidrográficas. Para tanto, a gestão integrada dos recursos hídricos, ambiental e de território é essencial e utiliza de modelos matemáticos para auxiliar nos processos de decisão. No entanto, algumas lacunas ainda precisam ser preenchidas no uso de ferramentas matemáticas de forma a diminuir as incertezas inerentes.

As instâncias responsáveis pelo gerenciamento e uso dos recursos da bacia têm a tarefa de analisar diferentes possíveis cenários e avaliar as prováveis consequências de propostas de estratégias de medidas de controle, bem como de uso e ocupação da terra. Isto passa pelo conhecimento das inter-relações entre os processos que ocorrem na bacia, tanto na superfície como na atmosfera e no subsolo. Dentro da área do gerenciamento dos recursos hídricos e meio ambiente, estas estimativas podem ser obtidas utilizando a modelagem matemática. Neste caso, os fenômenos são observados, medidos e os processos analisados para, depois, propor funções matemáticas que representem o processo e permitam reproduzir os eventos observados e, em uma segunda fase, servir como ferramenta de simulação e previsão.

Contudo, a complexidade e inter-relação entre processos físicos, químicos e biológicos é grande e se torna difícil modelar todos os processos envolvidos com a devida rigidez. Avanços em termos de informática e tecnologia permitem desenvolvimento de modelos determinísticos e distribuídos cada vez mais complexos que consideram tanto a variabilidade espacial como temporal (Tucci, 2005). Porém, os modelos são uma simulação simplificada da realidade nos quais muitos processos não são considerados. Ainda que os modelos contemplem todas as equações e escalas desejadas, a capacidade computacional pode ser uma limitante, especialmente em bacias hidrográficas de médio e grande porte.

Não é surpreendente, face a estas limitações, que existam diferentes modelos para um mesmo fenômeno, variando tanto na sua formulação como nos dados de entrada. Cada modelo pode ter o mesmo objetivo, mas deve lidar com diferentes graus de incerteza associados aos dados de entrada e às simplificações introduzidas no modelo. Os eventuais erros ou falta de dados de entrada se combinam dentro das etapas da modelagem, o que provoca a propagação da incerteza ao longo do modelo, do que decorre que o resultado tenha seu grau de incerteza aumentado (Wang e Solomatine, 2019).

Existe, então, um problema real associado ao uso de modelos. Por um lado, o adequado gerenciamento da bacia exige uma modelagem ágil e suficientemente confiável para justificar as decisões. Por outro lado, o engenheiro se defronta com as limitações dos dados e as simplificações ou suposições intrínsecas do modelo, que geram incerteza no resultado. Neste artigo se pretende avaliar a estimativa de cargas de poluentes de fósforo total para a bacia do rio Tibagi realizada com o modelo *Modeling of Regionalized Emissions* – MoRE (Fuchs, 2012), utilizando dados de monitoramento do Sistema Nacional de Informações sobre Recursos Hídricos – SNIRH.

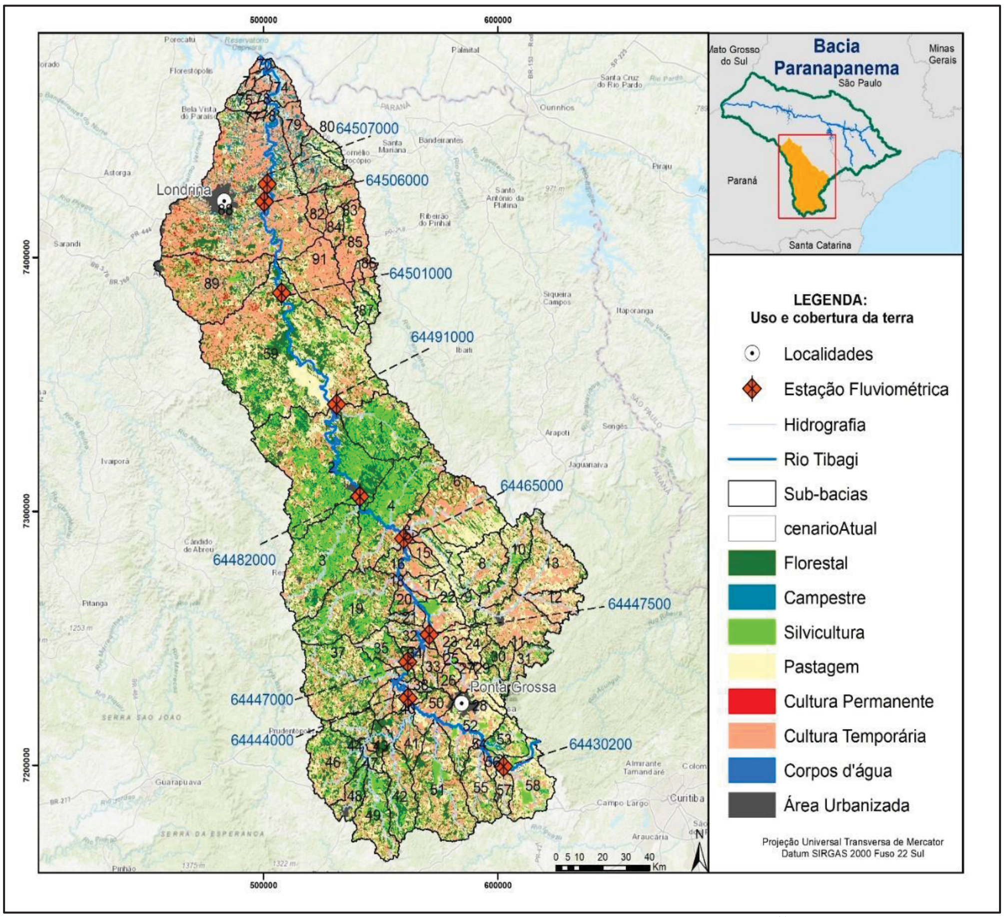
Esta pesquisa é parte de um projeto maior que desenvolveu um modelo de estimativa de cargas poluentes, para ser utilizado como uma ferramenta na definição e acompanhamento das metas de enquadramento, bem como na priorização de ações a serem tomadas para manter ou atingir a qualidade definida para cada porção do corpo hídrico.

4.1.2 Metodologia

A abordagem metodológica desta pesquisa consistiu no desenvolvimento de um modelo regionalizado para estimar as cargas poluentes baseado nas equações do modelo MoRE (Funchs et al., 2012). MoRE é um modelo utilizado para obter a caracterização da bacia através do levantamento das ameaças existentes dentro da bacia de drenagem, integrando suas vulnerabilidades, aspectos biofísicos, condições climáticas e características de influência.

A área de estudo é a bacia do rio Tibagi, contribuinte do rio Paranapanema. A bacia do rio Tibagi (Figura 4), é uma bacia com importância econômica para o Paraná. A área da bacia compreende 47 municípios das macrorregiões de Apucarana, Porecatu, Assaí, Cornélio Procópio, Ibaiti, Jaguariaíva, Londrina, Ponta Grossa, Prudentópolis e Telêmaco Borba, e corresponde a 80 sub-bacias com aproximado de 25 mil km2. Dentro do território analisado, encontram-se cidades importantes como Londrina e Ponta Grossa e um mosaico produtivo agrícola com culturas como cana-de-açúcar, café, trigo, milho, soja, fumo e feijão, silvicultura e pecuária correspondendo a 73% da área total da área de estudo. O restante 26%, é dividido em cobertura florestal e campestre (25% dispersos sobre todo o território), área urbana e outros (1%) segundo o mapa de cobertura e ocupação da terra do ano 2014 realizado sobre imagens de satélite Landsat 8 para PIRH Paranapanema (ANA, 2016).

FIGURE 4 – SUB-BACIA DO RIO DE TIBAGI. BACIA DE PARANAPANEMA



FONTE: DADOS DE PIRH PARANAPANEMA (ANA. 2016). ELABORAÇÃO: O AUTOR (2021)

A primeira etapa deste trabalho consistiu na obtenção de informações geográficas e tabulares relativas às características físicas, socioeconômicas e de monitoramento na bacia, disponíveis para compor a base de dados do modelo. Os dados usados na estimativa de cargas provenientes de bancos de dados institucionais, principalmente do Plano Integrado de Recursos Hídricos da Bacia Hidrográfica da bacia do Paranapanema (ANA, 2016).

Para realizar um comparativo com dados observados, foram selecionadas 43 estações disponíveis no Sistema Nacional de Informações sobre Recursos Hídricos (SNIRH) para a região do estudo, das quais 16 possuíam dados de vazão e 13 de qualidade da água, resultando em 10 estações com dados de fósforo e vazão na área de estudo não necessariamente concomitantes.

4.1.2.1.1 Cargas Pontuais

Os módulos de cargas provenientes da indústria e de ETEs baseiam-se na equação de estimativa de cargas e são calculados utilizando a equação 15.

$$M_{UA} = \sum Q \cdot C \qquad \text{Equação 15}$$

Onde:

M_{UA} – Estimativa da carga na unidade de análise (t/dia)

Q – Vazão de efluentes (industriais ou de ETEs) em m^3/s

C – Concentração do poluente nos efluentes (industriais ou de ETEs) em mg/l

O que diferencia a abordagem são as considerações realizadas para a estimativa e a agregação da informação, descritas a seguir.

As cargas pontuais provenientes da piscicultura foram levantadas pelo Grupo Integrado de Aquicultura e Estudos Ambientais - GIA, sendo considerada a localização geográfica dos parques aquícolas (GIA, 2013), e as concentrações anuais estimadas.

4.1.2.1.2 Cargas Difusas

O módulo de erosão se encontra baseado na metodologia desenvolvida por Wischmeier e Smith (1978) da equação universal de perda de solos (USLE). A estimativa de erosão é ajustada ao ano de análise com um fator relacionado à quantidade de chuva. Depois é utilizado o método de *Sediment Delivery Ratio* (SDR) e aplicado um fator de enriquecimento para calcular a exportação de sedimentos – $ER_{SED_{in}}$. Depois é aplicada a equação 16 para obter a emissão de fósforo via erosão das áreas agrícolas e cobertura natural. Detalhes do método em Acosta *et al*, (2013).

$$ER_{E_P} = \frac{ER_{CONT_{topsoil_P}}}{10^6} \cdot \left(ER_{SED_{in}} - ER_{NATCOV_{SL}}\right) \cdot ER_{ENR} + \frac{ER_{CONT_{geo_P}}}{10^6} \cdot ER_{NATCOV_{SL}} \qquad \text{Equação 16}$$

Onde:

ER_{E_P} *CEmissões de Fósforo via Erosão (t/a);*

$ER_{CONT_{topsoil_P}}$– Conteúdo de fósforo no solo superficial (mg/kg);

$ER_{SED_{in}}$– Exportação de sedimentos (t/a);

$ER_{NATCOV_{SL}}$– Perda de solo em áreas de cobertura natural (t/a);

ER_{ENR_P}– Taxa de enriquecimento de fósforo (adimensional);

$R_{CONT_{geo_P}}$– Conteúdo de fósforo no solo (geologia) (mg/kg);

As cargas geradas pelo esgoto difuso foram, portanto, consideradas como a soma de três parcelas, segundo a equação 17.

$$US_{E_{P;N}} = \left(US_{SI_{P;N}} \cdot C_{P;N} + US_{Rede_{P;N}} \cdot c_{P;N} + US_{Sem_{P;N}}\right) \qquad \text{Equação 17}$$

Onde:

$C_{P;N}$ *– Carga média por habitante (g)*

$US_{E_{P;N}}$ *– Cargas de esgoto sem tratamento que entram no sistema (pontuais e difusas).*

US_{SI_p}– Índice de população com atendimento por solução individual

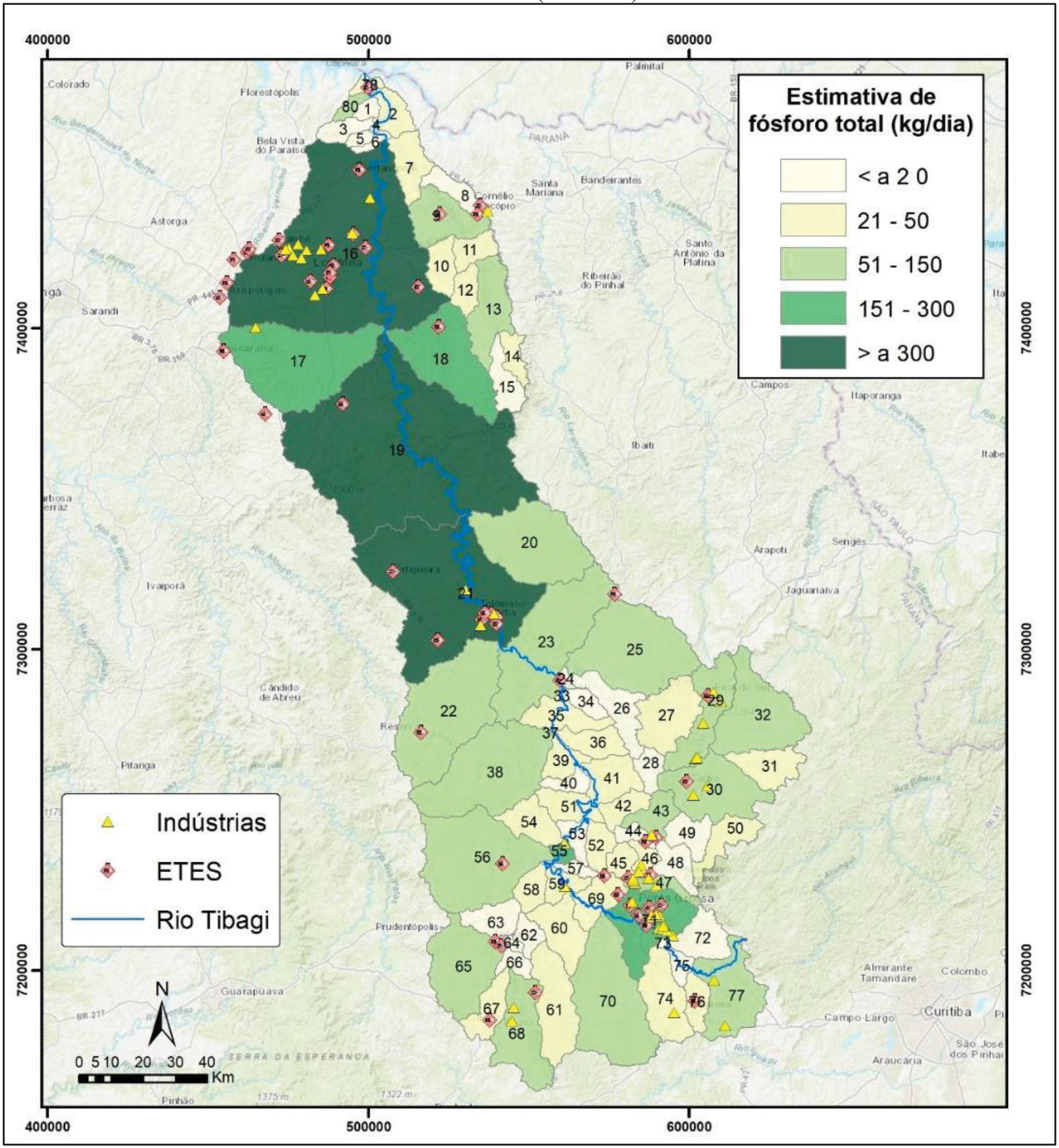
US_{Sem_p}– Índice de população sem atendimento

US_{Rede_p}– Índice de atendimento com coleta e sem tratamento

4.1.3 Resultados

A modelagem realizada estima as cargas potenciais que podem atingir o rio pelas vias pontuais e difusas. Os resultados da simulação fornecem um valor de fósforo total em quilograma por dia, valor médio para a bacia e não representa os picos de carga instantânea no caso de chuvas de intensidade alta. As faixas de carga mostradas na Figura 5 representam uma distribuição de quartil dos dados de cada uma das 80 sub-bacias da área de estudo.

FIGURE 5– ESTIMATIVA DE FÓSFORO TOTAL (KG/DIA) PARA A SUB-BACIA DE TIBAGI

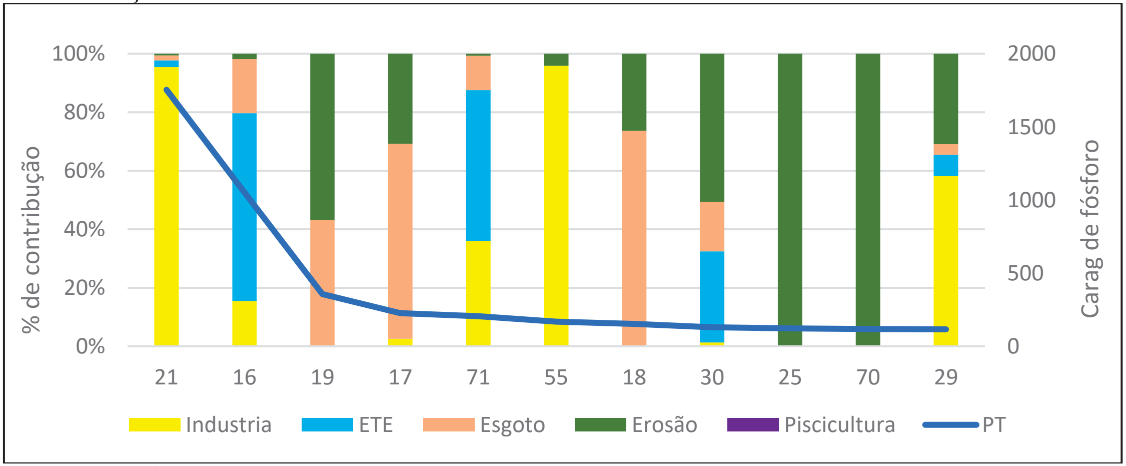


ELABORAÇÃO: O AUTOR (2021)

Só 3 bacias ultrapassam os 300 kg/dia, sendo elas, a bacia 16, a bacia 19 e a bacia 21 que correspondem às bacias onde foram identificados efluentes industriais e estações de tratamento com alta concentração de fósforo e uma vazão efluente alta. O principal ponto a destacar neste tipo de bacias com alta carga poluente via industrial, é que representam informações que são repassadas para as organizações ambientais, ou mesmo que foram estimadas baseadas na utilização de água que a indústria reportou. Levando-se a importância de ter um protocolo para a organização de dados georreferenciados e de licenciamento ambiental com os dados validados. Por outro lado, incentivar o setor industrial a repassar as informações reais para evitar superestimativas por falta de dados ou apresentação de dados incorretos. Além disso, levanta-se a questão da importância da transparência e compartilhamento das informações do licenciamento para o monitoramento das ações a serem feitas por cada setor, além de contar com estimativas mais acuradas.

Analisando as bacias que sobrepassam a taxas médias de 100 kg/dia de fósforo total (Figura 6), é possível notar tem uma proporção alta de cargas entrando no sistema de maneira pontual (cargas de indústrias e ETES) o que indica que na bacia hidrográfica do rio Tibagi existem problemas com cargas pontuais que poderiam ser diminuídas com ações voltadas a esse setor. Já as bacias 19, 18, 25 e 70 da mostram que a principal contribuição se deve a cargas difusas, seja por causa de esgoto não tratado ou ocupação agropecuária do terreno.

FIGURE 6 – FONTES DE POLUIÇÃO DAS BACIAS COM MAIS DE 100 KG/DIA DE EXPORTAÇÃO DE FÓSFORO TOTAL



ELABORAÇÃO: O AUTOR (2021)

As bacias com cargas de fósforo abaixo de 100 kg/dia representam, na sua maioria, áreas com menos população onde a principal fonte econômica é agricultura e pastagem. A ocupação agrícola, segundo Águas Paraná (2013), tem aumentado significativamente durante a década 2000-2010 com taxas de 3,53% ao ano, o que indica uma intensificação da agricultura na região. Como o mapa representa apenas um momento no tempo em 2012, é de se acreditar que atualmente, com o aumento da agricultura de irrigação e a tecnificação, a carga e a pressão sobre recurso tenha aumentado. Além disso, tem sido reportada a drenagem das várzeas (Águas Paraná, 2013), o que elimina o efeito de retenção de sedimentos desse tipo de ecossistema, podendo produzir um efeito sobre a velocidade e quantidade de carregamento de sedimentos para o rio.

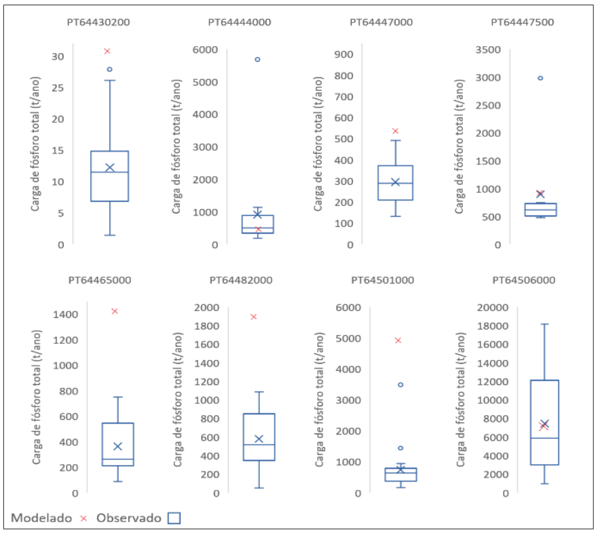
Para obter um comparativo dos resultados foram utilizados dados de monitoramento das estações disponíveis no SNIRH. Na Tabela 4, é apresentado um resumo dos dados existentes de vazão e concentração. Como pode ser visto, a quantidade de dados de concentração é muito pequena, o que torna a análise limitada a essa escassez.

TABLE 4 – RESUMO DOS DADOS DE MONITORAMENTO UTILIZADOS

Código da estação	Q_{10}	Q_{50}	Q_{90}	Média	Área afluente	Vazão	Fósforo Total	Fosfato Total
	----------------m^3/s		-------------		Km^2	----------Número de Registros		--------
64430200	23.5	5.7	1.2	9.1	426	275	20	24
64444000	389.0	121	36.5	184.1	4547	573	14	82
64447000	252.3	82.7	26.9	120.0	5727	11929	25	84
64447500	360.3	165.4	72.9	196.6	6258	1123	8	4
64465000	353.6	118.6	46.0	170.0	8925	24998	17	133
64482000	630.4	239.0	96.2	312.6	13778	3858	17	52
64491000	398.3	161.0	68.4	231.3	16106	11798	0	52
64501000	749.8	286.5	119.0	380.7	18948	13479	21	88
64506000	866.2	348.2	145.6	443.0	20444	9389	11	17
64507000	755.2	267.0	104.7	376.5	23029	24694	0	32

A carga observada conforme descrito na metodologia plotada em formato boxplot, junto com a carga estimada pelo modelo (Figura 7) para Fósforo total. Todas as cargas das sub-bacias contribuintes à estação de monitoramento foram somadas para compor a carga estimada. Os valores da modelagem em algumas estações se aproximam à mediana calculada, em outras o modelo superestima para suas respectivas estações.

FIGURE 7 – COMPARATIVO DOS RESULTADOS DE FÓSFORO TOTAL COM OS DADOS DE MONITORAMENTO



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4.1.4 Reflexões sobre a estimativa

O principal problema encontrado é que os dados de monitoramento são insuficientes para poder obter uma avaliação da performance da modelagem. Entre as possíveis causas de incerteza relacionadas aos dados de monitoramento podemos mencionar: i) O monitoramento da qualidade da água é escasso temporalmente. Os registros contam em média com 2 medidas por ano, ou seja, um dado semestral, sendo que a qualidade da água pode variar em eventos de chuva e dependendo do comportamento temporal das cargas pontuais. ii) Os dados de monitoramento de vazão e de qualidade não são concomitantes, uma vez que as campanhas de coleta de descarga de vazão e qualidade não são feitas em conjunto. O que traduz num erro na estimativa da carga observada, e sua vez gera uma incerteza sobre o dado utilizado no comparativo. iii) Além da pequena quantidade de dados de concentração, é desconhecida a condição climática do dia da coleta, que pode ser predominantemente em condição sem chuva, por exemplo, e a amostra ser tomada sem presença de cargas difusas pelo escoamento superficial e erosão, só de cargas pontuais. vi) Pode existir um fenômeno de histerese onde a concentração da substância pode ser diferente para uma mesma vazão. Sendo observado uma diferença da concentração coletada na vazão de subida e na vazão de descida. Acredita-se que esse fenômeno se deve aos processos de mobilização, transporte e deposição que ocorrem e ao tipo de fonte que gerou a substância (Minella, 2011 e Thomann & Mueller, 1987). v). Desconhecimento das variações do método de análise laboratorial da substância.

