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Effects of climate and land use changes on water ecosystem services: understanding the mitigating effect of green land use scenarios

PHELIPE DA SILVA ANJINHO

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Effects of climate and land use changes on water ecosystem services: understanding the mitigating effect of green land use scenarios

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ABSTRACT

ANJINHO, P. S. **Effects of climate and land use changes on water ecosystem services: understanding the mitigating effect of green land use scenarios**. 187p. Doctoral Thesis, Sao Carlos School of Engineering, University of Sao Paulo, Sao Carlos, 2024.

Water ecosystem services (WES) are crucial for preserving environmental quality and human well-being. Their degradation is primarily associated with climate and land use changes. This study aimed to understand how these factors affect WES in the Jacaré-Guaçu river basin, located in São Paulo, Brazil. Regional climate and biophysical models were used to investigate the effects of different climate and land use scenarios on erosion control, water supply, and purification services. Indicators such as sediment export and retention (erosion control), total nitrogen and total phosphorus export and retention (water purification), and quickflow and baseflow (water provision) were used to quantify these services. The research hypothesis involved testing whether green land use scenarios, based on increasing native vegetation, could enhance provision and mitigate adverse effects of climate change on WES. The research was structured into six chapters, with the first chapter presenting the general introduction, objectives, and research hypothesis. The second chapter involved a literature review on WES, aiming to identify potentials, limitations, and gaps in applying this approach to water resources planning and management. The third chapter assessed the performance of InVEST biophysical models in predicting observed values of WES, discussing important issues such as sensitivity, calibration of biophysical parameters, and validation of simulations. The fourth chapter investigated the effects of past land use changes on WES, proposing environmental zoning to identify priority areas for conservation and restoration of native vegetation, and evaluating the impacts of a planned land use scenario on WES. The fifth chapter assessed the individual and combined effects of four climate scenarios (RCP 4.5 2040-2069, RCP 4.5 2070-2099, RCP 8.5 2040-2069, RCP 8.5 2070-2099) and three land use scenarios (economic, trend, and green) on WES. Additionally, in the fifth chapter, the overall hypothesis of the research was tested. The results of all studies allowed understanding the individual and combined effects of climate and land use changes on WES, highlighting the positive effects of green land use scenarios on the provisioning of WES and mitigation of climate change impacts. The contributions and insights of this research are important for researchers and public managers interested in integrated planning and management of water resources.

Keywords: Ecosystem services. Climate change. Land use changes. Biophysical modeling. InVEST models.

RESUMO

ANJINHO, P. S. **Efeitos das mudanças climáticas e de uso do solo nos serviços ecossistêmicos hídricos: compreendendo o efeito mitigador de cenários verdes de uso do solo.** 187p. Doctoral Thesis, Sao Carlos School of Engineering, University of Sao Paulo, Sao Carlos, 2024.

Os serviços ecossistêmicos hídricos (SEH) são fundamentais para preservar a qualidade ambiental e o bem-estar humano. Sua degradação está associada principalmente às mudanças climáticas e de uso do solo. Este estudo buscou compreender como esses fatores afetam os SEH da bacia hidrográfica do rio Jacaré-Guaçu, localizada no interior do São Paulo, Brasil. Modelos climáticos regionais e biofísicos foram utilizados para investigar os efeitos de diferentes cenários climáticos e de uso do solo nos serviços de controle de erosão, provisão e purificação da água. Os indicadores exportação e retenção de sedimentos (controle de erosão), exportação e retenção de nitrogênio total e fósforo total (purificação da água) e quickflow e baseflow (provisão de água) foram utilizados para quantificar esses serviços. A hipótese da pesquisa envolveu testar se cenários verdes de uso do solo, baseado no incremento de vegetação nativa, podem ampliar a provisão e mitigar os efeitos adversos das mudanças climáticas nos SEH. A pesquisa foi estruturada em seis capítulos, o primeiro capítulo apresentou a introdução geral, objetivos e hipótese da pesquisa. O segundo capítulo consistiu em uma revisão da literatura sobre serviços ecossistêmicos hídricos, buscando identificar potencialidades, limitações e lacunas na aplicação dessa abordagem ao planejamento e gerenciamento dos recursos hídricos. O terceiro capítulo avaliou a performance dos modelos biofísicos do InVEST em prever os valores observados dos SEH, discutindo questões importantes como sensibilidade e calibração dos parâmetros biofísicos e validação das simulações. O quarto capítulo investigou os efeitos das mudanças pretéritas de uso do solo nos SEH, propondo um zoneamento ambiental para identificar áreas prioritárias à conservação e restauração da vegetação nativa, além de avaliar os impactos de um cenário planejado de uso do solo nos SEH. O quinto capítulo avaliou os efeitos individuais e combinados de quatro cenários climáticos (RCP 4.5 2040-2069, RCP 4.5 2070-2099, RCP 8.5 2040-2069, RCP 8.5 2070-2099) e três de uso do solo (econômico, tendencial e verde) nos SEH. Além disso, no quinto capítulo foi testada a hipótese geral dessa pesquisa. Os resultados de todos os estudos possibilitaram compreender os efeitos individuais e combinados das mudanças climáticas e de uso solo nos SEH da bacia hidrográfica estudada, destacando os efeitos positivos de cenários verdes de uso do solo no provisionamento de SEH e mitigação dos impactos das mudanças climáticas. As contribuições e insights desta pesquisa são importantes para pesquisadores e gestores públicos interessados no planejamento e gerenciamento integrado dos recursos hídricos.