Obviamente, não é possível descartar os problemas relacionados a dados de entrada, podendo mencionar: Falta de controle nos relatórios de descarga das indústrias. Falta da localização geográfica dos pontos de descarga dos efluentes provenientes de fontes pontuais, Falta de conhecimento sobre a realidade do saneamento rural e falta de saneamento básico nas localidades avaliadas. Desconhecimento dos métodos de boas práticas utilizados nas atividades agropecuárias. Este trabalho sugere a necessidade de avaliar a incerteza nas estimativas de cargas poluentes. É evidente que as simplificações dos processos físicos existentes nas bacias, são apenas uma representação limitada do mundo real. Fato que gera uma preocupação sobre as lacunas, transparência e incerteza desses modelos e como eles influenciam nas decisões a serem tomadas. Ainda assim, se destaca a importância da estimativa de cargas poluentes pode ser uma ferramenta valiosa para o suporte à decisão no gerenciamento de bacias hidrográficas. De acordo com Ma, (2019), o risco é que as decisões possam estar completamente eradas pode acontecer quando o problema é muito complexo e enquanto os dados são limitados em qualidade e quantidade.

Em conclusão, se espera que no final desta pesquisa se determinem os passos para avaliar as incertezas dos modelos utilizados para gestão. E verificar então, a incerteza de maneira justa e transparente a fim de garantir que as entradas utilizadas, assim como as suposições tomadas e as variáveis fornecidas pelos modelos sejam compatíveis com as decisões a serem tomadas.

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AGRADECIMENTOS - O estudo apresentado está inserido no projeto de auxílio ao Enquadramento dos Rios Paranapanema e Itararé, estabelecido em parceria entre a Agência Nacional das Águas (ANA) e a Universidade Federal do Paraná (UFPR). Os autores agradecem à ANA pelo suporte e a todos os pesquisadores e colaboradores envolvidos no projeto.

4.2 Paper II: Evaluating diffuse and point sources in sub-watersheds using an GIS-Based Pollutant Loads Estimative.

HIGHLIGHTS:

This part of the research concerns the generation of the computational algorithms and data processing processes necessary to perform the MoRE GIS estimates.

Corresponds to the article in preparation.

Abstract

In Brazil, water scarcity and quality issues are prominent, especially in semi-arid regions with inherent scarcity and in areas with high-water demand such as cities and irrigated zones. These challenges arise from both natural factors and climate pattern alterations, including a prolonged drought spanning from 2012 to 2017, and a widespread one in 2020 across most of Brazil (ANA, 2021; Grimm et al., 2020). To attend the complexity inherent to water quality mathematical models are often employed to assist in decision-making processes. In this research we enhance a regionalized model through a Geographic Information System (GIS) to estimate the pollutant loads from diffuse and point sources. In this article we discuss how modeling can effectively identify pollutant sources and prioritize actions in sub-watersheds to improve the water quality.

Keywords: GIS-based, pollutant loads, watershed modeling, Best Management practices.

4.2.1 Introduction

Pollutant load modeling is a transcendental process for the understanding and mitigation of environmental impacts. A holistic understanding of point and diffuse sources is essential to address interconnected issues and pathways that affect water quality (Pizella & Souza, 2007). To attend to the complexity inherent to water quality mathematical models are often employed to assist in decision-making processes (Cho et al., 2019; Hamel et al., 2020; Dinar & Quinn, 2022).

This discussion embarks on an exploration of diverse hydrological models designed to unravel the complexities of pollutant loads originating from agricultural, urban, and industrial sources. From the Water Erosion Prediction Project (WEEP) by USDA (1995) to the Integrated Valuation of Environmental Services and Tradeoffs

(InVEST) by Sharp et al. (2016), these models serve as indispensable tools in our pursuit of a clearer understanding of water quality dynamics.

As human's landscapes advance with increased industrial activities, rapid urbanization, and intensified agriculture, the demand for models capable of predicting pollutant loads from both diffuse and point sources becomes more pressing. Within this context, models like the Storm Water Management Model (SWMM) by Rossman (2015) and the Storage, Treatment, Overflow, Runoff Model (STORM) by US Army Corps of Engineers (1977) emerge as stalwarts, offering solutions tailored to the challenges posed by urban pollution.

The ongoing efforts in model development reflect a commitment to encompassing estimations from various sources, as evidenced by models like Soil & Water Assessment Tool (SWAT) by Neitsch et al. (2011), Modeling of Regionalized Emissions (MoRE) by Fuchs et al. (2012), and the Hydrological Simulation Program – Fortran (HSPF) by Tetra Tech (2017).

Case studies featuring the InVEST model mapping sediment production and SWAT evaluating the impact of land use classification in the Camboriú watershed illuminate how modeling not only informs but also influences decision-making processes (Kroeger et al., 2019 Fisher et al., 2018).

However, this journey through hydrological modeling contains its own challenges. The inherent uncertainties demand meticulous calibration efforts, as evidenced by studies comparing models such as SWAT and HSPF in predicting the impact of urban expansion and cropland reduction (Chen et al., 2019). It is within this intricate landscape that the importance of aligning model selection with decision-makers' requirements becomes paramount.

MoRE, POLAD, InVest, STORM, LSPC, WEEP, and SWIM lack a water routing algorithm. SWAT faces challenges in parameterization, calibration, and data requirements (Fuchs et al., 2017). Despite limitations, SPARROW and MoRE offer decision-making support for achieving ecological water quality standards on various scales (Fuchs et al., 2012; Schwarz et al., 2006). SPARROW requires a detailed station network, impractical for Brazil, while MoRE is open source and adaptable to local conditions.

The aim of this work is to underscore the indispensable role of these tools in shaping sustainable water resource management. In this research we enhance a model through GIS to estimate the pollutant loads from diffuse and point source and discuss how modeling can effectively identify pollutant sources and prioritize actions in sub-watersheds to improve the water quality.

4.2.2 Study area

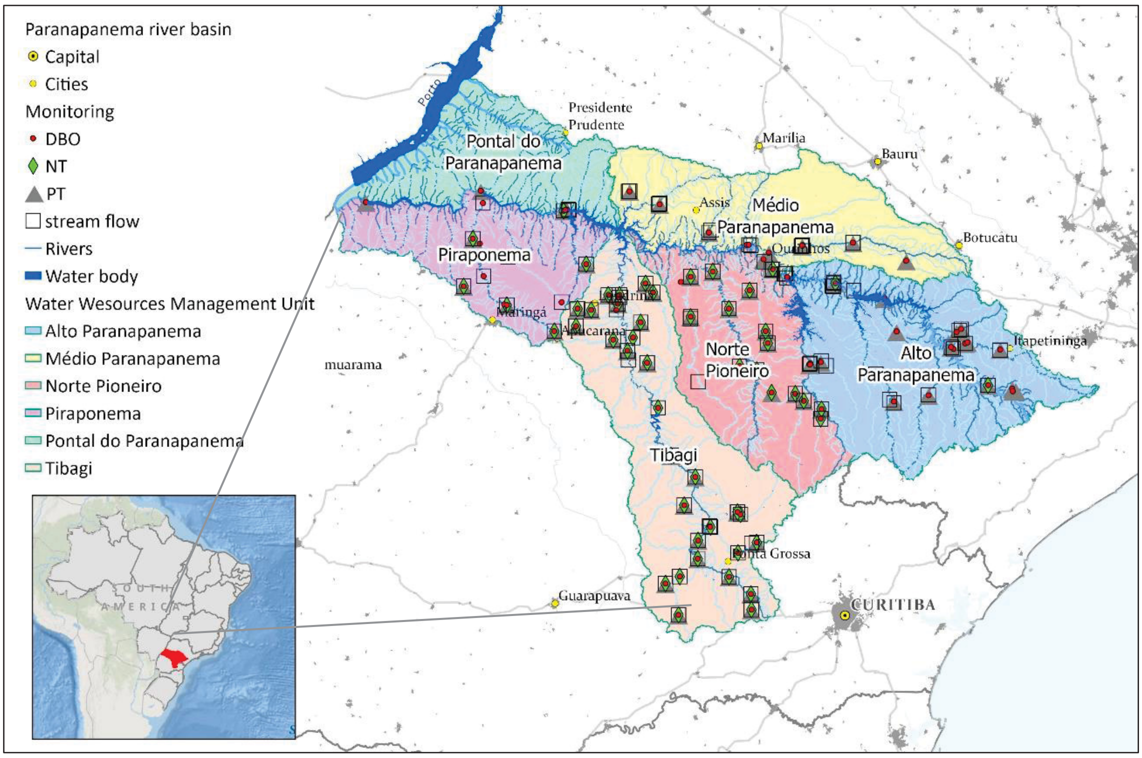
The Paranapanema River basin, situated in Brazil, is an interdepartmental basin that demands extensive organizational efforts from various institutions. The basin is a highly agricultural region. The 2020 land use and occupancy map revealed a breakdown of 75% for agricultural activities, 22% of the areas covered by vegetation, 1% for urban areas, and 2% for water bodies. The primary agricultural activity involves soybean cultivation, covering approximately 25% of the area. The second most significant cultivation is pastureland, accounting for 15%, alongside mosaic agriculture, also contributing 15% to the basin. The basin is divided into 6 watershed resources management units (UGRH by Portuguese translation of *Unidade de Gestão de Recursos Hídricos*) with different characteristics each.

The Norte Pionero has the highest average slope, reaching 13%. In this area, agricultural and livestock farming activities cover 65% of the region and forest plantations occupy 11% of the territory, while 20% is covered by natural vegetation. Tibagi and Alto Paranapanema, with average slopes of 12%, also have high percentages of agricultural coverage, reaching 58% and 53%, respectively. Forest plantations are a significant activity in these units, representing 11% and 16% of the area, while the largest natural vegetation coverages are concentrated in Tibagi (26%) and Alto Paranapanema (24%).

The Medio Paranapanema, Piraponema, and Pontal de Paranapanema units have average slopes of 7%, 6%, and 5%, respectively. In these areas, lands dedicated to agriculture and pasture cover 76%, 86%, and 84%, respectively. The Medio Paranapanema unit has 8% of its area dedicated to forest plantations, while the other two do not have this economic activity. In addition to having the largest agricultural areas, these units also exhibit the lowest natural vegetation coverage, with 11% for Medio Paranapanema, 8% for Piraponema, and 9% for Pontal de Paraná.

All management units have urban coverage of less than 2%, considering that the most important factor in determining sources of pollution is the number of people and not the coverage area. Alto Paranapanema has an urban population of 603,467 inhabitants, Medio Paranapanema has 582,408 inhabitants, Norte Pionero has 402,299 inhabitants, Piraponema has 727,796 inhabitants, Pontal de Paraná has 360,167 inhabitants, and Tibagi has 1,444,176 inhabitants.

FIGURE 8 – PARANAPANEMA RIVER BASIN AND LOCATION IN BRAZIL



SOURCE: ELABORATED THE AUTHOR

4.2.3 Data preparation

The data used in the load estimate is presented in Table 5. These data primarily come from institutional databases and the Integrated Plan for Water Resources of the Paranapanema River Basin (PIRH). In some approaches, it was noted that there are more representative load data available, but they are not accessible, such as pollutant load declarations from industry self-monitoring. Additionally, differences in available information were found between Paraná and São Paulo statal agencies, which hinders the application of methodologies. Standardizing basic data for management in Brazilian states in order to harmonize databases could facilitate the application of models in federal basins.

TABLE 5 – DATA DESCRIPTION AND SOURCES

	Pathway	Input data	Source	Descriptions
1	Pisciculture	Concentration of TP and TN	GIA, 2013	Local study in the Paranapanema basin

	Pathway	Input data	Source	Descriptions
2	Industry	Outflow rate	IAT, DAEE, and ANA	The discharged effluent was not accessible, the water concessions for discharge was used
		Concentration	IAT	Literature data for discharge limits by industrial type and effluent discharge limits permitted by legislation
3	WWTP	Population served; Per capita load Treatment efficiency	ANA	Sewer atlas: Treatment efficiency for TP andTNbased on literature and removal technology information for each WWTP
4	Erosion	Digital Elevation Model (DEM)	SRTM	Shuttle Radar Topography Mission: Data derived from the 30-meter base of the mission with void correction.
		Land use and land cover map (LULC)	PIRH Paranapanema	LULC, from MapBiomas 6, 2020, with a 30 meters pixel.
		Soil type	PIRH Paranapanema	Plano Integrado de Recursos Hídricos da Unidade de Gestão de Recursos Hídricos Paranapanema (PIRH Paranapanema)
			SNIRH e DAEE	Precipitation from 25 monitoring stations
5	Untreated Domestic Effluent	Population without WWTP service Per capita load Treatment average efficiency	ANA; IBGE.	Sewer atlas: Population without sewage collection and Population with sewage collection and treatment and Population served with individual sewage solution.
6	Surface runoff from natural areas with vegetation	Precipitation LULC	Hydrosheet (Linke. S, 2019)	Estimated using the Runoff curve number from Soil Conservation Service (SCS) model f in each sub-basin
7	Atmospheric Deposition	Atmospheric deposition rate of the substance		Literature from different studies
		Surface area of water bodies	PIRH Paranapanema	
8	Groundwater Flow	Substance concentration	CPRM	Wells readings data from Rede Integrada de Monitoramento das Águas Subterrâneas - RIMAS
		Outcropping aquifers layer	PIRH Paranapanema	
		Low rate flow (Q95)	Hydrosheet (Linke. S, 2019)	

For comparative purposes the observed data was acquired from the National Information System on Water Resources, including data from the National Agency of Water. A total of 64 stations where data on total phosphorus (TP) concentration could be found, 49 stations with total nitrogen (TN) concentration, and 81 with biochemical oxygen demand (BOD) data, where it’s possible to match with flow data. To estimate the loads, the concentration averages were used for all cases, and the median flow in the station (localization in Figure 8).

4.2.4 Description of the modeling framework "Modeling of Regionalized Emissions"

For estimating pollutant loads, we adapted the concepts and algorithms from the Modeling of Regionalized Emissions (MoRE) model, as proposed by Fuchs et al. (2012). This model, designed for decision-making, offers strategic guidance to attain a favorable ecological state in surface water bodies, aligning with predefined quality standards. Originating in response to the European Union Framework Directive 2008/105/EC (Fuchs & Brecht, 2022). MoRE plays a pivotal role in establishing environmental quality standards within the water policy domain. MoRE operates as a tabular model wherein all attributes are linked to a unique identifier. These attributes undergo algorithms within an open-access processor, forming the computational backbone of the model. Adaptations of MoRE's algorithms were made to suit data availability and the specific physical processes observed in Brazil (Rieke et al., 2021; Acosta et al., 2021). The principal algorithms are presented in Table 6.

TABLE 6 – LIST OF MORE EQUATIONS FOR ESTIMATING SUBSTANCE EMISSIONS VIA EROSION (TONS BY YEAR)

Name	**Algorithm**	**Description**
Erosion Equation 1	$RUSLE = R \cdot K \cdot CP \cdot LS$	$RUSLE$– Historical average soil loss per unit of area and time (t/(ha·year); R– Rainfall erosivity (MJ·mm/(ha·h· year)); K – Soil erodibility (t·h/(MJ·mm)); CP– Land use and land cover, management, and conservation practices. LS– Slope length and average gradient.
Erosion Equation 2	$ER_{SD_{corr}} = \Big(\big(ER_{AL_{sl}} \cdot IM_{AL_{total}} \cdot \big) + \big(BI_{GL_A} \cdot BI_{GL_{SL}} \big) + \big(BI_{SIL_{SL}} \cdot BI_{SIL_A} \big) + \big(ER_{NAT_{sl}} \cdot BI_{NAT_A} \cdot \big) + \big(BI_{CAM_A} \cdot BI_{CAM_{SL}} \big) \Big) \cdot 100 \cdot ER_{PREC_{corr}}$	$ER_{SD_{corr}}$ – Corrected erosion loss (t/ha); $ER_{AL_{sl}}$ – Average erosion rate for each crop according to slope (t/ha/year); $IM_{AL_{total}}$ – Areas within the analysis unit with agriculture (km^2); BI_{GL_A}– Areas within the analysis unit with pasture (km^2); $BI_{GL_{SL}}$– Average erosion rate for pasture (t/ha/ year); $BI_{SIL_{SL}}$– Average erosion rate for forestry (t/ha/ year); BI_{SIL_A}– Areas within the analysis unit with forestry (km2); $ER_{NAT_{sl}}$– Average erosion rate for native forest cover (t/ha/ year) BI_{NAT_A}.– Areas within the analysis unit with native forest cover (km^2); BI_{CAM_A}– Areas within the analysis unit with natural grassland cover (km^2); $BI_{CAM_{SL}}$– Average erosion rate for natural grassland areas (t/ha/year).

Name	Algorithm	Description
		$ER_{PREC_{corr}}$– Correction factor based on annual precipitation.
Erosion Equation 3	$ER_{SDR} = CE1 \cdot \left(BL_{slope} + CE4\right)^{CE2} \cdot (A_{al})^{CE3}$	ER_{SDR} – Sediment delivery rate (%); BL_{slope} – Average slope of the analysis unit (%); A_{al} – Percentage of agricultural soil within the Analysis Unit (%); CE_x– Model constants, CE1=0.00668; CE2=0.3; CE3=1.5; CE4= -0.25.
Erosion Equation 4	$ER_{SDR_{in}} = ER_{SD_{corr}} \cdot ER_{SDR}$	$ER_{SDR_{in}}$ – Sediment exportation (t/year); $ER_{SD_{corr}}$– Corrected erosion loss (t/ha); ER_{SDR} – Sediment delivery rate (%);
Erosion Equation 5	$ER_{ENR} = CE_7 \cdot \left(\frac{ER_{SDR}}{BI_{AU_A}}\right)^{CE_9}$	ER_{ENR} – Enrichment rate; $ER_{SDR_{in}}$ – Sediment exportation (t/year); BI_{AU_A} – Analysis unit area (km^2); CE_7 – Enrichment factor for phosphorus (18); CE_9 – Default value -0,47
Erosion Equation 6	$ER_{E_P} = \frac{ER_{CONT_{topsoil_P}}}{10^6} \cdot \left(ER_{SED_{in}} - ER_{NATCOV_{SL}}\right) \cdot ER_{ENR} + \frac{ER_{CONT_{geo_P}}}{10^6} \cdot ER_{NATCOV_{SL}}$	ER_{E_P} – Phosphorus emissions via soil loss on agriculture areas (t/ year); $ER_{CONT_{topsoil_P}}$– Phosphorus content in topsoil (mg/kg); $ER_{SED_{in}}$– Sediment exportation rate (t/year); $ER_{NATCOV_{SL}}$– Soil loss in natural cover areas (t/ year); ER_{ENR_P}– Phosphorus enrichment rate (dimensionless);; $ER_{CONT_{geo_P}}$– Phosphorus content in soil (geology) (mg/kg);
Erosion Equation 7	$ER_{E_N} = \left(\frac{ER_{CONT_{topsoil_N}}}{10^6} \cdot ER_{AGRL_{SL}} \cdot SR_{SDR} \cdot ER_{ENR}\right) + \left(ER_{NATCOV_{SL}} \cdot \frac{ER_{CONT_{geo_N}}}{10^6}\right)$	ER_{E_N} – Nitrogen Emissions via Erosion (t/a); $ER_{CONT_{topsoil_N}}$– Nitrogen content in topsoil (mg/kg) $ER_{SED_{in}}$– Sediment exportation (t/year); $ER_{NATCOV_{SL}}$– Natural cover loss from natural cover (t/a); $ER_{AGRL_{SL}}$– Soil loss in agricultural areas (t/ year); ER_{ENR_N}– Enrichment rate (dimensionless); $R_{CONT_{geo_N}}$– Nitrogen content in soil (geology) (mg/kg)
Untreated Domestic Effluent Equation 8	$US_{E_{P;N}} = \left(US_{SI_{P;N}} \cdot C_{P;N} + US_{Rede_{P;N}} \cdot c_{P;N} + US_{Sem_{P;N}}\right)$	$C_{P;N}$ – Average load per capita (g) N or P $US_{E_{P;N}}$– Loads of untreated sewage entering the system (not treated by WWTP) (t/year). US_{SI_p}– Index of population with individual sanitation solutions. US_{Sem_p}– Index of population without access. US_{Rede_p}– Index of population with collection systems but without treatment
WWTP loads Equation 9	$WWTP_{E_P} = Q_{ef} \cdot C_{wwtp} \cdot Coef_{unid}$	$WWTP_{E_P}$ – Substance exportation via WWTP (t/year); Q_{ef} – Effluent flow from WWTS m^3/s C_{wwtp} – Pollutant concentration in the effluent from WWTS in mg/l
Surface runoff Equation 10	$SR_{E_{P;N}} = \left(SR_{Q_{P;N}} \cdot SRC_{P;N}\right)$	$SR_{E_{P;N}}$– Substance exportation in overland flow (t/year); $SRC_{P;N}$ – Substance concentration in runoff from vegetation-covered surfaces (mg/l); $SR_{Q_{P;N}}$– Surface runoff flow (m3/s)

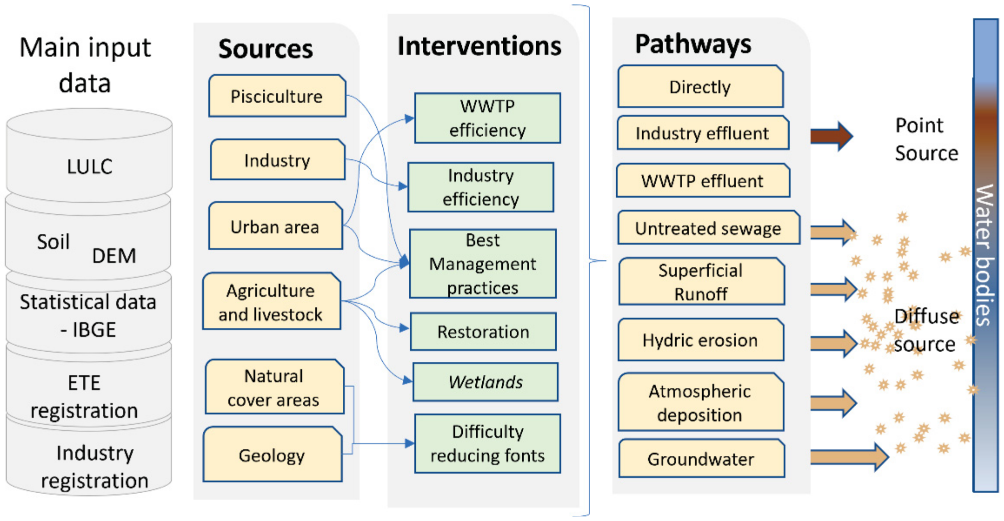
Name	Algorithm	Description
Industrial Load Equation 11	$ID_{E_P} = Q_{out} \cdot C_{subs} \cdot Coef_{unid}$	ID_{E_P} – Substance exportation via industrial discharge (t/ year); Q_{out}– Licensed flow rate (m³/s); C_{subs}– Concentration of the substance in industrial effluent (mg/L); $Coef_{unid}$ – Unit conversion coefficient (t·s·L/(mg·year·m³)).
Atmospheric Deposition Equation 12	$AD_{E_{P;N}} = \left(AD_{r_{P;N}} \cdot IM_{ws}\right)$	$AD_{E_{P;N}}$– Substance loads via atmospheric deposition (t/a); $AD_{r_{P;N}}$ – Substance deposition rate (mg/m^2); IM_{ws} – Water Surface Area, Total (km^2)
Pisciculture Equation 13	$Ps_{P;N} = PSC_{P;N} \cdot Aq_a$	$PS_{P;N}$ – Substance loads by pisciculture; $PSC_{P;N}$ – Quantity of substance input into the water body (kgP/ha/ano); Aq_a – Area of the aquaculture site (ha)

Three routines address point sources, incorporating effluents from treatment plants, industrial effluents, and aquaculture, while five routines refer to diffuse sources. The last includes untreated sewage, diffuse loads from land use and natural cover (divided into water erosion and surface runoff paths), atmospheric deposition, and groundwater. Despite the model's predominantly tabular structure, its effectiveness is contingent on processing a substantial volume of data. Recognizing this challenge, we implemented data processing routines utilizing the Model Builder tool within ArcGIS, with the USLE methodologies incorporated into Google Engine (GEE). The code and visual representations of these routines can be found in the Appendix 1.

4.2.5 Strategies for Load Reduction and Basin Prioritization

To determine the strategies for load reduction first were ranking the watershed with the mayor loads estimative and recognizing the principal sources. Figure 8 shows the main sources and pathways of the model and highlights the possibilities of strategies of reduction.

FIGURE 8 - SCHEME OF THE POLLUTANT LOAD ESTIMATION MODEL REDUCTION



SOURCE: ELABORATED BY THE AUTHOR

A specific portfolio of strategies was defined including three types of interventions (Table 7). First the improvements in the efficiency of Wastewater Treatment Plants (WWTPs). Second, improvements in the treatment of industrial effluents, and for agricultural areas, a reduction of erosion lost using the restoration of Riparian Protection Areas (identified in the study of environmental constraints) and good agricultural practices.

TABLE 7 – DEFINITIONS AND VALUES USED FOR REDUCTION STRATEGY

Source	Base line	Definitions	
Industry	Concentration used was 5mg/l for TP, 10mg/l for TN and BOD 50 mg/l	Reduction of phosphorus concentration in industries with water use more than 500 m3/h	Reduction in 50% the concentration in effluent to 5 mg/l For total phosphorus incorporate de reduction with treatment 2,5 mg/l
Erosion and surface runoff		Increase in agricultural practices by 20%	Factor P of USLE equation modified in -.2% for agriculture and pasture areas.
WWTP		Efficiency of treatment plants	Increase the efficiency to 90% for BOD, in 50% for TP and 75% for TN.

Initially, the potential load reduction was estimated by comparing the results of scenarios with the reductions achieved when interventions were applied in the basin through the overlay of maps. To estimate the reduction in the basin the differential between scenarios was calculated with the equation 18.

$$\Delta_r = Loads_{i,j} - Loads_{i,j,m} \qquad \text{Equation 18}$$

Where:

Δ_r – is potential reduction in kg by day $\left(\frac{kg}{day}\right)$ in each basin;

$Loads_{i,j}$ – is the estimate of loads in the basins for each scenario "i" and for each parameter "j";

$Loads_{ij,m}$ – is the load estimate resulting from the application of alternative pollution control measures in the basins "m", for the scenario"i" and each parameter "j".

The achieve a relevant basin priority definition of areas where the implementation could be necessary. The equation 19 was used to estimate the

$$\beta_p = \frac{\sum \Delta_{rj}}{n} \qquad \text{Equation 19}$$

Where:

Δ_{rj} – is potential reduction in kg by day (%) in each basin for each parameter.

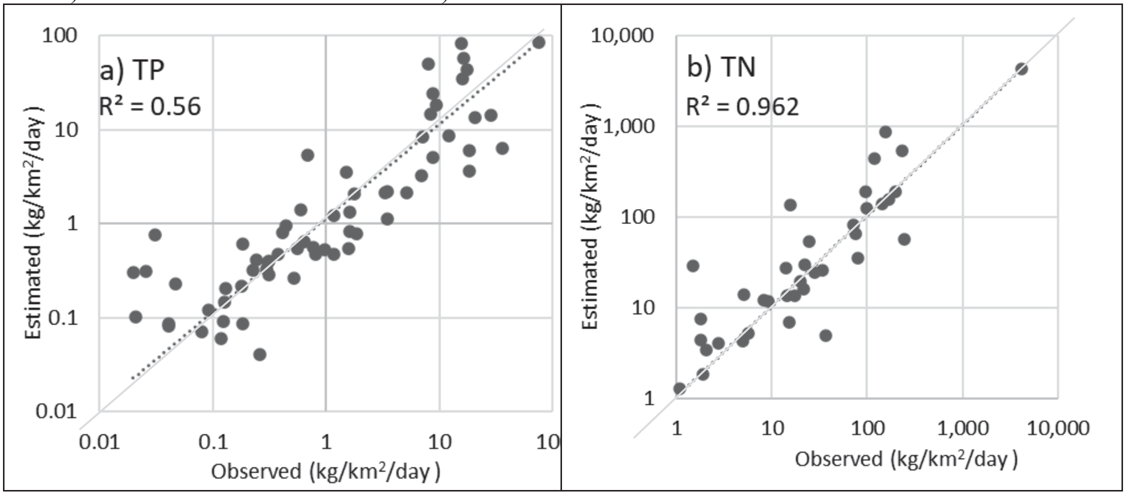
n – the number of substances evaluated in the basin.

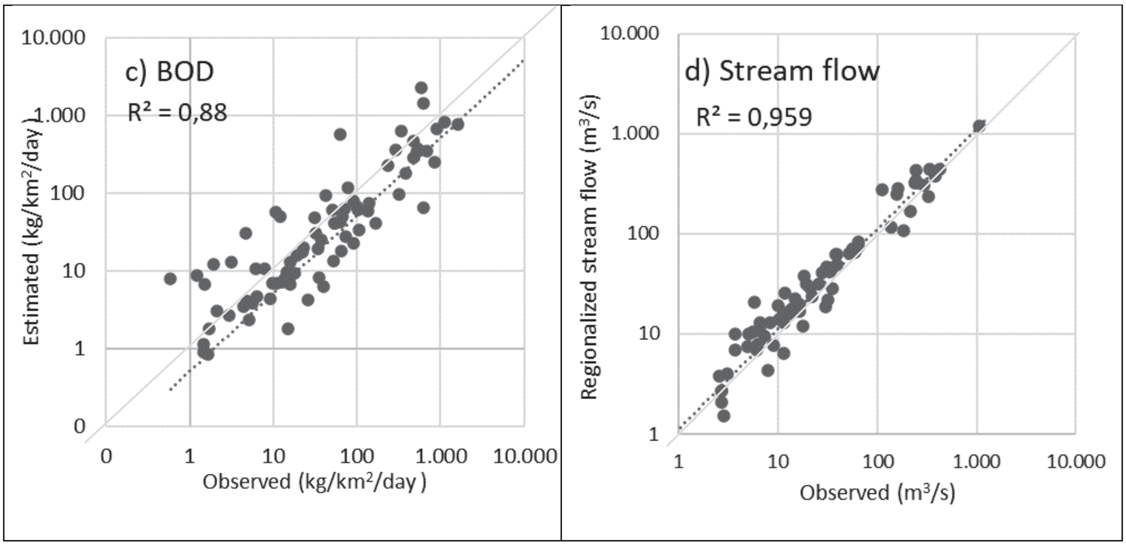
4.2.6 Results

4.2.6.1 Model performance

Figure 9 shows the comparative for the model for the 3 substances (TN, TP and BOD) and the comparative also for water flow. Each point represents the cumulative load in the watershed estimative (kg/km^2/day) and its respective observed data in the principal river of the watershed. The results show an expected trend with R^2 > a 0.5 for PT, 0.96 for TN and 0.8 for BOD and > 0.9 for stream flow. While the model implemented lacks the capacity to accurately represent intricate processes within the water body, such as sedimentation, resuspension, and bank erosion. It is important to note that a one-to-one linear tendency is not anticipated, and the graphs are better suited to explain adjustments in rank order rather than serving as a calibration.

FIGURE 9 – COMPARATIVE OBSERVED DATA AND ESTIMATED LOADS FOR A) PT; B) TN AND C) BOD IN KG/KM2/DAY AND D) STREAM FLOW IN M^3/S





SOURCE: ELABORATED THE AUTHOR

However, the improvement is not only to the model uncertainty but also in the observed data. There is a lack of temporal data in the stations and some of them don't have enough observed measures to represent all the hydrologic periods, some of them with just 2 samples in a year.

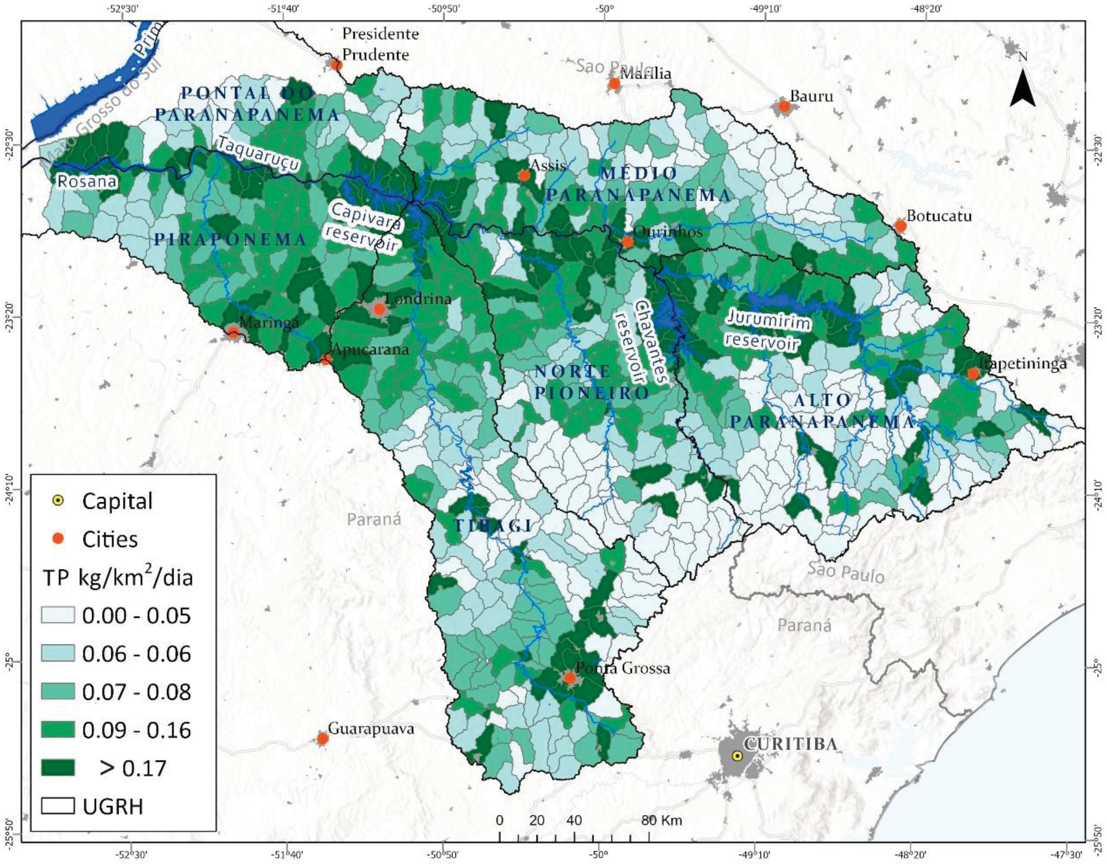
An additional aspect to highlight is that, despite the possibility of updating land use and land cover data annually, certain databases, such as census data, industry effluent information, and wastewater treatment plant (WWTP) efficiency data, pose challenges for regular updates. The availability of these data depends on various agencies and institutions, and acquiring this information may not be feasible on an annual basis.

4.2.6.2 Spatial distribution of nutrient exportation (PT and NT) and BOD

The estimation of pollutant loads was conducted in analysis units, totaling 784 sub-basins with an average area of 129 km^2. We also subset the Water Management Units (UGRH for *Unidade de Gestão de Recursos Hídricos* in Portuguese) to determine the main contribution to Paranapanema river.

In Figure 10, a range of load values is represented, with darker tones signifying greater substance production. Specifically for phosphorus, 30 basins exhibit loads surpassing 0.5 kilograms per square kilometer per day (kg/km2/day), distributed among planning units. This includes 12 basins in Tibagi, 12 basins in Tibagi, 4 in Alto Paranapanema, 4 in Medio Paranapanema, and 4 in Piraponema, along with 3 basins in Norte Pionero and 3 in Pontal de Paranapanema. Basins exhibiting elevated phosphorus loads are primarily located in regions characterized by dense urban populations and intensive agricultural activities, notably in proximity to cities with populations exceeding 100,000 inhabitants. These cities include Ponta Grossa, Apucarana, Londrina, Ourinhos, Assis, and Itapetininga, where both wastewater treatment plants (WWTP) and untreated wastewater contribute significantly to the phosphorus load.

FIGURE 10 – ESTIMATIVE OF LOADS PRODUCTION OF TOTAL PHOSPHORUS IN KG/KM²/DAY



SOURCE: ELABORATED THE AUTHOR

Figure 11 shows the total nitrogen estimates for the entire Paranapanema basin. When analyzing basins with loads exceeding 2,1 kilograms per square kilometer per day, Tibagi analysis unit has the highest number of watersheds in the range, containing 22 sub-basins with high nitrogen exports. In 13 of them, effluents from treatment plants account for over 50% of exports, while in the others, the contribution is shared between effluents and erosion from agricultural areas. Three of the basins located in the Tibagi planning basin, situated in the main river (Tibagi river), show significant loads related to industries, with percentage values of 83%, 50%, and 80%, respectively.

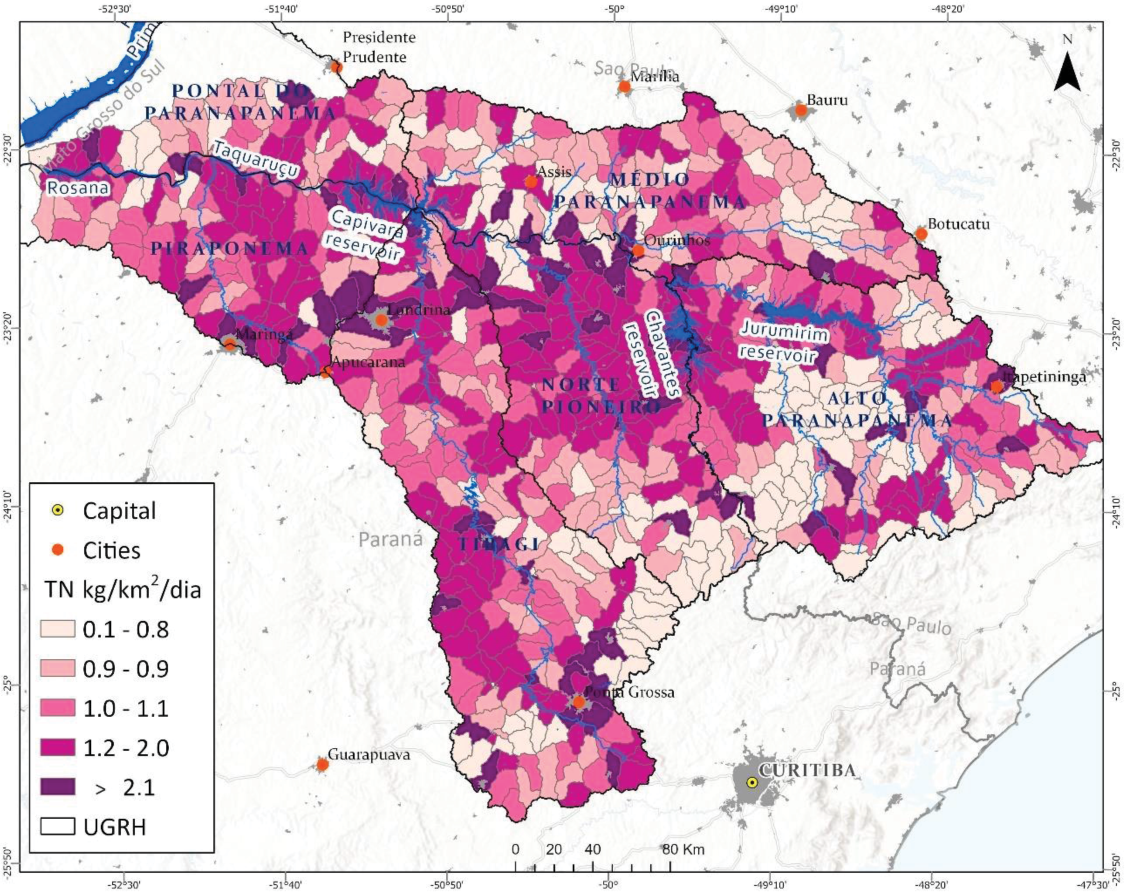
The Norte Pionero region exhibits 15 sub-basins within this export range, of which 8 have exports of over 50% from wastewater treatment plant effluents. In the others, the distribution is more diffuse, with pollutants coming from water erosion, ranging from

19% to 48%.

The Alto Paranapanema has 13 basins with loads exceeding 2 kg/km^2/day, with 4 of them having point WWTP source effluents as the main contributors. On the other hand, some sub-watershed with over 60% of the territory covered by water have high percentage contributions from atmospheric deposition and fish farming.

The Piraponema unit, totaling 11 sub-watersheds, the Meio Paranapanema, with 7 sub-basins, and the Pontal de Paranapanema, with 4, exhibit a more equitable distribution of loads, with significant contributions from wastewater treatment plant effluents and water erosion from agricultural lands.

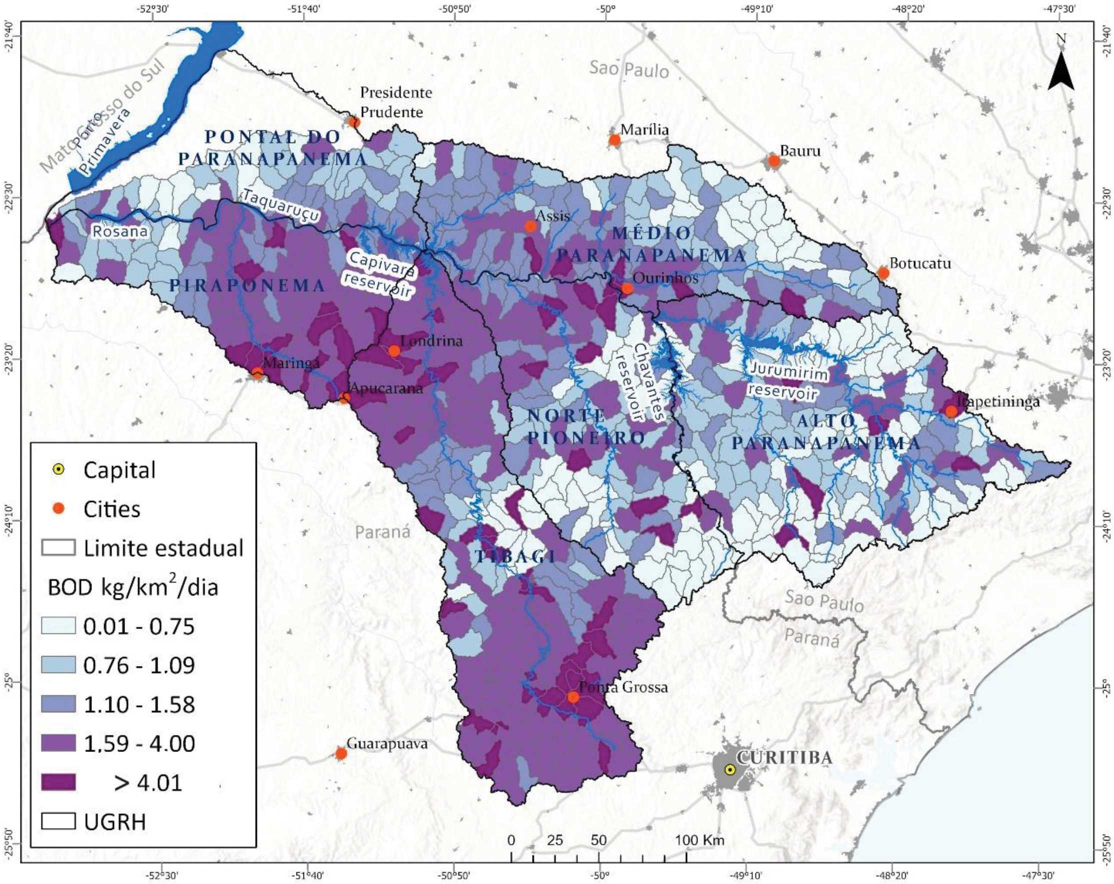
FIGURE 11 – ESTIMATIVE OF LOADS PRODUCTION OF NITROGEN, IN KG/KM^2/DAY



SOURCE: ELABORATED THE AUTHOR

Figure 12 illustrates the spatial distribution of nutrient exportation and BOD in watersheds. The Tibagi Unit is where there is the greatest contribution of BOD loads. Analyzing those sub watershed where the load exceeds 4 kg/km^2/day, we find that 32 sub-watersheds are in Tibagi, without a notable trend of origin. Six basins have more than 60% industrial sources, seven basins have over 50% contribution from wastewater treatment plants (WWTP), five basins where the main contribution is surface runoff, and three basins with a high percentage from untreated sewage. The others have distributions from all sources less than 50%. The second unit with higher load rates is Piraponema, with 14 basins above 4 kg, including five basins where the main source is effluent from the treatment plant with over 60% of the contribution. The Norte Pionero takes the third place with 11 sub-basins, of which two have contributions greater than 60% from WWTP, two from industrial sources exceeding 69%, and one from untreated sewage in an urban area with 76% of the contribution. The rest do not have a representative source and are distributed in various sources. The Alto Paranapanema has five sub-basins where the main source is industrial, and the Medio Paranapanema has three basins with high concentrations from WWTP and one with an industrial source exceeding 83% of BOD export.

FIGURE 12 – ESTIMATIVE OF LOADS PRODUCTION OF BOD, IN KG/ KM^2/DAY.



SOURCE: ELABORATED THE AUTHOR

4.2.6.3 Sources of Phosphorus, Nitrogen and BOD

One of the focal points of the work involved the identification of the main sources of pollutants to characterize the basin and make the best decision to achieve the goals of water quality. In the figure 13 it is possible to analyze which are the principal contributions by UGRH and which source is the most important to the contribution for Paranapanema river and the maps on the right show a representation of the accumulated substance in the river.

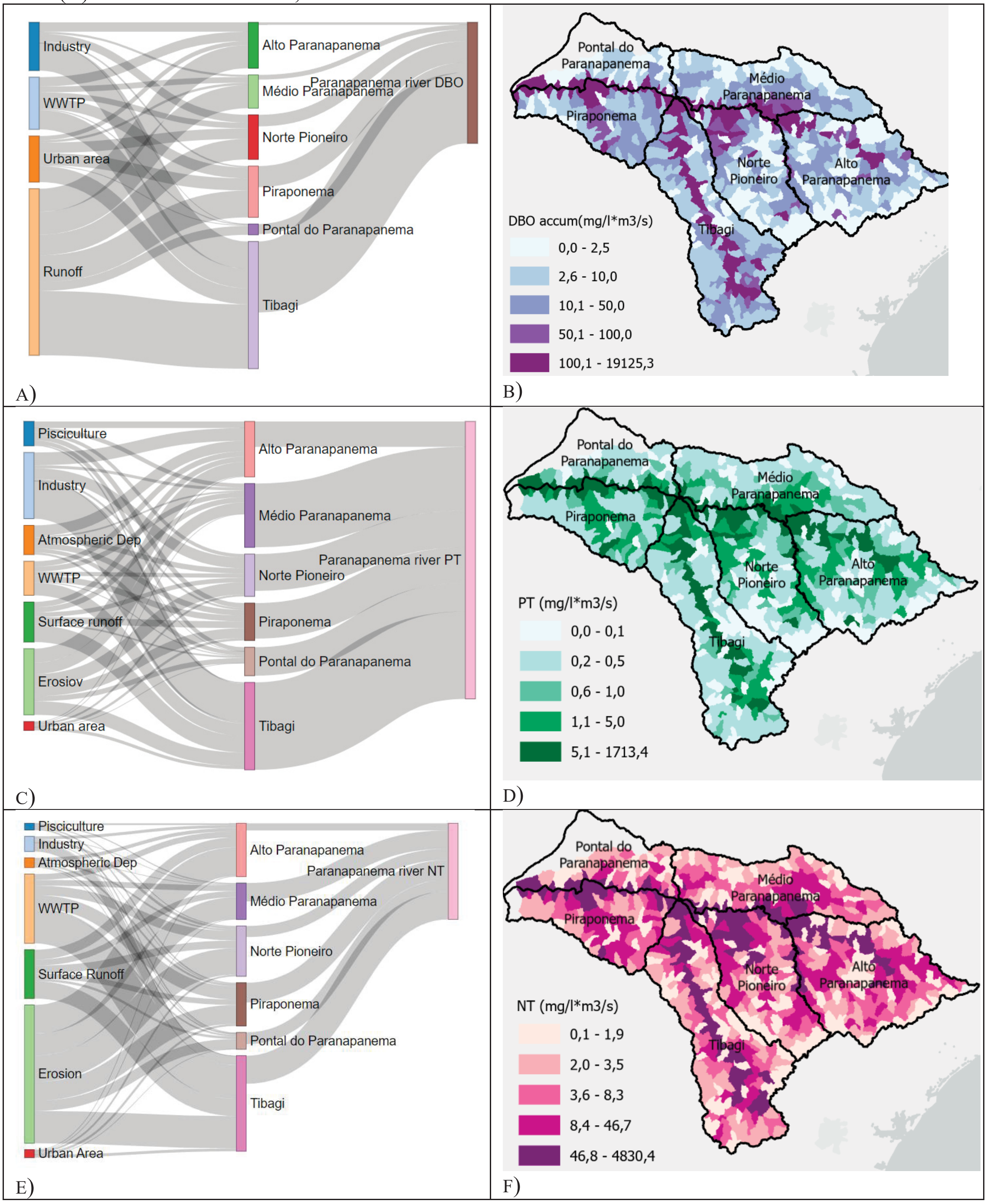
In the case of BOD (figures 13.a and 13.b), the largest contributor is the Tibagi unit, representing 41%, where the highest BOD load occurs by surface runoff accounting for 51% of the total. The Pontal do Paranapanema, Alto Paranapanema, and Norte Pionero units represent 16%, 15%, and 14%, respectively of the total of BOD, also having surface runoff as the main contribution to the river load, with 52%, 50%, and 46%, respectively. The other units, Médio Paranapanema and Pontal de Paraná, represent 11% and 3% of the contribution to the main river, with the principal source in about 69% and 83% coming from surface runoff. Other point sources such as industries and WWTP have a more point impact, as discussed in the previous section. The same applies to untreated urban runoff, which depends on the location of the urban area in the basin.

In Figures 13.c and 13.e, the main cumulative phosphorus loads for the basin are illustrated, with the Tibagi unit again having the highest contribution, accounting for 32% of the phosphorus reaching the main river. In this case, the main phosphorus source refers to the industry within the unit, constituting 43% of the total unit. In second place is Alto Paranapanema, with 21%, where the main contribution comes from sediments exported by agricultural water erosion (25% of the total). The third-largest contribution is Norte Pionero, with 16%, also coming from erosion (27%) and industrial effluent with 26% as the major phosphorus sources. The Piraponema, Meio Paranapanema, and Pontal de Paraná units account for 16%, 11%, and 6% of the contribution to the main channel, respectively, with the principal source being erosion from agriculture areas with 29%, 37% and 32% of each.

In Figures 13.e and 13.f, the main contributions and sources of total nitrogen are shown, with the Tibagi unit presenting the highest cumulative pollutant loads, approximately 32% of the total. The main sources for this unit are effluents from treatment plants with 35% and loads from agricultural erosion with 34%. In second place is Alto Paranapanema, with 54% of the total nitrogen loads coming from hydric erosion and 18% from surface runoff. Another planning units: the Norte Pionero with 17%, Piraponema with 15%, Meio Paranapanema with 12%, and finally Pontal do

Paranapanema with 6%, all of them with the main source being water erosion in agricultural areas, with 52%, 44%, 60%, and 60%, respectively. Secondary top sources for these last four units come from treatment plants and surface runoff.

FIGURE 13 –LOADS CONTRIBUTIONS TO PARANA RIVER (A) BOD (B) TOTAL PHOSPHORUS AND (C) TOTAL NITROGEN, SUBDIVIDED BY SOURCE AND PLANNING HYDROLOGIC UNIT

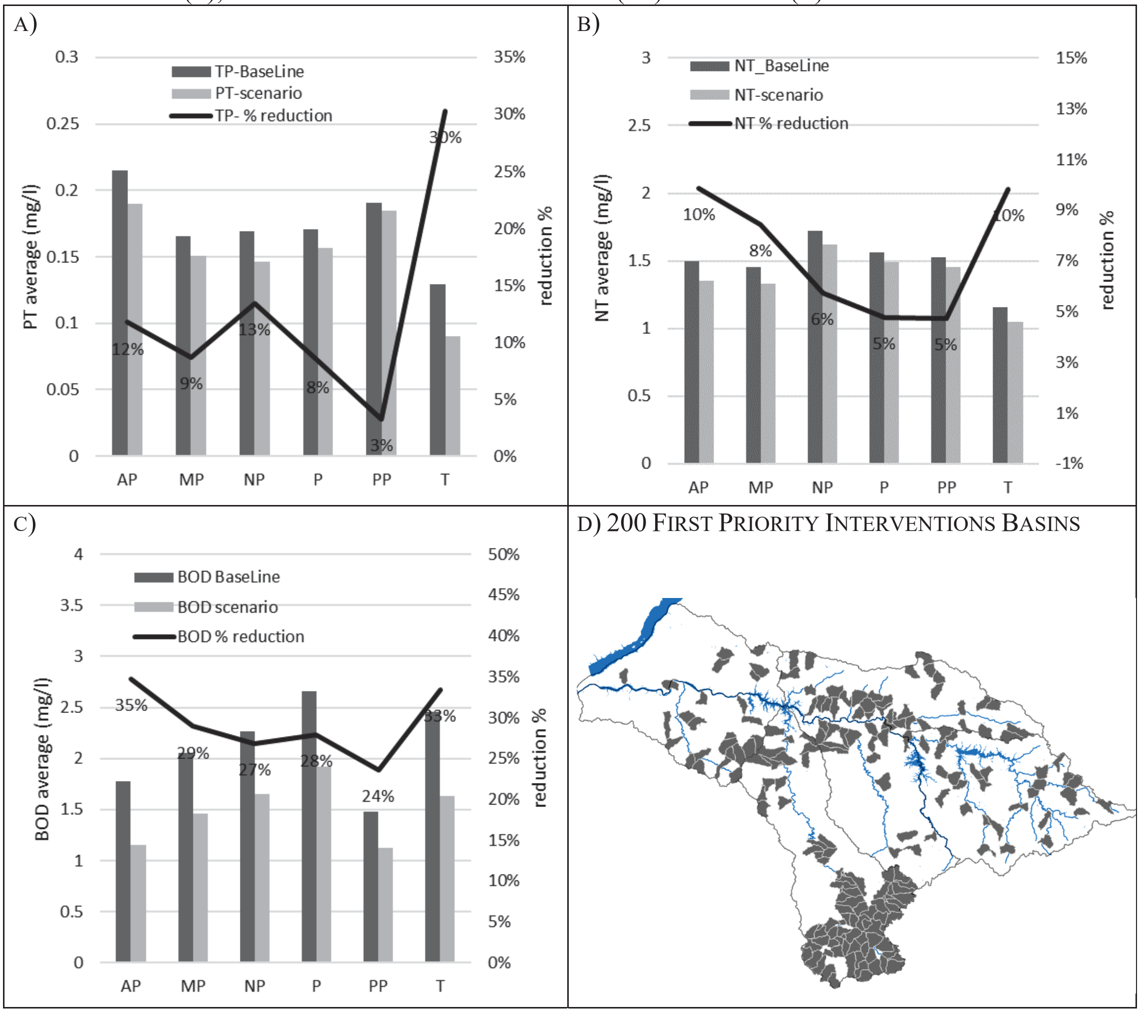


SOURCE: ELABORATED THE AUTHOR

To achieve a relevant interpretation of the possibilities of reduction in the basin two scenarios where compared, the baseline referent a 2012, and an optimistic scenario with all the interventions described in the methodology. The comparative results are presented in Figure 14, showing the potential reduction for all the UGRH. For the Tibagi unit it’s possible to reduce more than 30% in phosphorus and BOD loads in, and 10% for nitrogen total.

The representation of reductions was analyzed in milligrams per liter to enable comparison with the water classes defined in Brazil. The Class 2 limits adopted for comparison were BOD ≤ 5 mg/L, total phosphorus ≤ 0.10 mg/L, and total nitrogen ≤ 2.18 mg/L. In the figure, it is observed that, in the case of BOD and Nitrogen on an annual average, it is possible to stay within the acceptable range. However, for Phosphorus there is a need for reductions to attend the normative. The Figure 15d, also shows the prioritization of the first 200 sub-watersheds selected in the ranking, including the areas where the basins have more reductions for the three substances.

FIGURE 14 – LOADS CONTRIBUTIONS TO PARANA RIVER (A) TOTAL PHOSPHORUS (B) TOTAL NITROGEN AND (C) BOD, SUBDIVIDED BY SOURCE AND PLANNING HYDROLOGIC UNIT.ALTO PARANAPANEMA (AP); MÉDIO PARANAPANEMA (MP); NORTE PIONEIRO (NP); PIRAPONEMA (P); PONTAL DO PARANAPANEMA (PP) E TIBAGI (T).



D) 200 FIRST PRIORITY INTERVENTIONS BASINS

SOURCE: ELABORATED THE AUTHOR

4.2.6.4 Modeling loads for waterbody framework

This study emphasizes the significance of employing models to estimate pollutant loads, permitting the identification of key sources, estimation of potential reductions, and prioritization of basin. The modeling results align with findings from other studies, that consider the importance of knowing the sources origination for water management (Robertson et al., 2019 Fernandes et al., 2021; Marques et al., 2019).

The proposed methodology holds significance for resource allocation and the establishment of framing goals, particularly in large basins like the Paranapanema. The model was developed using harmonized geospatial datasets, allowing estimates of pollutant loads and their spatial distribution, letting the understanding from the source until they reach the river.

In Brazil, efforts are being made to generate high-quality institutional data through monitoring and information compilation. This data is, for the most part, readily accessible. Consequently, the proposal to develop a model utilizing pre-existing data arises from the necessity to transform this data into easily an accessible information for decision-makers. While the model is still not able to conduct an automatic translation capability for the data, the algorithm developed is able to process the data to information and estimated the loads in each sub watershed. This capability helps decision-making understanding the characteristics and possibilities for each watershed to have an effectively manage and preserve water quality. The analysis of estimative loads could assist managers in making informed decisions and adjusting strategies based on the specific conditions and needs of each water body.

The proposed method can save time and money while guaranteeing the definition of actions. Currently, economic resources are invested to make models that are difficult to replicate to evaluate the actions carried out in the basin. The proposal of this model is to be able to use data such as land use and occupation from MapBiomas that is generated each year, institutional data such as the wastewater atlas "*Atlas de esgoto*", or the inventory of industries that once updated can be run again to evaluate in the same model being able to guarantee the evaluation of the results obtained after the actions are implemented. The managers could be focus more on the action than planning. Another notable advantage is that the model could run with national base data and employs a simple algorithm, making it applicable to large basins and the entire country. This adaptability is particularly essential for a continental-sized country like Brazil.

The suggested assessment not only offers source analysis but also aids in identifying trends, patterns, and the potential effectiveness of future policies and interventions. Taffarello et al. (2016) also emphasize the importance of integration qualitative and quantitative data to provide a holistic understanding of water quality and quantity in water bodies. This adaptability is crucial for addressing challenges and ensuring the sustainability of water resources. Insights gained from such analyses are invaluable for informing public policies that aim to adopt sustainable water resource management.

Despite significant efforts to mitigate the impact of land use changes and occupation, controlling diffuse loads from urban areas (due to a lack of sewage treatment) and agriculture (via water erosion or surface runoff) is a complex challenge, not unique to Brazil. Wu et al. (2023) highlight a similar situation in the Pearl River, China. Their analysis, reach over ten years of monitoring and evaluating water quality, reveals that, despite measures implemented by the government and ministry, guaranteeing water quality in rivers stays a persistent challenge.

This paper wants to underscore the importance of implementing integrated water policies, where exist collaboration between researchers, managers, and community, like the efforts realized by ANA, (2022b) to implement a project about water frame modeling incorporating different actors. The project elaborated also involve sharing scientific knowledge and practical experiences in a simpler way, at last leading to better decisions and more effective water resource management policies.

The results also evidence that despite efforts to monitor water quality in basins, there remains a lack of clear indicators and monitoring definitions specific to the goals of water quality. This includes considerations not only for concentration values but also for flow across different periods of the year to reduce uncertainty like also appointed by Meals et al. (2013) and Marques et al. (2019). A key point to be address for water quality monitoring is the irregular frequencies and lack of representative, to accurately and reliably capture the load pattern, like also mentioned by Coelho et al. (2019).

The monitoring data utilized in this study indicates that, while an adequate number of stations are available, it is fundamental to maintain the standards of the frequency and spatial representativeness of the quality data. Simultaneously, integrating the collection of data with flow causes challenges in validating regionalized models comprehensively, such as the one employed in this study. In addition, monitoring must be incorporated into to guarantee an evaluation system to track the progress and effectiveness of implemented policies and interventions.

Finally, involving local actors (e.g., municipalities, river basin authorities) and inter-basin entities (e.g., states or countries) in water policy requires efficient tools to manage mutual dependence across government levels, also mention by Stein et al., (2023). It encourages a spatial approach in water policy design and implementation. Options for enhancing policy coordination include frameworks for combining tools, funds, and organizations or establishing a multi-stakeholder platform for dialogue on integrated water policy at all levels.

4.2.7 Concluding remarks

This paper describes the enhancement of the Modeling of Regionalized Emission (MoRE) for application in Brazil. The findings show the Paranapanema basin's estimative load production for three parameters: NT, TP and BOD. The results show spatially where the highest watershed contributions of loads in kg/km^2/day are.

The model can identify the main sources and the percentage of contributions to the total river basin, highlighting that the main contributor is the Tibagi basin, due to its high percentage of agricultural production, industrial use and population density. Also, it presents the delivered incremental yields of the 3 substances (BOD, TN and PT) with which it is possible to identify the expected river water quality in each section.

The paper also presents a novel approach with routines in GIS that were created in the model builder in ArcGIS to facilitate the update of the estimate in the future. An important aspect is to be able to compare and validate the results of the watershed management actions that were implemented.

The access to a prioritization result can be utilized by decision-makers to set necessary framing goals. It also enables the estimation of areas requiring intervention, the definition of intervention types, and an assessment of whether the applied reduction can contribute to framing goals for the river. In total, 780 sub-basins were evaluated, demonstrating the potential for an average reduction that ranged from 3 to 30% in total phosphorus, 5 to 10% of total nitrogen, and 24 to 35% of BOD concentration in the scenario evaluated.

The model results demonstrate a ranking of all sub watersheds that could be employed to determine the priority order. The approach is based on the expected effects on the watershed and not only in the watersheds that have the highest loads, because sometimes the use and conditions of the basin didn't permit an effective implementation of the strategies of reduction.

Nonetheless, some limitations of the study must be recognized. Firstly, there is a necessity to implement a hydrologic model to model processes in the river and reservoir as addressed by Acosta; et al. (2023) and applied by ANA (2022a). Secondly, it will be important to dedicate time to transfer the algorithm model in a free software like QGIS, or python.

Finally, due to concerns regarding the accuracy and accessibility of the data, the study was limited to typical parameters of water quality. To effectively monitor water quality with the aim of achieving reduction targets at the appropriate temporal and spatial scales, future monitoring efforts should focus on setting up stations within the basin that adhere to the requisite requirements.

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4.3 Paper III: a Web-GIS for decision making to achieve water quality standards of water bodies through collaborative watershed modeling.

Eileen Andrea Acosta; Regina Tiemy Kishi; Marcelo Luiz de Souza; Gabriel Henrique de Almeida Pereira; Cristóvão Vicente Scapulatempo Fernandes; Tobias Bernward Bleninger; Danieli Mara Ferreira; Bruna Arcie Polli; Arthur Humberto Rocha Ferreira; João Marcos Carvalho; Alexei Nowatzki; Camila Bergmann Goulart; Alana Louise Werneck Lassen.

HIGHLIGHTS

The paper represent the principal investigation related to specific objective 4, about development a WEB-GIS for decision marking. Presented in Qualification 3.

The paper was published in the Brazilian Journal of Water Resources (RBRH, 28, e 29)

- 1. Submitted: 14/04/2023
- 2. revision 1: 26/06/2023
- 3. Accepted: 27/07/2023
- 4. https://doi.org/10.1590/2318-0331.282320230038

Abstract

Ensuring compliance with the minimum Water Quality Standards stipulated by law demands the implementation of strategic measures within the watershed. Water pollution modeling serves as a tool to guide the formulations of effective pollution control strategies. However, the inherent complexity of calibration, spatial-temporal variability, and uncertainty, in addition to effective communication of technical information to decision makers, makes it challenging to prioritize actions, implement them, and allocate resources efficiently. This paper presents the implementation of a Web-GIS for decision making support which combines collaborative hydrological and hydrodynamic modeling results with an interactive visualization of the Paranapanema river basin in the South of Brazil. The Web-GIS aimed to overcome the difficulty of presenting scientific results to decision-makers, gathering and harmonizing diverse datasets. Combining information from the watershed, the pollutant loads estimations for three substances (phosphorus, nitrogen, and BOD), the resulting concentrations in rivers and reservoirs, as well as the results for different future scenarios into a unified platform. It is expected that decision-making regarding water bodies framework will be facilitated by identifying the primary sources and pathways of pollution, prioritizing basins with the highest load production, and determining realistic possibilities of load reduction through effective measures.

Keywords: Web-GIS, Water Framework, Water Quality Standards, decision making, Paranapanema.

WEB-GIS COMO SUPORTE À DECISÃO PARA ENQUADRAMENTO DOS CORPOS DE ÁGUA ATRAVÉS DE MODELAGEM COLABORATIVA NA BACIAS HIDROGRÁFICA.

Resumo

Garantir o cumprimento dos padrões mínimos de qualidade de água estabelecidos por lei exige medidas estratégicas na bacia afluente. A modelagem da poluição de água serve como ferramenta para orientar a formulação de estratégias eficazes de controle de poluição. No entanto, a complexidade inerente à calibração, à variabilidade espacial-temporal e a incerteza, aliadas ao repasse ineficaz de informações técnicas para os tomadores de decisão, dificultam não apenas a priorização se não a própria efetivação das ações e aplicação dos recursos eficientemente. Sendo assim, este estudo apresenta o desenvolvimento de um Web-GIS que reúne os principais resultados das modelagens hidrológicas para conceder uma visão interativa da bacia do Rio Paranapanema no sul do Brasil. O sistema supera a dificuldade de apresentação de resultados científicos para o gestor, reunindo e harmonizando conjuntos de dados diversos. Combinando informações da bacia hidrográfica, estimativas de carga de poluentes para três substâncias (fósforo, nitrogênio e DBO), as concentrações resultantes em rios e reservatórios, bem como os resultados para diferentes cenários futuros em uma plataforma unificada. Espera-se que a tomada de decisão em relação ao enquadramento de corpos d'água seja facilitada pela identificação das principais fontes e vias de poluição, priorizando as bacias com maior produção de carga e determinando possibilidades realistas de redução da carga por meio de medidas eficazes.

Palavras-chave: Web-GIS, enquadramento dos corpos d'água, padrões de qualidade da água, suporte à decisão, Paranapanema.

4.3.1 Introduction

The formulation and implementation of strategies in the basin depend on the agility in decision-making processes to establish goals that ensure water quality in rivers, even for the most demanding uses. In Brazil, the Water Quality Standards (WQS), depend on the agreement between water users at the watershed, including the landowners, government agencies, non-governmental organizations, and community's members (ANA, 2007). Nevertheless, there are several challenges related to it, the first one is to achieve a consensus among these groups who have different backgrounds and interests, which requires a good understanding of the impacts of human activities on water bodies (Pahl-Wostl *et al*., 2007). The second is the substantial time required for the stakeholder to understand and analyze the multiple stages involved in this process such as i) the basin diagnosis that implies the understanding of the current conditions characteristics and challenges of the basin, ii) the basin prognosis, that refers to the assessment and projection of future conditions, trends, and scenarios for a river basin or watershed; iii) the elaboration of a framework proposal that involves the development of a structured plan or set of guidelines to manage and improve the quality of water resources, and finally iv) the analysis and deliberation by the basin committee and the Water Resources council that includes the revision of the proposal and review scientific data, technical reports, stakeholder inputs, and other relevant information for take a decisions referent to the viability of the goals proposed (ANA, 2009, Machado et al., 2019; ANA, 2020).

Another challenge lies in effectively assimilating the models that support the decision for defining WQS goals, ensuring their relevance and achievability. This interpretation depends on the expertise of technicians and scientists to communicate relevant and simplified information dynamically to all the stakeholders in the basin. To overcome these challenges, it is crucial to utilize tools or frameworks that can effectively synthesize scientific information. In the present context, Web-GIS (Web Geographic Information Systems) tools are employed as intuitive interfaces for results interpretation, providing systematic visualization of different alternative scenarios and their implications on water quality, resulting in adequate information for decision-making (Lins et al., 2012; Machado et al., 2019 & Quinn et al., 2022).

Recent studies have explored the potential regarding the use of Web-GIS for visualization and sharing geospatial data highlighting the possibility of simplifying access to information for decision-making processes (Botha et al., 2023; Quinn et al., 2022; Bedair et al., 2022 & Kourgialas et al., 2022). A Web-GIS allows the incorporation and understanding of various biophysical processes, such as land use and land cover patterns, slope, soil types, or geology distribution, and the relationships between these factors and water quality. Furthermore, it enables the establishment of spatial relationships between the impact of chosen actions and scenarios involving contaminants that can reach rivers (Quinn et al., 2022). Another study describes an approach that can facilitate the real-time management of water quality based on forecasts using the WARMF (Watershed Analysis Risk Management Framework) (Dinar & Quinn, 2022). The methodology combines a Multi-Criteria Decision Analysis (MCDA) with the GIS environment. This approach allows different basins to be assessed and prioritized based on multiple factors that are relevant to improve water quality, including point and diffuse pressures and landscape metrics. By applying this methodology, they can rank the basins that should be targeted for interventions to improve water quality and mitigate the risk of contamination (Fernandes et al., 2021). Likewise, the engagement of partners, even in the development of a sediment model, can be very important for decision-making, as those involved can have more transparency and understanding of the processes, thus generating more confidence in the results (Cho et al., 2019).

In this context, the objective of this research was the implementation of a Web-GIS for decision-making support which combines collaborative hydrological and hydrodynamic modeling results with a geospatial visualization of the basin. By integrating and summarizing the complexity of the models within the prioritization of actions it enables a better interpretation of the relationship between an action and the maintenance or improvement of water quality. This research is part of a larger project that developed a set of models to estimate pollutant loads in the watershed and hydrodynamic models for rivers and reservoirs. These models serve as the foundation for defining progressive goals, as well as prioritizing actions and ranking basins to maintain or achieve the defined quality standards for each section of the water body.

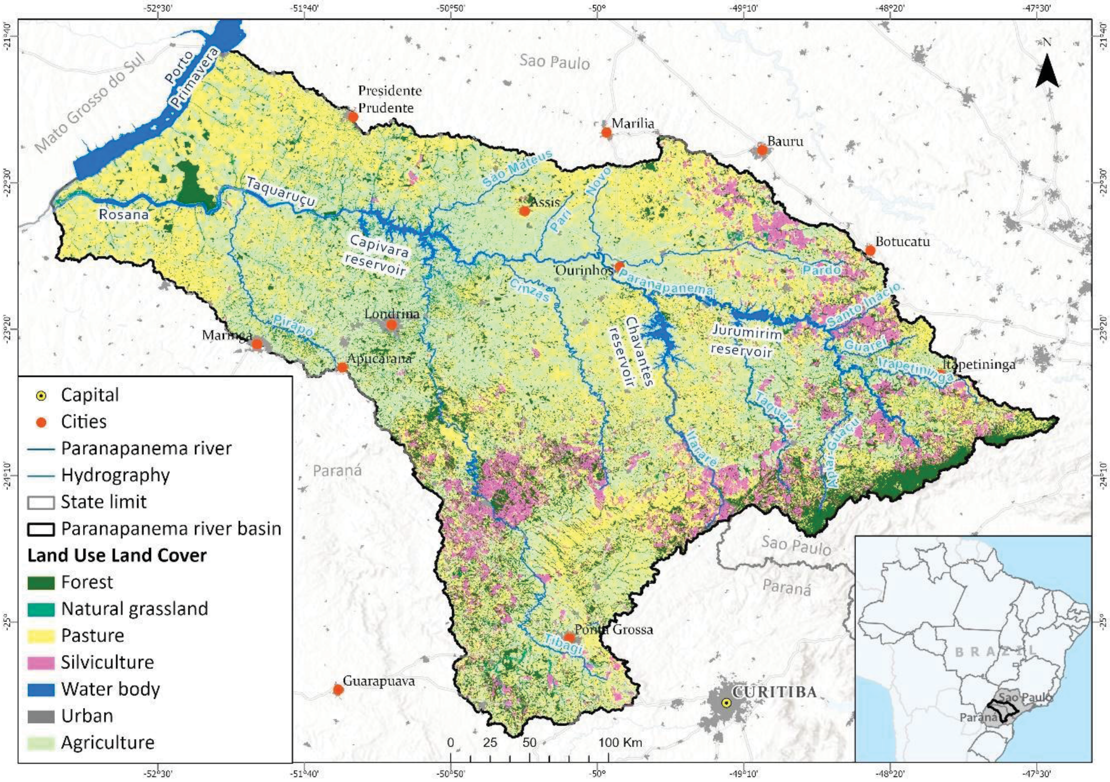
4.3.1.1 Case Study:

In Brazil the definition of WQS was based on the stipulation of two federal resolutions: CONAMA Resolution nº 357/05 and CNRH Resolution nº 91/08. CONAMA Resolution nº 357/05 classifies rivers into four classes (ranging from Class 1 as highest quality to Class 4 as the lowest quality) and establishes specific limits for various parameters within each class. These standards serve to assess and classify the environmental quality of rivers according to their preponderant uses (Brazil, 2005).

The National Council of Water Resources Resolution CNRH nº 91/08 presents the steps to be followed in a framing study. The framework should be based on the quality established by the required water uses (current and future) and should not just be based on the current quality presented by the river (Brazil, 2008). In this way, the instrument should ensure that the water quality is compatible with the most demanding water users located in the basin, thus ensuring pollution reductions according to the needs established by society (Machado et al., 2019).

The study area is the Paranapanema River basin (Figure 15), which is about 900 km long, with a drainage area of about 100,800 km² (ANA, 2016). It is an interstate basin of great economic importance for two Brazilian states (São Paulo and Paraná). It contains almost 4.7 million habitants, who are mainly concentrated in urban areas. The main economic activities are agriculture and cattle ranching (which occupies almost 70% of the basin), and forestry (with 8% of the basin). The natural areas are composed of 14% forest cover and 4% grassland. The remaining territory, which corresponds to 4%, presents other types of activities such as industries, urban areas, and water bodies.

FIGURE 15– STUDY AREA: PARANAPANEMA RIVER BASIN



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The Paranapanema Basin is part of Brazil's interconnected electric power production and transmission system, contributing to approximately 6% of the capacity of the southeast/central-west subsystem (ONS - Operador Nacional do Sistema Elétrico, 2022). Three large multipurpose hydroelectric plants have been installed, as follows: Jurumirim, Chavantes, and Capivara, which modified the riverbed and, along with human activities, required good basin management to guarantee water quality for all users.

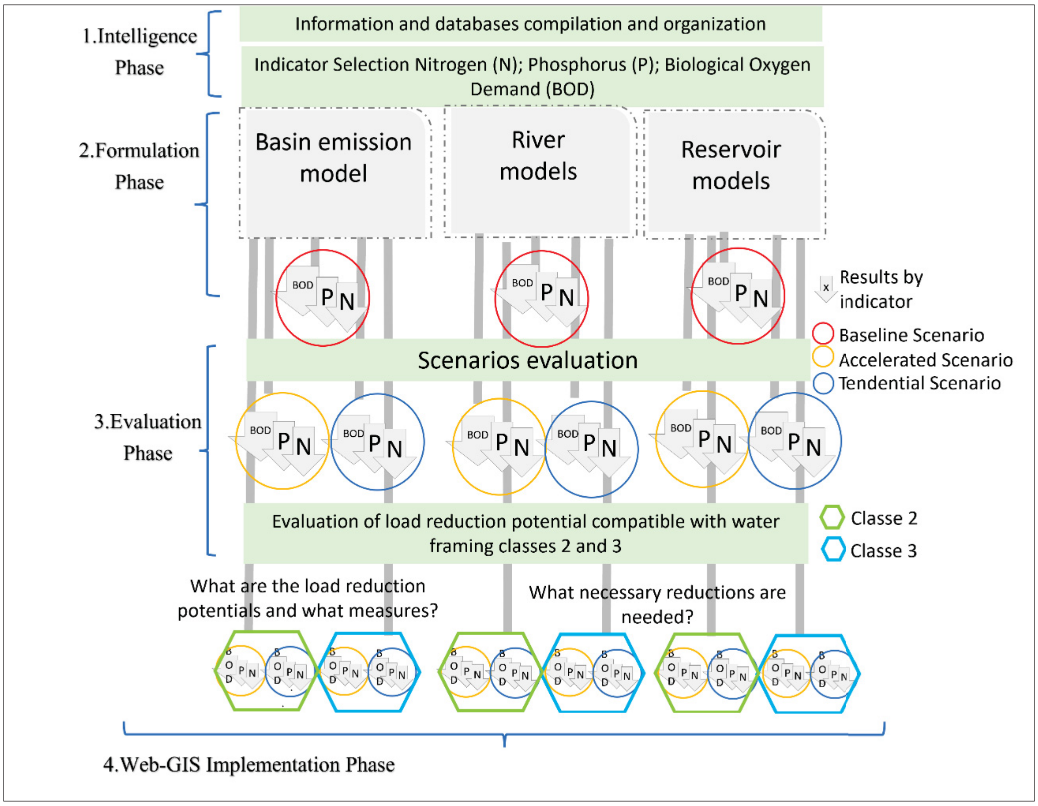
4.3.2 Methods

The Web-GIS was developed as part of the project called "Modeling of Water Quality in the Paranapanema Basin: Base for the water quality standards", between ANA and UFPR (ANA, 2022), and it was created with the aim of harmonizing and visualizing the results of the modeling of the basin load emission estimates, hydrodynamic modeling of rivers, and substance concentration estimates in the reservoirs. This section presents a brief description of the previous stages, data preparation and modeling, and the development of the Web-GIS platform to support decision-making. The models are available for future research in the following repository: <https://sites.google.com/view/paranapanema-openmodels/home> and the Web-GIS is available at the link <https://bit.ly/paranapanema_modelagem>

4.3.2.1 Data preparation and modeling

The steps involved for the development of the Web-GIS are illustrated in Figure 16. The process was divided into four phases. The first step, or intelligence phase, involves the compilation of a spatial database, climate data and water quality data. Additionally, during this stage the parameters Total Nitrogen (TN), Total Phosphorus (TP) and BOD (Biochemical Oxygen Demand) were selected as indicators of water quality. These indicators were chosen based on data availability and their significance as sources of information about pollution. The year 2012 was selected as the baseline due to the availability of data encompassing land use and land cover, socioeconomic factors, as well as monitoring data. The second step was the formulation phase, which involved the modeling of rivers, reservoirs, and basins. This modeling aimed to organize complex environmental and biophysical information, estimating the basin loads, their propagation in rivers and reservoirs. The third part or evaluation phase, consists in the evaluation of future scenarios that could influence the water quality, as well as evaluating measures aimed at reducing pollutant loads. Two scenarios were selected for presenting in the Web-GIS, a trend scenario, and an accelerated scenario. The scenarios were based on the projections proposed for the long term (2035) in the Integrated Water Resources Plan of the Paranapanema Basin Management Unit (ANA, 2016). The trend scenario under the assumption that public policies and the cultural socioeconomic framework will not differ from the current ones, and that the economy maintains a recovery process. The accelerated scenario, on the other hand, considers a combination of favorable conditions such as economic growth which later will increase the demands on water resources. The final and fourth phase refers to the WebGIS implementation which consists of building a series of interactive panels to be used in the decision-making process.

FIGURE 16 – PHASES OF DATA PROCESSING AND MODELING NECESSARY TO IMPLEMENT THE WEB-GIS



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4.3.2.2 Intelligence phase: Preparing the database

The Paranapanema Basin already had a large amount of spatial information that was produced in the studies of the Integrated Plan of Water Resources of the Paranapanema River (PIRH Paranapanema) and the Study/Report of the Integrated Group of Aquaculture and Environmental Studies – GIA ANA (2022a).

Data collection was conducted to gather information representing the main biophysical characteristics of the basin. First, the geospatial data was organized according to the following steps: i) evaluation of geospatial data, ii) systematization by topics, iii) quality control and iv) application of the database. These four steps generated a functional arrangement with a Geospatial Databases (BDG) structure following the methodology previously described by other authors (Da Paz et al., 2020).

This process involved identifying and recognizing various data sources such as land use, land cover (LULC), topography, hydrology, soil types, vegetation cover, socioeconomic and other relevant environmental factors for the basin model. Additionally, the diagnoses and categorization of areas with land use restrictions and special designations areas such as ecological reserves or with some environmental requirement, were also conducted by Nowatzki et al. (2021). Climate and rainfall data was collected to calculate rainfall erosion as well as quality data from monitoring wells to assess pollutant load from groundwater. Data regarding water flow and water quality was analyzed and used to define which stations would be used for calibration and validation of the models. The river models were calibrated using 11 fluviometric stations and 8 water quality monitoring stations available in the National System of Information on Water Resources (SNIRH) for the base year (2012). For the hydrodynamic and the water quality simulation in reservoirs, water level and water discharge data available in the Reservoir Monitoring System (SAR), and meteorological data from the Avaré station (A725), Joaquim Távora (A821) and Nova Fátima (A842) of INMET were used (Goulart et al., 2023) as well as the load results provided by the Modeling of Regionalized Emissions - MoRE basin modeling (Lassen et al., 2021; Acosta et al., 2021), and the synthetic series generated from the available monitored data (UFPR & ANA, 2020a).

4.3.2.3 Formulation phase: Basin-river-reservoir modeling

The formulation phase, which involves understanding the sources of pollution and their pathways, was carried out using a collaborative modeling approach. This approach incorporated three models for river, reservoir, and load estimation from the watersheds.

To prepare the pollutant load estimation, the *Modeling of Regionalized Emissions* – MoRE by Fuchs et al. (2012) was customized to align with the data availability and physical processes specific to Brazil. With the ArcGIS Model Builder, a total of eight algorithm routines were generated including three routines focuses on point sources such as effluent from treatment stations, industrial effluent, and aquaculture and five routines to estimate the diffuse sources (soil erosion, surface runoff, atmospheric deposition and groundwater loads). More details can be found in a study carried out by Lassen et al., (2021) and Acosta et al., (2021).

The flow and concentration river estimates were carried out using the Hydrodynamic Simulation and Water Quality models – SihQual (Ferreira et al., 2020; Ferreira et al., 2021) and the Hec-Ras model (Ferreira et al., 2021; D. M. Ferreira & Fernandes, 2022) more details of the process can be found in previous studies (Ferreira et al., 2021).

The Paranapanema river is characterized by the presence of eight reservoirs, including five run-of-river (usually lotic systems) and three storage reservoirs (usually lentic systems). In order to select the appropriate approach for each section, the water residence time was used as a determining factor (Goulart et al., 2023). Sections with residence time greater than 40 days were modeled as lentic water bodies, thus Jurumirim, Chavantes and Capivara reservoirs followed this classification (ANA, 2022a). To evaluate the spatial variations, a computational simulation was carried out using the Delft3D model (Deltares, 2014). Additionally, the need for reservoir zoning was assessed, using remote sensing and a load ranking approach to define a classification. These classifications correspond to sectors that needed different strategies for reducing pollutant loads (Goulart et al., 2023).

4.3.2.4 Assessment phase: Load reduction estimative in basins, rivers, and reservoirs

The scenarios were simulated by the UFPR-ANA project team using three models (basin, river, and reservoir) to assess three indicators: TN, TP and BOD. Two different scenarios along with a baseline scenario were considered. Based on the simulation results, the required load reduction in the basin, river and reservoir was determined.

To estimate load reduction and strategies for prioritization of actions in the sub-basins, the results from scenarios were compared with future scenarios that incorporate different measures (equation 20).

$$rb = Loads_{i,j} - Loads_{i,j,m} \qquad \text{Equation 20}$$

Where:

rb – Is a load reduction estimative in kilograms by day $(\frac{kg}{day})$ for each sub-basin

$Loads_{i,j}$ – the estimate of loads in the basins for each scenario "i" and for each parameter “j";

$Loads_{ij,m}$ – is the load estimate resulting from the application of alternative pollution control measures in the basins “m”, for the scenario"i" and each parameter "j".

Four types of interventions were applied to carry out the evaluation, such as: improvements in the efficiency of effluent treatment stations (ETE's) and treatment of untreated sewage (97%, 70% and 70% for removal of BOD, TP and TN, respectively), as well as improvements in the treatment of industrial effluents (load reduction by 50% for the 3 parameters) and for agricultural areas, a 30% reduction in diffuse loads due to the adoption of good practices (ANA, 2022a). The results of this process showed the ranking of sub-basins where load reduction is feasible. Identifying the sub-basins with the highest load reduction potential provides valuable guidance on where the most significant reductions in pollutant loads can be achieved.

For the evaluation of the necessary load reduction in rivers to achieve or maintain the target class of water framework, duration curves of the hydrodynamic modeling results were constructed for each parameter "j" and for each "i" scenario, as well as suitable duration curves for each section of river (ANA, 2022a). The duration curve, derived from the hydrodynamic model, was compared to the maximum tolerable load curve corresponding to different water quality classes (ANA, 2022a). This analysis resulted in the determination of the percentage of load reductions necessary to attain the desired water quality class *“k”* for the scenarios "i" as follows in equation 21:

$$rr\,(\%) = 100 \cdot \left(1 - \frac{Permissible\ Load_{\ i,j,k}}{Calculated\ Load_{i,j}}\right) \qquad \text{EQUATION 21}$$

Where:

$rr\ (\%)$ – is the load reduction in rivers necessary to achieve or maintain the target of water class for water framework;

$Permissible\ Load_{\ i,j,k}$ – is the load duration curve calculated for each parameter “j” is for each water quality class “k”;

$Calculated\ Load_j$ – is the load calculated from the hydrodynamic modeling for each parameter "j".

By modeling the allocations of estimated loads for each scenario within the sectors of the reservoir, it was possible to understand how load variations can potentially impact water quality (ANA, 2022a). The necessary reduction results were presented for each sector of the reservoir, considering the two scenarios and the resulting classification of water quality classes (equation 22).

$$rs = 100 \cdot \left(1 - \frac{F_{j,limix,k}}{F_{j,k}}\right) \qquad \text{EQUATION 22}$$

Where:

rs – Percentage of necessary load reduction required for each sector of the reservoir;

$F_{j,limix,k}$ – is the admissible load for the critic parameter *"j"* for each water class *"k";*

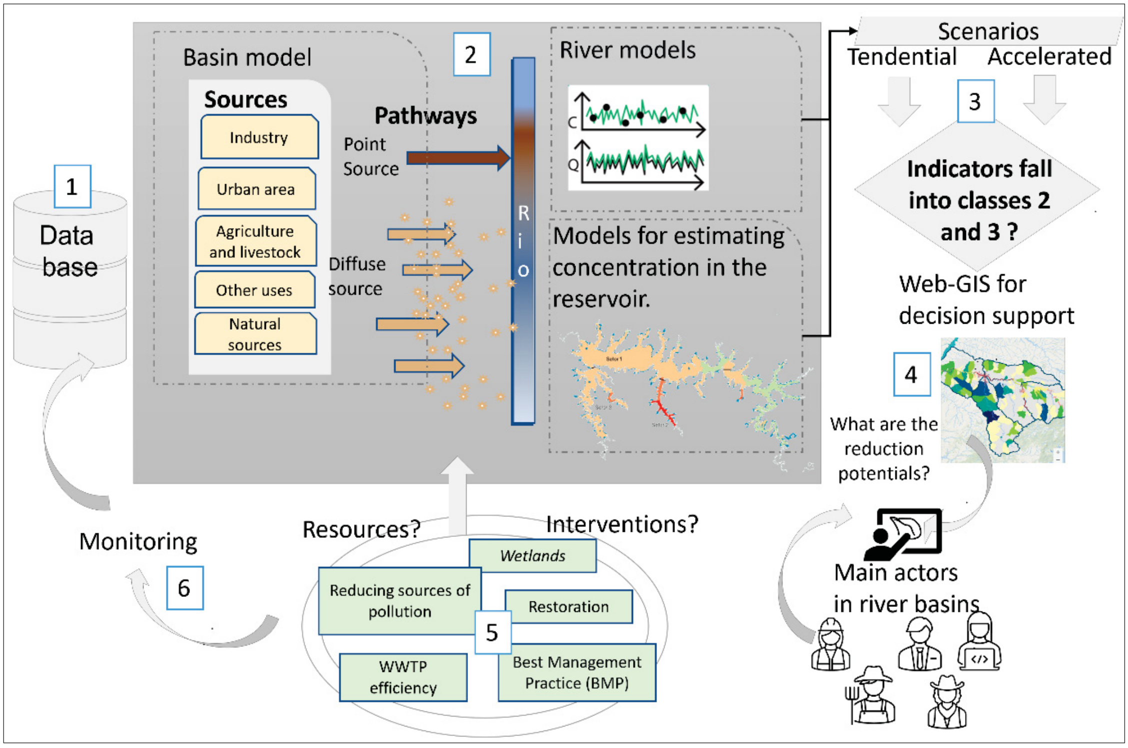
$F_{j,k}$ – is a calculated annual load of the critical parameter *"j"* for each water class *"k"*.

4.3.3 Web-GIS: Translating Information for Decision Makers

For the development of the Web-GIS, the ArcGIS online portal was used, which is a geographic information system software (Esri's web-based) used to create and use maps, compile geographic data, analyze mapped information, as well as manage geographic information in cloud databases (Figure 17.1). The information and results considered most relevant for decision-making were compiled. A link between the need to understand the substances that are emitted in the basin and how they behave in rivers and reservoirs when they reach the water bodies was established (Figure 17.2). The Web-GIS was designed to explore the potential for reducing pollutant loads in the sub-basins and the necessary reductions in river sections to achieve water quality compatible with classes 2 and 3 in different scenarios (Figure 17.3).

Results are presented in an interactive and user-friendly manner to facilitate public and stakeholder participation in decision-making processes (Figure 17.4). Facilitating the decision to define resource use priorities and the definition of goals and intervention strategies in the basin, that guarantee the maintenance of water quality according to the most restrictive use (Figure 17.5). Additionally, the analysis can be used to prioritize and determine the locations and parameters that should be monitored to ensure the attainment of the defined framing goals (Figure 17.6).

FIGURE 17 – PROCESSES TO DEVELOP A DECISION SUPPORT SYSTEM FOR DEFINING WATER QUALITY GOALS IN THE BASIN



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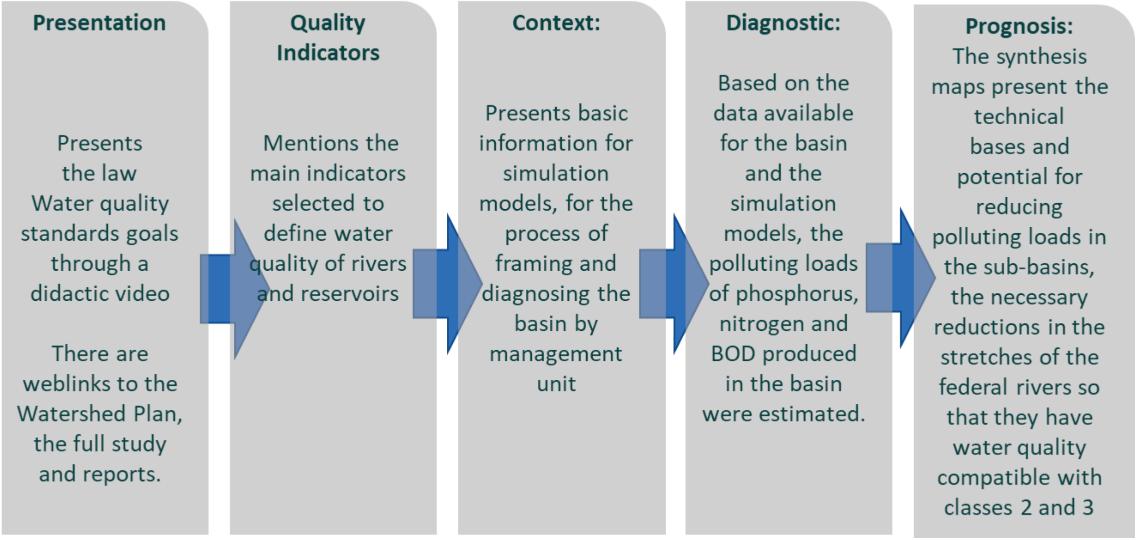
4.3.3.1 Narrative Interface Development

The narrative interface was developed using the Story Maps web application from the ArcGIS online portal. The definition of the structure was a participative process, through weekly meetings (from September 2020 to February 2021) between the modeling and geoprocessing teams, project coordinators and ANA agents. In the meetings, the concept and purpose of the system were discussed, the type of information it should have and the main objectives it should achieve to contribute to the needs of decision makers.

The structure of the narrative interface was defined based on the essential information and steps required to define the Water Quality Standards goals (Figure 18).

FIGURE 18 – STRUCTURE OF THE NARRATIVE INTERFACE FOR THE WEB-GIS



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4.3.3.2 Interactive panels development

To present data and results in the Web-GIS platform, a series of three interactive panels were constructed. The first panel provides a comprehensive overview of the current situation and serves as a general diagnosis of the basin. The second panel shows the results obtained from the estimation of polluting loads for the base year (2012). Finally, the third panel outlines the priorities for reducing polluting loads and the corresponding reductions required to meet the classification categories.

First, the data was prepared and organized to be individually uploaded in .zip format to the online ArcGIS cloud. A total of 10 web maps were prepared, such as: four with general characteristics of the Water Management Units (UGH), map of land use and coverage, map of restricted areas, map of water concessions, tree maps of load estimation and tree synthesis maps, one for each of the selected parameters (total phosphorus, total nitrogen and BOD). Finally, the three panels with the respective combination of maps were loaded to the platform according to Figure 18.

4.3.3.2.1 Context dashboard

The first set of maps name “context panel” was structured using the ArcGIS dashboard application. In order, to display all the information, a series of tabs were incorporated to show the four web maps with general information on the Paranapanema River basin. Dynamic dialog boxes with information that changes according to the selection of the Water Management Unit (UGH) to be analyzed were placed on the panel. The breakdown of information included the area in kilometers, the total population, the urban and rural population, as well as the demographic density. For aggregation of information, 3 levels of aggregation were used: municipal, by UGH, and by sub-basins. The necessary bases for the elaboration were loaded in shapefile format, and the attributes were integrated in a comma-separated values files (.csv) table with a unique identifier that allowed linking the shapefiles and attributes (Table 8).

TABLE 8 – INPUT DATA FOR BUILDING THE PANEL ON THE BASIN CONTEXT.

Input data	Format type	Source
Water Management Units	Shapefile	ANA
Reservoirs	Shapefile	ANA
Main Hydrography	Shapefile	ANA
City Hall	Shapefile	IBGE
Land Use Land Cover	Shapefile	XX
Table with social and territory attributes	.csv	IBGE
Priority areas for conservation	Shapefile	GIA
Conservation Units	Shapefile	GIA / IAT / MMA / ICMBio
Devonian Escarpment	Shapefile	
Protection Areas	Shapefile	
Water Concessions	Shapefile	ANA / DAEE/
Attributes table of water concessions grouped by UGH containing type and concession purpose	.csv	Project results UFPR/ANA

Links were added between data tables and web maps to establish functions such as selection, filters, zoom and dynamic text changes. For this panel, capabilities for selecting Water Management Units were added in the side panel to display information, for each of the UGHs, both about general characteristics, such as the display of percentage and area of use and land cover by UGH and display of information related to the number of water concessions.

4.3.3.2.2 Diagnostic dashboard

The diagnosis interactive panel presents the results of the pollutant load estimates for the base year scenario that was elaborated in the basin modeling. The results were grouped into sub-basins and organized as demonstrated in Table 9. The web maps used to create the panel show the total load in kg/day estimated for the water quality indicators showing the areas with highest emission in darker tones. The function of filtering by UGH was added to the estimation panel, making it possible to visualize the priority basins for each parameter. Graphs were also generated showing the ranking of the basins with the highest loads and the characterization of the main sources of each type of pollutant.

TABLE 9 – INPUT DATA FOR BUILDING INTERACTIVE PANELS

Input data	Format type	Source
Water Management Units	Shapefile	ANA
Basins with handle from Ottobacia	Shapefile	ANA

Attribute table of basin modeling results (current condition) containing in the columns: Ottobacia Identifier, UGH, results for each Parameter in kg/day, both total and by type of source.	.csv	Project results UFPR/ANA

4.3.3.2.3 Synthesis maps dashboard

In the summary map panel, the required reductions to achieve the water quality classification of water bodies (class 2 and class 3) as well the magnitude of the reduction in the basins are presented. The panel functionalities also provided filters to show the results by UGH, for each scenario (trend and accelerated) and for the desired Water Quality Standard. The input data was prepared as demonstrated in Table 10.

TABLE 10 – INPUT DATA FOR BUILDING INTERACTIVE PANELS

Input data	Format type	Source
Table containing the required reduction for rivers and reservoirs grouped by sector of the reservoir and river section. Containing UGH information, results per scenario and reduction for each parameter and for each class.	.csv	Project results UFPR/ANA
Reduction potential for each sub-basin with a table of attributes containing the following information for each Otto: UGH, reduction for each parameter, for each scenario and according to the class that needs to be achieved.	*Shapefile* and attribute table	Project results UFPR/ANA

4.3.4 Results Web-GIS

The Web-GIS for Water Quality Standard definition is an innovative and user-friendly tool designed specifically for management stakeholders seeking for effective solutions. It provides an intuitive visualization of the study area, and the model results, enabling managers to explore several scenarios and simulate the potential outcomes of different actions. By utilizing this tool, managers can conduct objective analyses to ensure that their actions align with environmental objectives and regulations and to identify viable alternatives to define goals for maintaining the water quality.

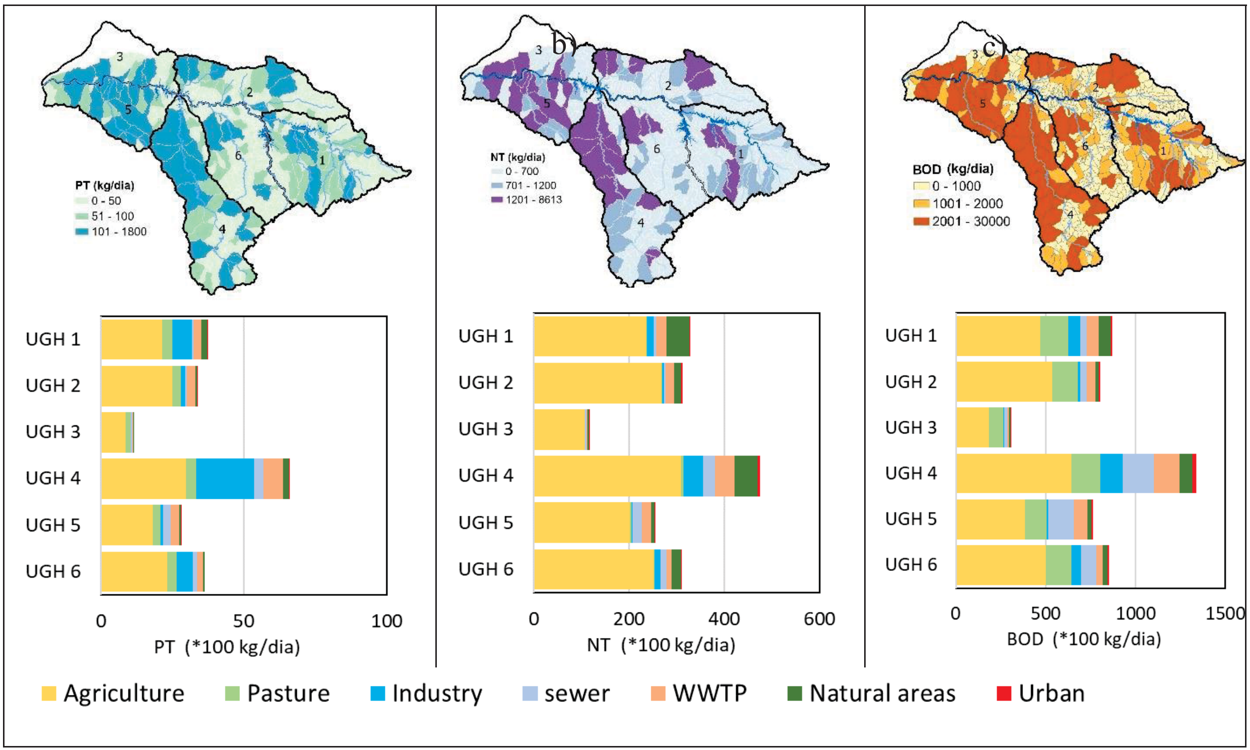
4.3.4.1 Collaborative modeling estimation basin – river - reservoir

4.3.4.1.1 Basin pollutant load modeling

The spatial distribution of the results related to the estimation of pollutant loads for the baseline and for each parameter a) Total Phosphorus; b) Total Nitrogen and c) Biochemical Oxygen Demand can be found on Figure 21. Additionally, the graphs show the estimative grouped by load sources. The diffuse loads are produced especially from areas with crops, natural areas including forest, countryside, and pasture areas. In addition, the point sources include the estimation of untreated sewage and drainage from urban areas, as well as effluents discharged by industries and effluent treatment stations

(WWTP). In the provided example, the results are grouped by UGH, but they can also be presented by municipality or by sub-basin. The Paranapanema River basin has a high percentage of occupation by agriculture with a percentage exceeding the 70%. This agricultural influence is clearly depicted in the emissions presented in the graphs. The basins with the highest loads are related to high urban and industrial occupation in addition to agricultural activities, such as UGH 4, where 2 large cities with a population greater than 100,000 inhabitants are located IBGE (2019).

FIGURE 19 – SPATIAL DISTRIBUTION OF THE RESULTS FROM THE POLLUTANT LOAD MODELING. DAILY AVERAGE IN KILOGRAMS BY DAY FOR TOTAL PHOSPHORUS (A); FOR TOTAL NITROGEN (B) AND FOR BOD (C). THE GRAPHS SHOW THE RESULTS FOR THE PARANAPANEMA WATERSHED AGGREGATED BY SOURCE AND BY UGH



SOURCE: ELABORATED THE AUTHOR

Figure 20.a provides insights about the influence of land use land cover to the phosphorus loads. It demonstrates that agriculture, pasture, or/and urban development, can have a substantial effect on the phosphorus levels in the basin. This suggests that the practices associated with these land uses, such as fertilizer application or stormwater runoff from urban areas, significantly contribute to the phosphorus load in the river basin.

By analyzing Figure 20.b it is possible to identify the presence of industries and treatment plants located near areas where the basin has high phosphorus loads. This indicates that point sources are still a major contribution to the overall phosphorus levels to the river.

FIGURE 20 – A) SHOWS THE LAND USE AND LAND COVER AND LOCALIZATION OF MOST POPULATED CITIES; B) RESULTS OF THE POLLUTANT LOADS ESTIMATIVE FOR TOTAL PHOSPHORUS IN DAILY AVERAGE (KG/DAY) AGGREGATED BY SUB-BASIN IN UGH TIBAGÍ.

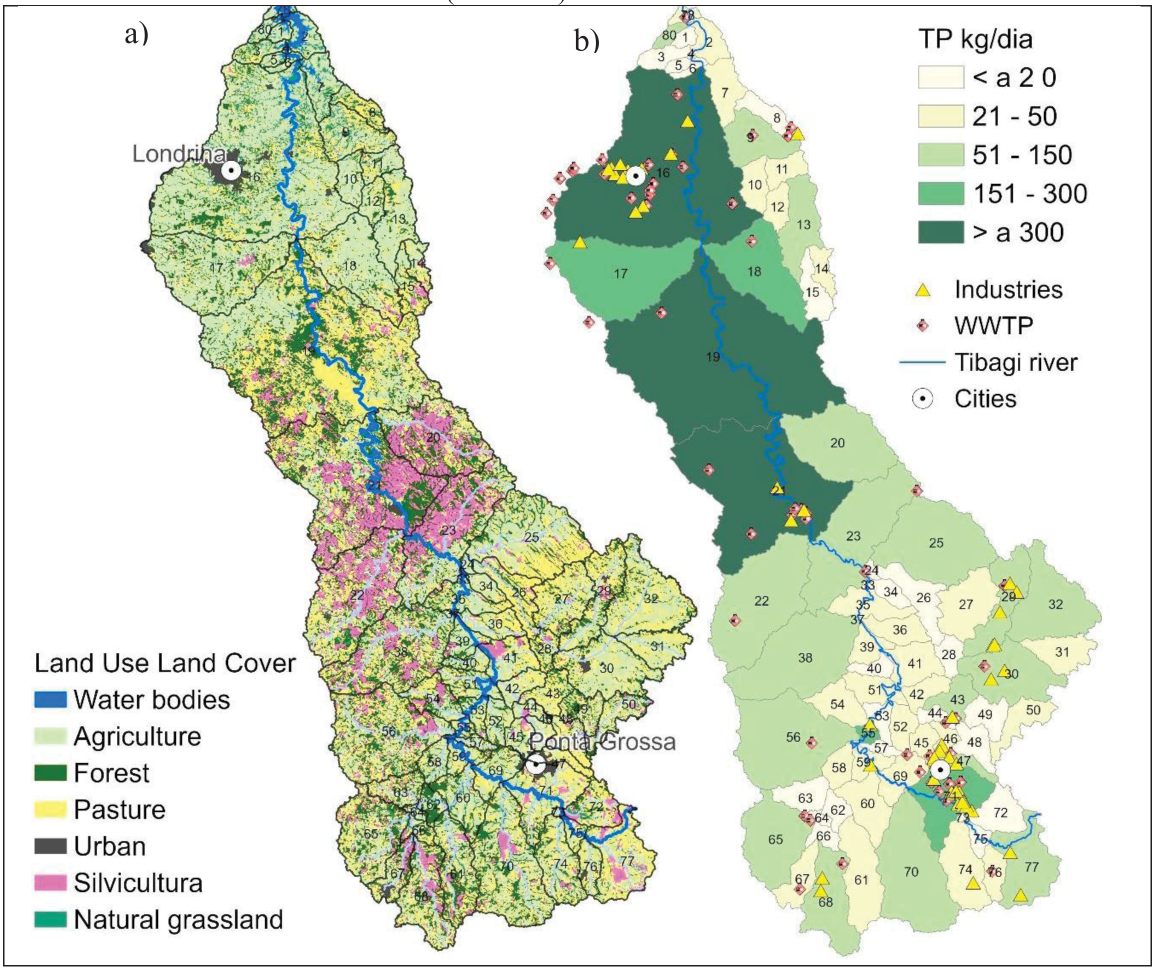


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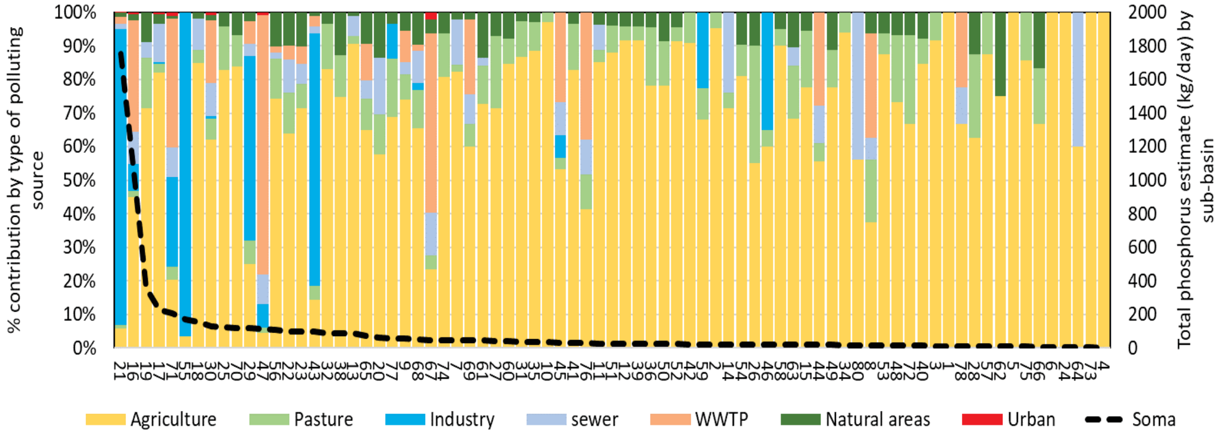
Figure 21 presents the results by sub-basin for UGH 4, showing the respective assessment of polluting sources in percentage of contribution by source (left axis). In total, 80 sub-basins were evaluated, and ranked based on the basin with the highest pollutant load (right axis).

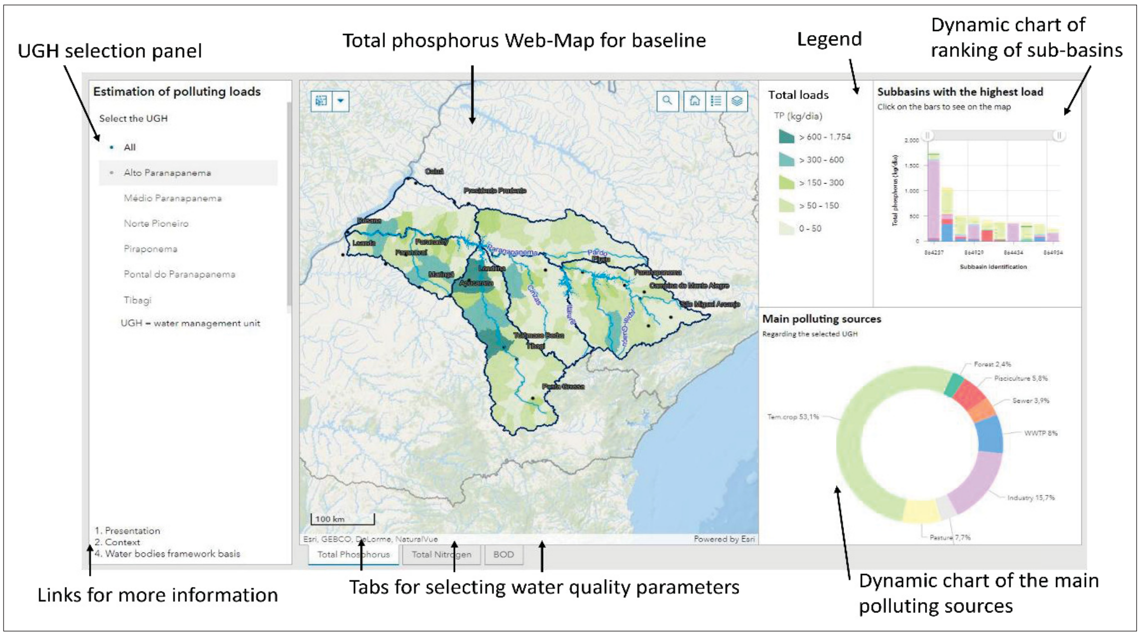
FIGURE 21 – POLLUTANT LOADS ESTIMATIVE: AVERAGE PHOSPHORUS DAILY LOADS IN KG/DAY AND SUMMARIZED BY SUB-BASIN (RIGHT AXIS), AND THE PERCENTAGE CONTRIBUTION BY TYPE OF POLLUTANT SOURCE IN RELATION TO A TOTAL CONTRIBUTION OF POLLUTANTS (LEFT AXIS)



SOURCE: ELABORATED THE AUTHOR

Figure 22 showcases the outcomes presented through the Web-GIS, where it is possible to compile the most relevant information within a single platform. This functionality allows users to explore various features including location proximity, information filtering, map comparison, and ranking the basins with the highest loads. Moreover, users can visualize the primary sources for all UGH and the sub-basins. In this way, the filters used are passed on to the tabs of the other substances showing the results for each indicator. Additionally, the chart data changes interactively as the UGH or basin to be analyzed is selected.

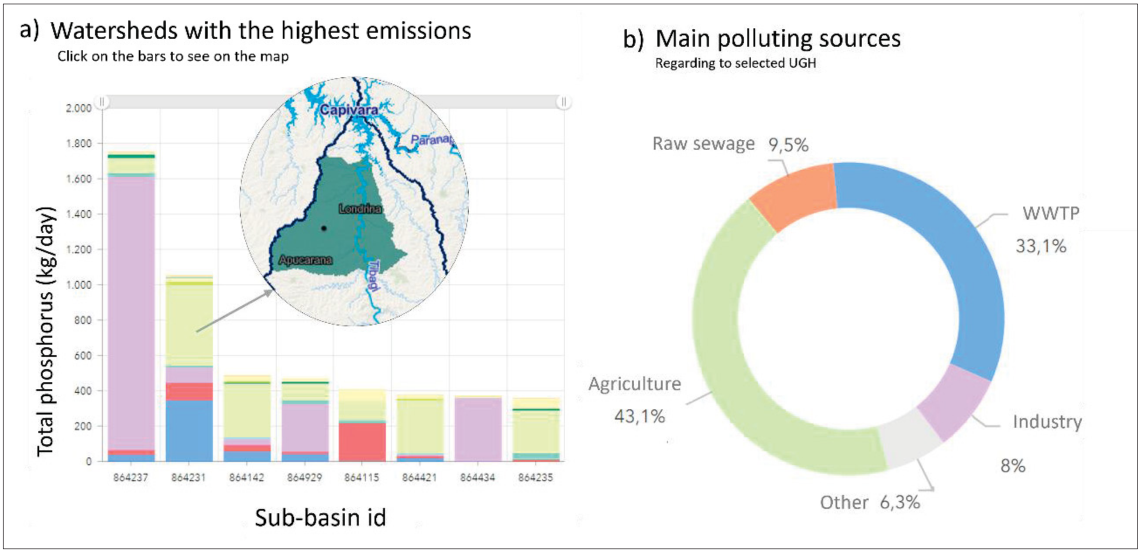
FIGURE 22 – SCREENSHOT OF THE POLLUTANT LOADS ESTIMATIVE PANEL SHOWING: THE MAPS WITH THE AVERAGE PHOSPHORUS DAILY LOADS IN KG/DAY; THE SELECTION PANEL; THE BAR CHART WITH THE RANKING AND THE PIE CHART SHOWING THE CONTRIBUTION PERCENTAGE BY SOURCES



SOURCE: ELABORATED THE AUTHOR

This tool helps to obtain a clearer discussion about where it is possible to act and what kind of action may be necessary to modify the current and/or future scenario. For example, in Figure 23.a. a ranking of the basins with the highest phosphorus load is observed. When selecting the second basin with identification (id) 864231, it is possible to observe the main polluting sources (Figure 23.b) related to loads coming diffusely from agricultural areas (43%) and from sewage treatment plants (33%), the first due to the use of fertilizers and soil erosion and the second possibly where the treatment has low total phosphorus removal efficiency. This knowledge provides tools for decision makers pointing out where interventions can be carried out as a priority to achieve the framework goals.

FIGURE 23 – SCREENSHOT OF THE GRAPHICS A) RANKING OF SUB-BASINS WITH THE HIGHEST LOAD AND THEIR RESPECTIVE SOURCES AND; B) THE DISTRIBUTION OF THE MAIN POLLUTING SOURCES IN THE SELECTED SUB-BASIN



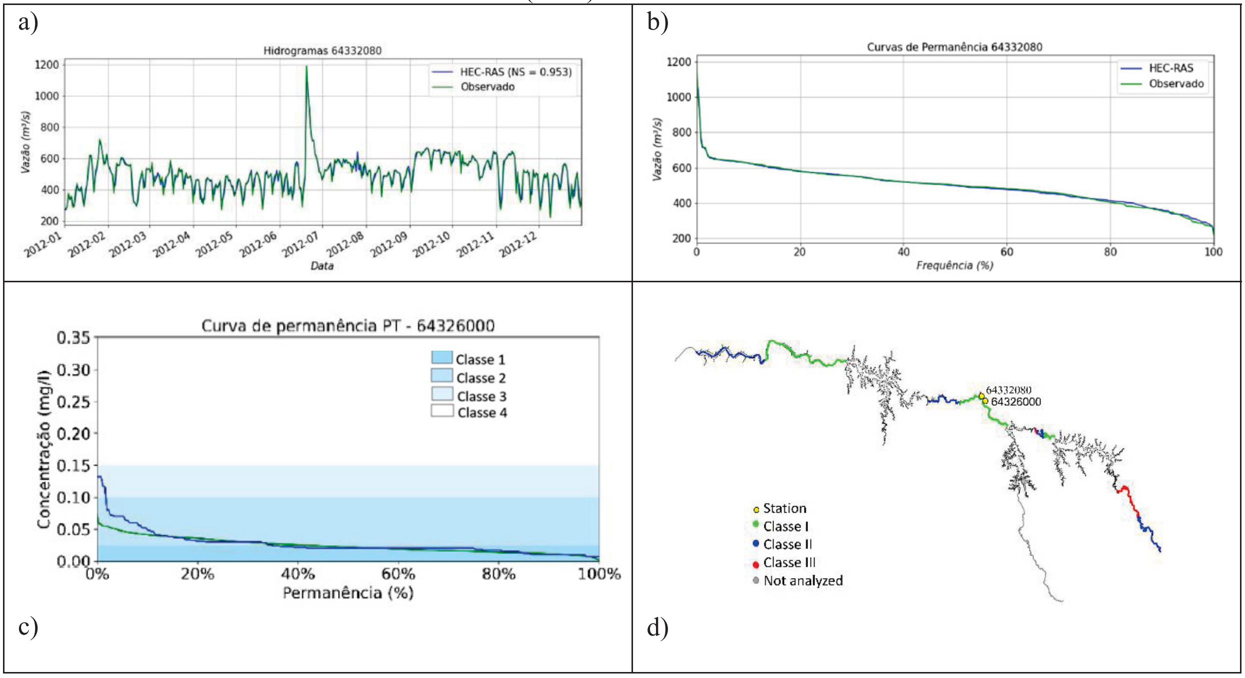
SOURCE: ELABORATED THE AUTHOR

4.3.4.1.2 Hydrodynamic models rivers and reservoir

To evaluate the temporal and spatial concentration of pollutants in the rivers, the flows and concentrations of the parameters in different sections of the rivers were simulated. First, the model was calibrated with observed data for the base year of 2012 and then modeled based on the selected future scenarios. A subset of the results is presented on Figure 24, highlighting the comparisons between simulated and observed for the calibration period. The modeling results are expressed in hydrographic curves (Figure 24.a) and duration curves (Figure 24.b). The Figure 24.c demonstrates the comparison of the quality data with the water classification ranges defined in CONAMA resolution nº 357/2005 Brazil (2005). The probability of exceeding the limit value for class 1 (below 0.05 mg/L) is 65%, while the probability of exceeding class 2 (exceeding the limit of 0.10 mg/L) is about 3%. Finally, Figure 24.d. shows the spatial distribution by sections of the simulation of total phosphorus concentrations and their classification into water quality classes.

The hydrodynamic results for the base years are the basis for the diagnosis of the current condition of the water quality in the river. Evaluations conducted using the future scenarios illustrate the expected behavior in the water quality classes. Both simulations are needed to understand and to define the goals for Water Quality Standards. Full results are available on studies (A. H. R. Ferreira et al., 2021; UFPR & ANA, 2020b), for the scenarios (trend and accelerated), analyzed parameters (total phosphorus, total nitrogen and BOD) and for each of the reference stations used for calibration.

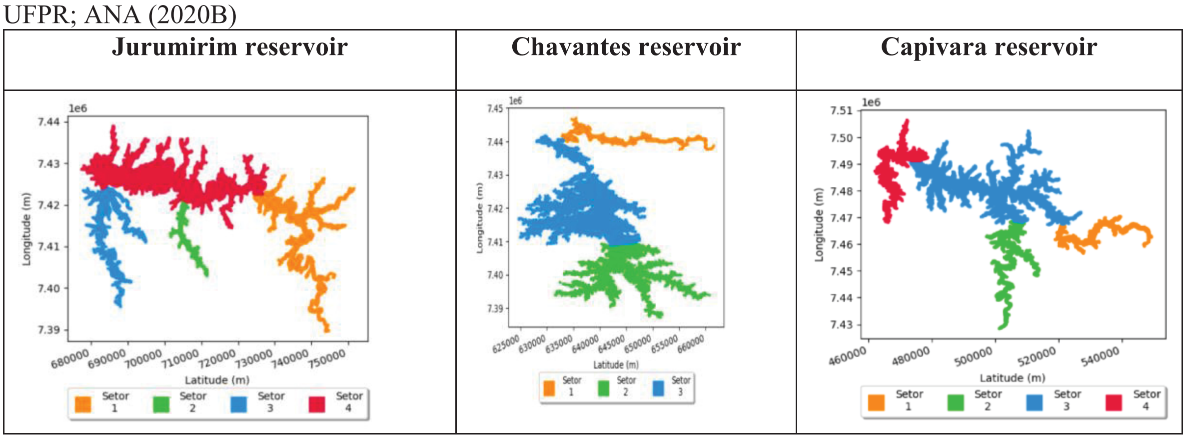
FIGURE 24 –RESULTS OF HYDRODYNAMIC AND WATER QUALITY SIMULATIONS FOR TOTAL PHOSPHORUS IN THE BASE YEAR (2012).



For a station located in the middle of the Paranapanema River (quality nº 64326000 and flow nº 64332080). a) Modeled versus observed comparative hydrographs; b) Presentation of the same result in the form of a duration curve; c) comparison of observed total phosphorus duration curves versus modeled for the base year and d) Total phosphorus concentrations in the year 2012 in the simulation stretches on the Paranapanema River. Source:(A. H. R. Ferreira et al., 2021; UFPR & ANA, 2020b)

The evaluations conducted using reservoir modeling have revealed that the need for complex simulation processes is not justified, because the interannual and extreme events do not interfere in the definition of goals to frame the water quality. However, in the case of evaluations that include long-term modifications such as changes in land cover and climate change, it is important to perform hydrodynamic modeling that allows to analyze the seasonal behavior of the reservoirs UFPR; ANA (2020a). Additionally, the evaluation conducted using hydrodynamic and water quality models identified the need of implementing a zoning approach to determine the water quality framework. The zoning exhibits distinct water quality characteristics and behaviors. Figure 25 shows the results of the different sectors obtained after applying temporal and spatial evaluation of the behavior of substances in the reservoirs UFPR; ANA (2020a); UFPR & ANA, 2020a).

FIGURE 25– ZONING OF THE PARANAPANEMA RIVER STORAGE RESERVOIRS. SOURCE: UFPR; ANA (2020B)


Jurumirim reservoir **Chavantes reservoir** **Capivara reservoir**

4.3.4.1.3 Load reduction in rivers and reservoirs

To understand the necessary reduction of loads in rivers and reservoirs, an analysis was conducted on 7 sections of the Paranapanema and Itararé rivers and 11 sectors of the reservoirs. The analysis revealed the required reductions to reach classes 2 and 3 in the trend and accelerated scenarios for the projection of 2035 (Table 11). Negative values indicate that no reduction is necessary, while positive values indicate the percentage of reduction required for each section.

TABLE 11 – ASSESSMENT OF LOAD REDUCTION FOR WATER QUALITY CLASSES 2 AND 3 FOR THE ACCELERATED AND TREND SCENARIOS OF 2035

Scenario	River-Reservoir section	Water Class 2			Water Class 3		
		TP	TN	BOD	TP	TP	BOD
TENDENTIAL 2035 - LOAD REDUCTION	Capivara-1	75%	0%	n/a	58%	0%	n/a
	Capivara-2	81%	0%	n/a	68%	0%	n/a
	Capivara-3	57%	0%	n/a	28%	0%	n/a
	Capivara-4	37%	0%	n/a	0%	0%	n/a
	Chavantes-1	64%	0%	n/a	41%	0%	n/a
	Chavantes-2	49%	0%	n/a	15%	0%	n/a

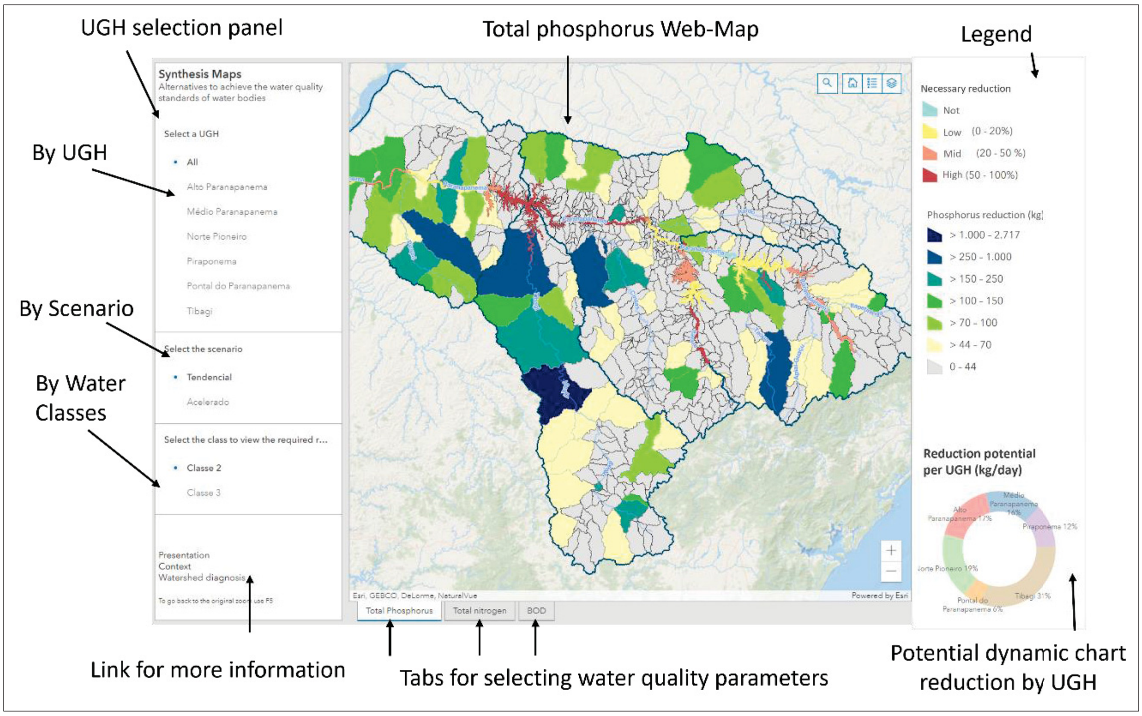
	Chavantes-3	11%	0%	n/a	0%	0%	n/a
	Jurumirim-1	6%	0%	n/a	0%	0%	n/a
	Jurumirim-2	95%	0%	n/a	92%	0%	n/a
	Jurumirim-3	54%	0%	n/a	0%	0%	n/a
	Jurumirim-4	6%	0%	n/a	0%	0%	n/a
	River section 1	55%	27%	0%	32%	0%	0%
	River section 2	0%	0%	0%	0%	0%	0%
	River section 3	2%	63%	18%	0%	45%	0%
	River section 4	68%	13%	12%	52%	7%	0%
	River section 5	1%	0%	3%	0%	0%	0%
	River section 6	47%	0%	11%	21%	0%	0%
	River section 7	11%	0%	0%	7%	0%	0%
	River section 8	89%	85%	0%	83%	77%	0%
ACCELERATED 2035 - LOAD REDUCTION	Capivara-1	84%	0%	n/a	73%	0%	n/a
	Capivara-2	89%	0%	n/a	82%	0%	n/a
	Capivara-3	74%	0%	n/a	56%	0%	n/a
	Capivara-4	62%	0%	n/a	36%	0%	n/a
	Chavantes-1	74%	0%	n/a	57%	0%	n/a
	Chavantes-2	70%	0%	n/a	50%	0%	n/a
	Chavantes-3	39%	0%	n/a	0%	0%	n/a
	Jurumirim-1	32%	0%	n/a	0%	0%	n/a
	Jurumirim-2	96%	12%	n/a	94%	0%	n/a
	Jurumirim-3	67%	0%	n/a	45%	0%	n/a
	Jurumirim-4	34%	0%	n/a	-10%	0%	n/a
	River section 1	67%	59%	23%	51%	38%	0%
	River section 2	0%	0%	0%	0%	0%	0%
	River section 3	31%	64%	41%	0%	46%	0%
	River section 4	80%	19%	33%	70%	14%	0%
	River section 5	29%	16%	25%	5%	0%	0%
	River section 6	55%	16%	29%	48%	0%	0%
	River section 7	35%	14%	23%	14%	0%	0%
	River section 8	93%	94%	40%	90%	91%	0%
High reduction (50 - 100%)		🟧	Low Reduction (0 - 20%)				🟨
Medium Reduction (20 - 50%)		🟨	Reduction not necessary (< 0%)				🟦

N/A - Not analyzed
Source: Modified from ANA (2022).

In the summary map panel (Figure 26), the compiled information showcases the necessary reductions to achieve the classification of water bodies into class 2 and class 3. The panel highlights the basins that require prioritization for reducing pollutant loads, and the corresponding value of loads that could be reduced for each scenario. Furthermore, the maps provide detailed information on the percentage reductions necessary for each river section and reservoir sector under each scenario.

The left selection panel allows the user to visualize the UGH of interest, in addition to being able to perform combinations between future scenarios and the desired classes.

FIGURE 26– SCREENSHOT WITH THE SUMMARY MAP PANEL. THE PANEL SHOWS THE TOTAL PHOSPHORUS LOAD REDUCTIONS REQUIRED FOR THE PARANAPANEMA BASIN, THE RIVERS AND RESERVOIRS.



4.3.5 Concluding remarks

In the current study, it was demonstrated how it is possible to integrate basin-river-reservoir models within a decision support system, creating an easy-to-operate and flexible tool that effectively presents complex processes to the basin actors from different sectors.

In order to understand the pollutant load using this Web-GIS system developed, deep knowledge about geographic information systems is not necessary, which provides the user with the opportunity to interact with the information without extensive training.

The information used for water quality framing is currently presented through reports and geographic databases, which prove to be effective in generating valuable data and supporting the overall process. Nevertheless, to empower decision-makers with actionable insights, there is a requirement for synthesizing the available documentation and working with the technicians to gather information into a more accessible system. The platform can be used as a tool for the basin stakeholders who still do not have GIS knowledge to interact with the information presented in the Web-GIS.

The Web-GIS provides vital information to evaluate the best actions within the basin. Even though it was not tested during this project, it is relatively simple to update the panels with new information. Additionally, it’s possible to create new ways to better represent the changes in the basin by land use, land cover changes or by implementation of the interventions.

There exists an opportunity to implement platforms like these to integrate information from institutions involved in data generation, enabling automatic feed processes that provide real-time updates every time new information is generated. One of the author's suggestions is the incorporation of the water concessions showing the allocated water quantity per basin, being fed by the responsible institution in real-time. Given how easy the use and capability to adapt the modeling part of the framework, this could also be seen as a first step to the creation of a digital models of a large water resources system in Brazil.

The Web-GIS represents the initial version of a proposed solution to create a comprehensive data set to be utilized for water quality framework. By understanding the dynamics of both upstream and downstream basin, it can be an alternative to avoid conflicts. By finding the necessary information for the decision-making process only within one platform, it is possible to communicate the modeling results more quickly to define the prioritization of actions that can make adequate use of resources to really be able to assess the river's framework.

Next steps: In the next stage of this research, it is intended to create a routine within the MoRE model that allows testing how different interventions within the basin can reduce the export of polluting loads, this function being useful for prioritizing areas and defining actions.

***Author contributions**:* Conceptualization: E.A., R.K., M.S., C.F., T.B; Web-GIS Preparation: E.A, M.S.; Funds acquisitions: M.S., C.F., T.B.; Project coordination: R.K., M.S, C.F, T.B.; first draft: E.A.; revision and editions: E.A., R.K., M.S., C.F., T.B.,C.G, G.P.; data curation: A.N; Reservoir modeling: B.P., C.G., J.C.; Rivers modeling: D.F; A.F.; Basin modeling: E.A.,A.L.,G.P.

Project financing: This study was financed by the project for Elaboration of Study of Implementation and Application of Hydrodynamic and Quality Models of Surface Waters of Federal Domain as support for Decision Making in Framework Proposal carried out by UFPR and National Water Agency (ANA).

Acknowledgments: To the multidisciplinary team that formed part of the project for the Elaboration of a Study for the Implementation and Application of Hydrodynamic and Quality Models of Surface Waters in the Federal Domain as support for Decision Making in a Framework Proposal carried out by UFPR and the National Water Agency (ANA).

The opinions expressed in this document are those of the authors and do not necessarily reflect the opinions of the National Water Agency (ANA) or UFPR.

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5 DISCUSSION

Interpreting the results of pollution pathway diagnosis requires consideration of diverse pollution sources and their respective environmental impacts, which can be a complex task (Robertson et al., 2019). Models are utilized to determine various pollutant loads, but accessing adequate information can sometimes pose challenges to the process (Yuan et al., 2020). Although models are developed for specific objectives, they may not always be adaptable to different works. Sometimes, a lack of information prevents the completion of the process, further complicating the overall task. In this context, MoRE is a regionalized modeling approach that allows for the modification of algorithms to facilitate estimations (Fuchs et al., 2017). For this study, eight algorithms were developed based on the MoRE framework to estimate the primary sources of pollutants in the Paranapanema basin, considering intrinsic regional characteristics such as tanks for pisciculture, a distinctive feature of the area. Three substances, Nitrogen, Phosphorus, and BOD, were chosen as indicators, representing some of the most critical substances in the basin.

Phosphorus is often the limiting factor in many regions in Brazil, so detecting high concentrations serves as an indicator of soil modifications, agriculture, and the presence of urban areas. Similarly, nitrogen is present in industrial effluents and treatment facilities. Estimating its loads is crucial for water quality management, aiding in evaluating the pollutant load a waterbody can tolerate before impairment and measuring changes in response to implemented management measures (Meals et al., 2013).

One of the significant challenges in Brazilian basins is the absence of an updated basin information system that contains all the necessary data to assess the impact of human activities on rivers. Consequently, it became imperative to develop approaches capable of determining loads originating from diverse sources.

The study was able to produce an intrinsic characterization of the basins that allows decision-makers to have knowledge of the areas with the highest contribution. With the available data and expertise, it was possible to develop a better understanding of the area's most contributing to pollution. The model helps in setting water quality goals and understanding the necessary management strategies to achieve and maintain water quality standards.

By assessing intrinsic characteristics, decision-makers can prioritize basins and actions to be taken to protect the river segments within the study area. This approach can be particularly useful in areas where data on pollution sources and levels are limited.

The diagnostic approach should prioritize actions to be taken to reduce pollution levels in the river basin. This information can be used to develop a comprehensive management plan that addresses the most significant sources of pollution and pathways of pollution (Grison et al. (2023). The results should be presented in a manner that is easy to understand, highlighting the most significant actions to be taken.

The assessment evaluates the potential of actions and the contribution of load modeling to basin management through the creation of GIS implemented routines for MoRE. Develop a Web-GIS for decision making support, that facilitated the identification of the primary sources and pathways of pollution, prioritizing basins with the highest load production, and determining realistic possibilities of load reduction through effective measures.

The diagnostic approach should communicate the results in a manner that is accessible to decision-makers and stakeholders. The results should be presented in a clear and concise manner, highlighting the most significant sources of pollution, pollutant loads, pathways of pollution, and actions to be taken. The communication of results should be tailored to the needs of decision-makers and stakeholders, ensuring that the information is relevant and actionable.

By adopting a comprehensive approach, decision-makers can develop a management plan that addresses the most significant sources of pollution and pathways of pollution, ensuring the protection of the river basin and the health of the surrounding communities. The loads in the waterbody framework requires regular monitoring and evaluation of water quality to assess the effectiveness of implemented management strategies. Understanding these interactions is crucial for developing adaptive management strategies to address the changing water quality conditions.

The loads in the waterbody framework encourages public involvement and collaboration among various stakeholders, such as municipalities, industries, and environmental agencies. This collaboration helps in developing and implementing effective water quality management plans.

Currently, watershed managers and decision-makers face numerous challenges, with one of the most relevant being the understanding of the dynamics of land use and occupation in the basin, the interpretation of pollution pathways, and the definition of prioritized areas. When decision-makers assess their financial capabilities, they are confronted with the urgent need to prioritize areas or define actions quickly, often without sufficient knowledge to achieve the selected goals. The same complexity arises when defining progressive action goals, often having to set goals based on assumptions or a lack of knowledge of the region. This is why the National Water Resources Policy incorporates the Water Resources Information System as one of its instruments, aiming to create a comprehensive system for the collection, processing, storage, and retrieval of information crucial for management.

To address this gap and provide managers with a more comprehensive and dynamic overview of estimated loads, a portal was developed in the ArcGIS Online environment that allows such interaction (Acosta et al. 2023). The portal not only displays maps but also integrated graphs with key loads and polluting sources, as well as a ranking of basins with the highest load. The portal is a replicable tool that is user-friendly for management decision-makers, offering easy interaction and providing an intuitive view of the basin from various perspectives (municipal or by basin; by water quality parameter; by load or by land use), visual scales (entire basin or zoomed into a specific area), and various combined information options to choose from (hydrography, municipalities, monitoring stations, etc.).

The autonomy provided by the portal to decision-makers will allow an assessment of the study area and a more dynamic diagnosis of the main sources and pathways of pollution. Thus, managers can evaluate, understand, and have decision-support tools that will help prioritize and assess alternative actions, ensuring the maintenance of the water body and, consequently, the well-being of the population dependent on this resource.

6 CONCLUSIONS

In conclusion, the findings of this study serve as a valuable tool for identifying areas where existing policies may fall short in effectively addressing pollution pathways, underscoring the imperative for the formulation of new or revised policies. Furthermore, the results offer insights that can be instrumental in raising awareness regarding the potential efficacy of a policy and informing the decision-making process for its modification or adjustment.

Additionally, by comparing the results with counterfactual exposure levels, representing recommended exposure thresholds or a scenario without policy, this study provides a robust means to assess the effectiveness of current policies and their potential impact on pollution pathways. Such insights empower policymakers to prioritize targeted actions aimed at reducing pollution levels within the river basin, with a specific focus on mitigating the most significant sources and pathways of pollution.

Importantly, the results offer valuable guidance for the development and implementation of policies and interventions targeting air pollutants. These efforts aim to reduce emissions, lower concentrations, and prevent individual exposure, ultimately contributing to the enhancement of public health.

Furthermore, the findings provide a foundation for fostering collaboration among diverse stakeholders, including local communities, researchers, and governmental organizations. This collaborative approach is essential for the development and implementation of effective management strategies to address the identified pollution pathways. By bringing together various perspectives, this collaborative effort ensures a comprehensive and sustainable approach to mitigating pollution and safeguarding environmental and public health.

7 FUTURE PERSPECTIVES

For future work, we plan to examine the feasibility of integrating a streamlined transport and sedimentation routine within aquatic systems. Develop a model adaptable to both rivers and reservoirs. The model is currently implemented using Python algorithms within the model builder framework. Transitioning this model to an open-source environment in the future represents a significant advancement, enhancing accessibility and adopting broader utilization.

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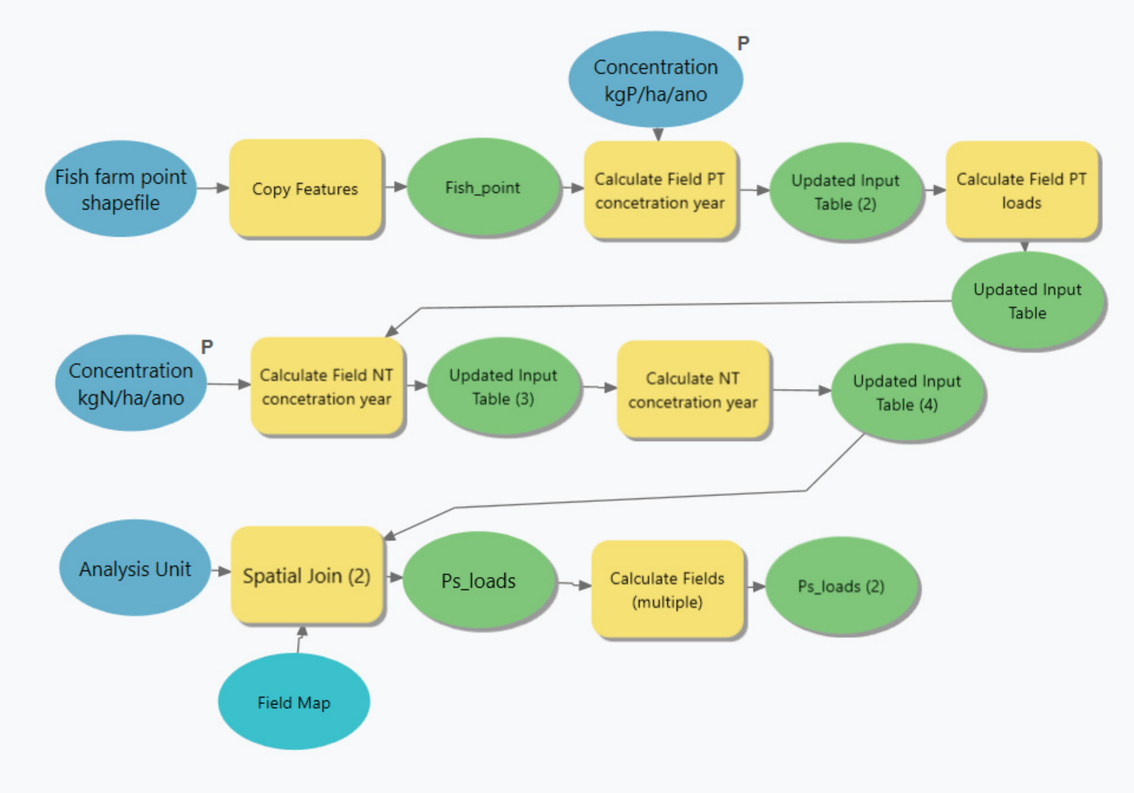
9 APPENDIX I - FORMULATION AND IMPLEMENTATION OF GEOSPATIAL ROUTINES WITHIN THE GIS

9.1 Load modeling GIS based for (update for ArcGIS Pro 3.1.3)

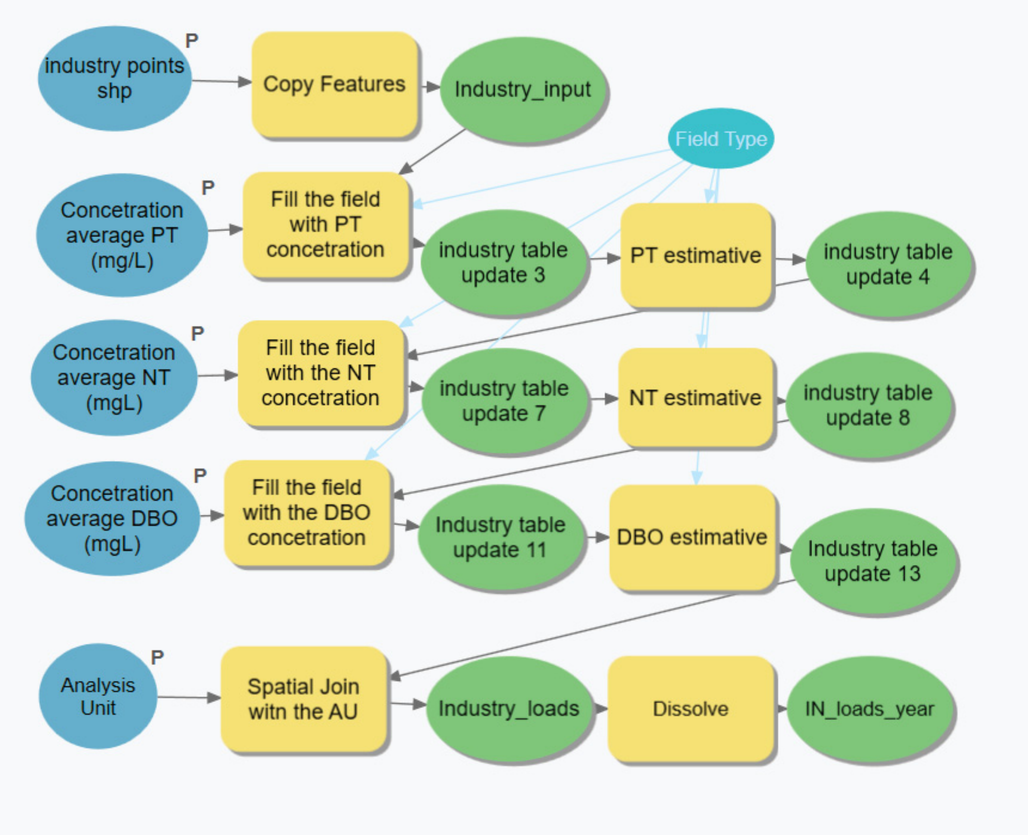
9.1.1 Loads estimative from Pisciculture

FIGURE 27– MODULE FOR THE DEVELOPMENT OF POINT LOAD ESTIMATION FROM PISCICULTURE



9.1.2 Input of pollutants from industrial source

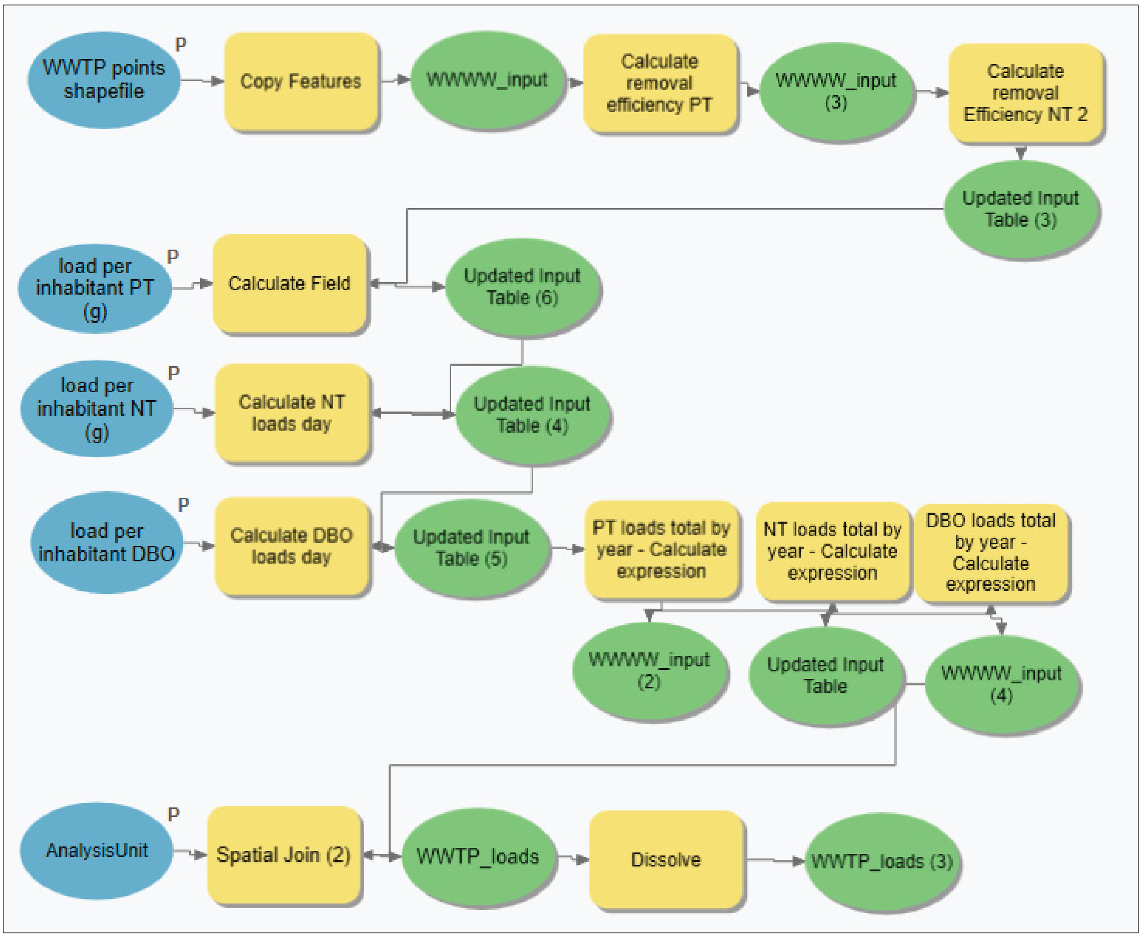
FIGURE 28– MODULE FOR THE DEVELOPMENT OF POINT LOAD ESTIMATION FROM INDUSTRIAL EFFLUENT



9.1.3 Module to estimate point source residual loads from treatment plants

The input data shown in blue in the figure were the analytical units (AU), the shape with the location of the Wastewater Treatment Plants (WWTP) with data on served population and efficiency, as well as the average load rate per inhabitant. In the processing performed, the calculation model shown in Figure 29 was developed, which contains the equations to estimate the annual loads of Total Phosphorus (TP), Total Nitrogen (TN), and BOD, in tons, from the WWTPs for each of the analysis units.

FIGURE 29 – MODULE FOR THE DEVELOPMENT OF POINT LOAD ESTIMATION VIA WWTP



9.1.4 Erosion based loads

9.1.4.1 Estimation of soil erosion map

A routine was developed to define the historical erosion map using the Universal Soil Loss Equation in Figure 32. The main difference from modeling done by other models is that MoRE has adjustment factors to calculate erosion for the specific year, modifying soil cover and rainfall erosivity factors, adjusting the equation for the year being analyzed. This does not occur in other models where the average erosion remains the same over the period. In other countries, it may not be necessary to perform this algorithm in the case of an existing ready-made raster map of average soil losses from already developed basins, so Part 1 of the model is considered optional.

TABLE 12 – GEE CODE USED TO CALCULATE THE ESTIMATE OF SHEET EROSION SOIL LOSS USING THE RUSLE EQUATION 1.

```
//Calcula o factor K
var clay = ee.Image("OpenLandMap/SOL/SOL_CLAY-WFRACTION_USDA-
3A1A1A_M/v02").select('b0');
var sand = ee.Image("OpenLandMap/SOL/SOL_SAND-WFRACTION_USDA-
3A1A1A_M/v02").select('b0');
var silt = ee.Image('users/eileenandreaacosta/T_SILT');
```

```
var mo = ee.Image("OpenLandMap/SOL/SOL_ORGANIC-CARBON_USDA-
6A1C_M/v02").select('b0').multiply(0.58);
var co = ee.Image ("OpenLandMap/SOL/SOL_ORGANIC-CARBON_USDA-
6A1C_M/v02").select('b0');
var sn1 = sand.expression('1-x/100',{'x':sand});
var soil = ee.Image([sand,silt,clay,mo,sn1,co]).rename(['sand','silt', 'clay', 'mo','sn1','co']);
var factorK = soil.expression
('(0.2+0.3*exp(-0.0256*SAND*(1-(SILT/100))))*((SILT/(CLAY+SILT))*exp(0.3))*(1-
((0.25*CO)/(CO+exp(3.72-2.95*CO))))*(1-((0.7*SN1)/(SN1+exp(-5.51+22.9*SN1))))',
{'SAND':soil.select('sand'),'SILT':soil.select('silt'),
'CLAY':soil.select('clay'),'MO':soil.select('mo'),
'SN1':soil.select('sn1'),'CO':soil.select('co')
});
```

```
//Calcula o factor C
var MAX_CLOUD_PROBABILITY = 65;
var s2_lv1 = ee.ImageCollection('COPERNICUS/S2');
var s2Clouds = ee.ImageCollection('COPERNICUS/S2_CLOUD_PROBABILITY');
var s2SrWithCloudMask = ee.Join.saveFirst('cloud_mask').apply({
 primary: s2_lv1,
 secondary: s2Clouds,
 condition:
   ee.Filter.equals({leftField: 'system:index', rightField: 'system:index'})
});
function maskClouds(img) {
 var clouds = ee.Image(img.get('cloud_mask')).select('probability');
 var isNotCloud = clouds.lt(MAX_CLOUD_PROBABILITY);
 return img.updateMask(isNotCloud);
}
var addIndexBands = function(image) {
 return image
  .addBands(image.normalizedDifference(['B8', 'B4']).rename('NDVI'))
  .addBands(image.metadata('system:time_start'));
};
var s2CloudMasked = ee.ImageCollection(s2SrWithCloudMask)
var s2020_1 = s2CloudMasked.filterDate('2020-01-01','2020-12-
31').filterBounds(geometry).map(maskClouds).map(addIndexBands).median()
var NDVI = s2020_1.normalizedDifference(['B8', 'B4'])
var factorC = NDVI.expression('((-NDVI+1)/(2))',{'NDVI':NDVI,});
```

```
//Calcula o factor R
var pp = ee.Image("OpenLandMap/CLM/CLM_PRECIPITATION_SM2RAIN_M/v01");
var annual_pp = pp.reduce(ee.Reducer.sum())
var
Monthly_pp=ee.Image(10).pow(ee.Image(1.5).multiply(pp.pow(2).divide(annual_pp).log10().
subtract(-0.08188))).multiply(1.735)
var factorR=Monthly_pp.reduce(ee.Reducer.sum())
```

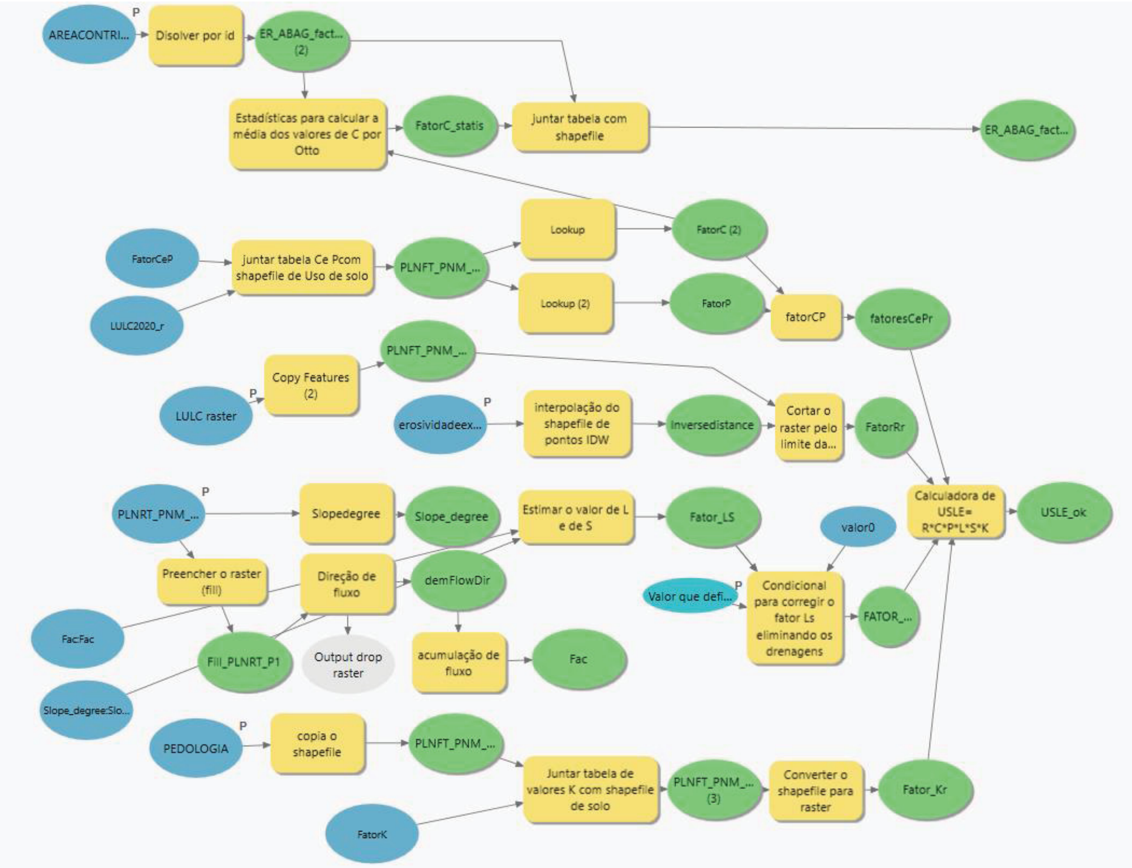
```
//Calcula o factor LS
var facc= ee.Image("WWF/HydroSHEDS/15ACC").clip(geometry);
var flowAccumulation = facc.select('b1');
var dataset = ee.Image('WWF/HydroSHEDS/03CONDEM').clip(geometry);
var dem = dataset.select('b1');
var slope = ee.Terrain.slope(dem);
var slope_percent = slope.expression('tan(SLOPE/180*3.14)*100',{'SLOPE':slope});
//// Calculate aspect. Units are degrees where 0=N, 90=E, 180=S, 270=W.
var aspect = ee.Terrain.aspect(dem);
//Calculando o LS usando o artigo de (https://doi.org/10.1016/j.mex.2019.01.004 e
//https://naldc.nal.usda.gov/catalog/CAT10698097)...........
var seno = slope.expression('sin(b)',{'b':slope});
var Bf =
slope.expression('((abs(SENO)/0.0896)/(0.56+3*(abs(SENO))*exp(0.8)))',{'SENO':seno});
```

```
VAR M = BF.EXPRESSION('BFX/(BFX+1)',{BFX:BF})
VAR X_VARIAVEL = EE.IMAGE([ASPECT]).RENAME (['ASPECT1']);
VAR X = X_VARIAVEL.EXPRESSION('ABS(SIN(ASPECT1))+ABS(COS(ASPECT1))',
{'ASPECT1':X_VARIAVEL.SELECT('ASPECT1')});
VAR L_FACTORS = EE.IMAGE([FLOWACCUMULATION,SLOPE,BF,M,X]).RENAME
(['FLOWACC','SLOPE','B','M','X']);
VAR FACTORL = L_FACTORS.EXPRESSION('((((FACC+(450*450))*EXP(M+1)-
FACC*EXP(M+1)))/(450*EXP(M+2)*X*EXP(M)*22.13*EXP(M)))',
{'FACC':L_FACTORS.SELECT('FLOWACC'),
 'M':L_FACTORS.SELECT('M'),
 'B':L_FACTORS.SELECT('B'),
 'SLOPE':L_FACTORS.SELECT('SLOPE'),
 'X':L_FACTORS.SELECT('X')});
VAR S_FACTORS = EE.IMAGE([SLOPE_PERCENT,SENO]).RENAME (['SLOPE_PER','SENO']);
VAR FACTORS = S_FACTORS.EXPRESSION('(0.044+0.10*SLOPE_PER-0.00073*SLOPE_PER*EXP(2))',
{'SENO':S_FACTORS.SELECT('SENO'),
 'SLOPE_PER':S_FACTORS.SELECT('SLOPE_PER')});
VAR LS = FACTORS.MULTIPLY(FACTORL);
```

```
\/CALCULANDO O USLE___________________________
VAR ERO = FACTORR.MULTIPLY(FACTORK).MULTIPLY(LS).MULTIPLY(FACTORC);
LINK:
(Https://Code.Earthengine.Google.Com/?Scriptpath=Users%2feileenandreaacosta%2fcod_Psa%3ausle
%2fusletotal)
```

A routine was generated to define the historical erosion map using the Universal Soil Loss Equation in Figure 32. The main difference from modeling done by other models is that MoRE has adjustment factors to calculate erosion for the specific year, modifying soil cover and rainfall erosivity factors, adjusting the equation for the year being analyzed. This does not occur in other models where the average erosion remains the same over the period. In other countries, it may not be necessary to perform this algorithm in the case of an existing ready-made raster map of average soil losses from already developed basins, so Part 1 of the model is considered optional.

FIGURE 32 – GRAPHICAL MODEL FOR ESTIMATING SOIL EROSION MAP



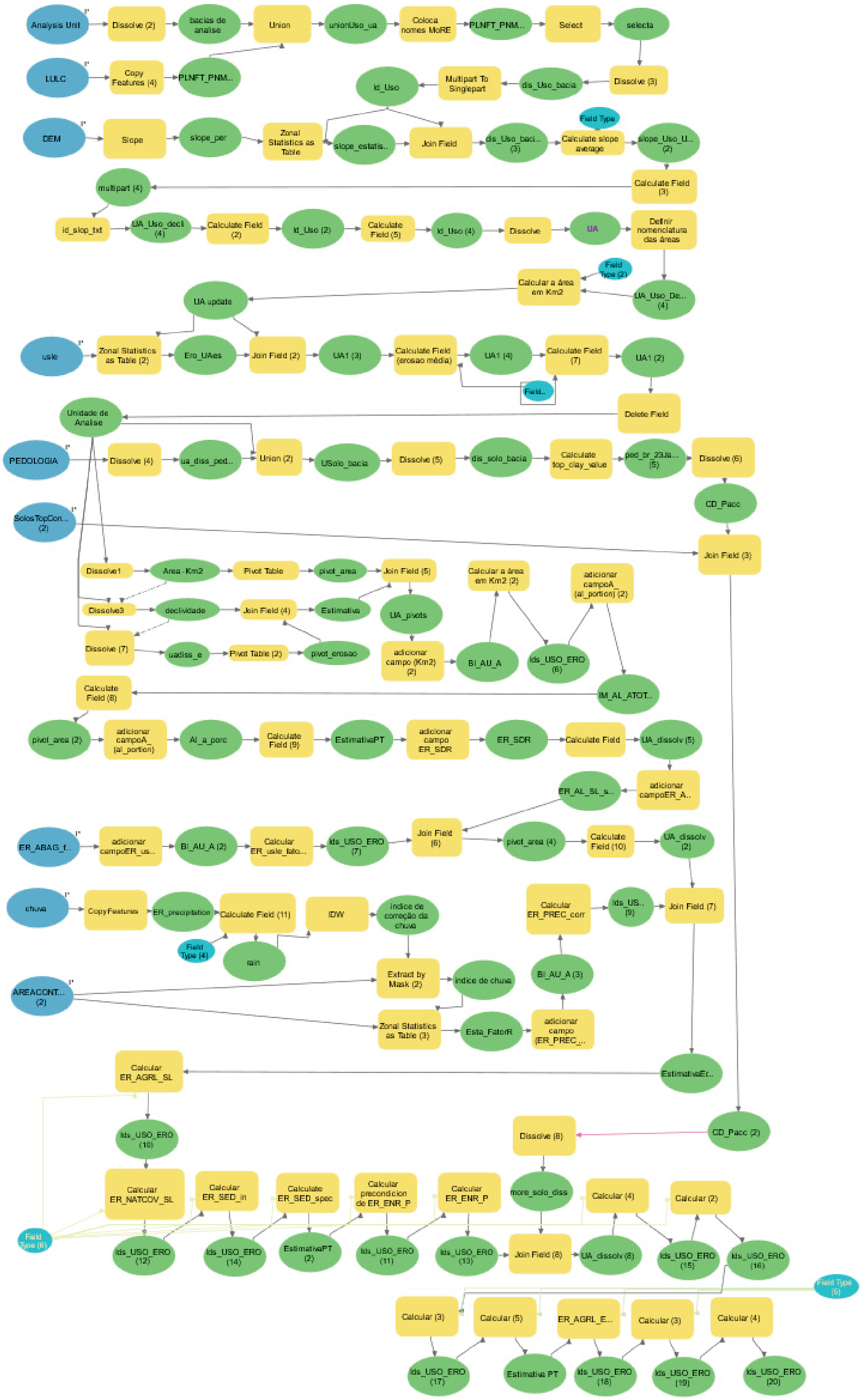
9.1.4.2 Input of pollutants from water erosion

The definition of the main information to define the tables of the analysis unit (Figure 33). As inputs for this part of the model, we have the digital elevation model, land use and cover, and a delineation of selected basins with a unique identifier code (ID), as well as the map estimating historical average erosion, which was generated in the previous flowchart. In the processes represented in orange, the tables and information necessary for the modeling are calculated, including: land use nomenclature coding, slope in percentage, average slope of the analysis unit, nomenclature for the slope, area in square kilometers, and the average erosion for each type of land use within the analysis unit (t/ha/year). The result of this process is an information layer of the analysis units with their respective linked information.

In the modeling, soil is an important factor. MoRE considers both the accumulation of the substance in the soil over the historical period and the amount that can be accumulated each year. Therefore, the accumulations of phosphorus were estimated according to the flowchart in Figure 33. The inputs in blue are the analysis unit, pedology, and the accumulated phosphorus and nitrogen content in the surface layer of the soil.

The analysis unit was defined for this work as level 6 of the ottocoded basins of ANA. The ottobasins are the current official division of Brazilian watersheds and are divided into various levels. The size of the analysis unit directly influences the processing time of the models and depends on the spatial resolution of the input variables (Figure 33).

FIGURE 33 – GRAPHIC MODEL OF THE EROSION MODULE



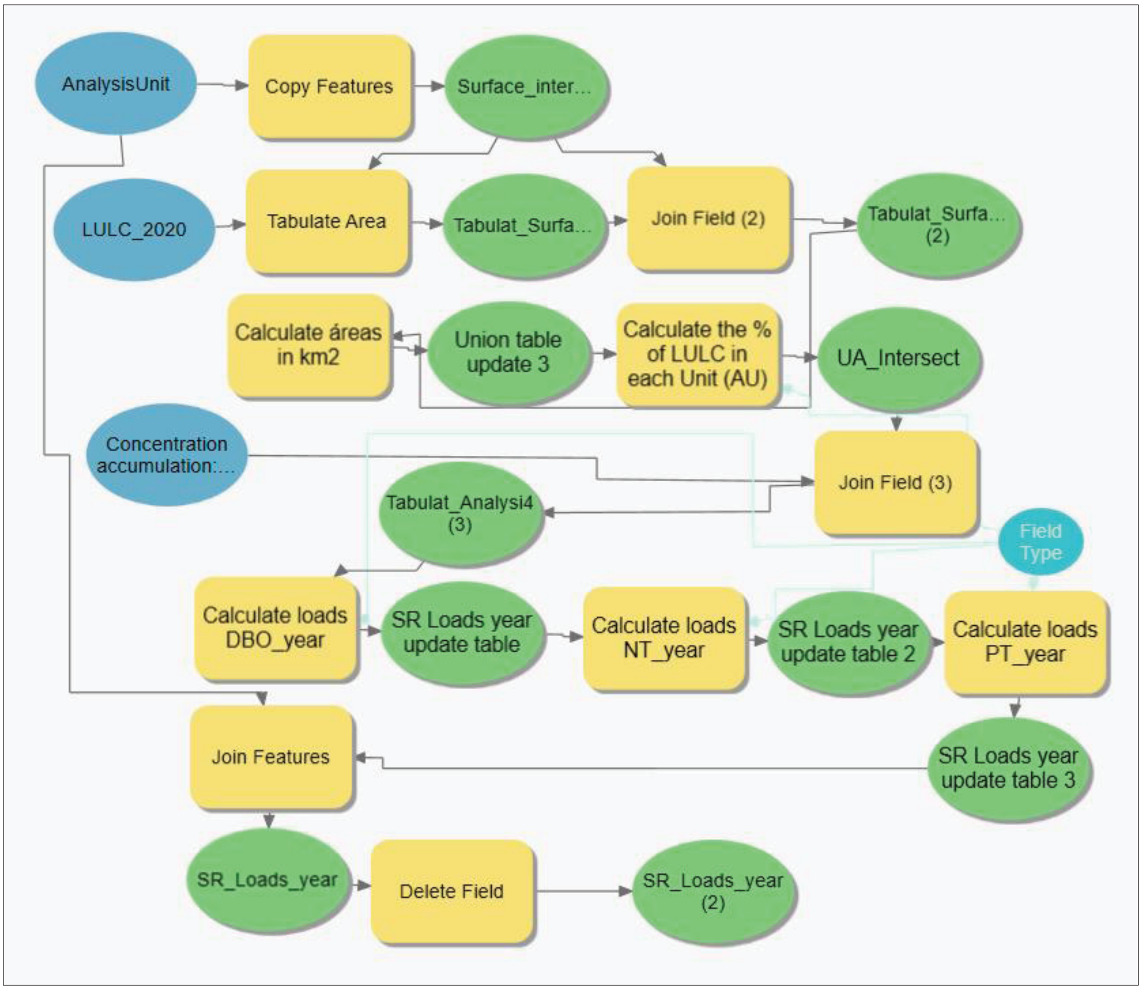
9.1.5 Module to estimate untreated domestic effluent

This source of pollution, 'untreated sewage,' is calculated using data provided in the IBGE census, chosen because they are based on census zones, while others are based on municipalities, making it difficult for discretization by ottobasin. Therefore, untreated sewage was considered all domestic sewage generated that is not collected and is being treated as a diffuse module. The IBGE information pertains to the number of residents in permanent private households with a bathroom for exclusive use of residents or a toilet. These are classified as: general sewage or rainwater system (when there is a sewage collection system, whether or not treated in a Wastewater Treatment Plant), septic tank (individual solution), or rudimentary septic tank (individual solution)

FIGURE 34 – MODULE FOR ESTIMATING UNTREATED SEWAGE IN URBAN AREAS

9.1.6 Surface runoff module - diffuse loads transported in surface runoff

FIGURE 35 – MODULE FOR ESTIMATING SURFACE RUNOFF



9.1.7 Module to estimate the loads from Atmospheric Deposition

FIGURE 36 – MODULE FOR ESTIMATING LOADS FROM ATMOSPHERIC DEPOSITION