Palavras-chave: Serviços ecossistêmicos. Mudanças climáticas. Mudanças de uso do solo. Modelagem biofísica. InVEST models.

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Chapter 1

INTRODUCTION AND GENERAL CHARACTERIZATION OF THE RESEARCH

1.1. Introduction

Since the mid-20th century, the planet has undergone intense and continuous changes in its natural characteristics to promote economic development and the population's well-being (FOLKE et al., 2021; JØRGENSEn et al., 2024). These changes have led to greater development and technological innovation, facilitating progress in various sectors such as agriculture, health, education, energy, transportation, and sanitation, commonly associated with human well-being. While providing multiple benefits to society, modifications to the Earth's surface cause environmental impacts that affect biodiversity and humanity (ROCKSTRÖM et al., 2009; STEFFEN et al., 2017).

The term "global changes" refers to anthropogenic transformations on a planetary scale that alter the natural cycle of the planet, generating impacts on society, the economy, and the environment (STEFFEN et al., 2017; FOLKE et al., 2021). Among these transformations, climate and land use changes stand out as the main drivers associated with global changes (SALES et al., 2020; ASAMOAH et al., 2021; DAVISON et al., 2021). These changes have altered the planet's cycles of matter and energy (ELLISON et al., 2017; SUN et al., 2017), causing diverse impacts, especially on Water Ecosystem Services (WES), which in this study are related to the hydrological, nutrient, and sediment cycles (erosion control, water provision, and purification).

Climate and land use changes are two processes with significant effects on ecosystem functioning. Not only are these processes interconnected, meaning changes in one can affect the other, but they can also generate synergistic impacts on ecosystems, sometimes more intense than individual effects (SEGURADO et al., 2018; BAI et al., 2019). Regarding WES, climate change affects them due to changes in precipitation and temperature patterns. These factors directly influence the flow of water, nutrients, and sediments in watersheds (SUN et al., 2017). In turn, the conversion of natural vegetation for agricultural expansion, urbanization, mining, and other anthropogenic uses alters key ecohydrological processes related to WES, including energy, water, sediment, and nutrient cycles, due to the biophysical characteristics of each plant species (ELLISON et al., 2017).

Understanding the impacts of these changes is crucial for developing mitigation and adaptation strategies. The global challenge lies in finding solutions that enhance ecosystem resilience and the provision of their services. Forests and other types of native vegetation play a crucial role in regulating ecohydrological processes and, consequently, WES (CAPON et al., 2013; ELLISON et al., 2017; RIIS et al., 2020). Studies suggest that native vegetation has the potential to control erosive processes, improve water infiltration and aquifer recharge, regulate base flow, ensuring water availability during droughts, and purify water in watersheds (FERREIRA et al., 2019; WEN; THÉAU, 2020; GHIMIRE et al., 2021).

Biophysical modeling is a fundamental element for understanding the impacts of climate and land use changes, using mathematical equations in computational environments to quantify ecosystem services (PALOMO et al., 2017). These models are crucial for elucidating ecohydrological processes in watersheds and for the assessment and prediction of multiple environmental pressures (GRIZZETTI et al., 2016). When properly calibrated and validated, they provide a valuable tool in the planning and management of water resources, significantly contributing to the development of effective policies aimed at watershed conservation, including ecological restoration projects.

The surface and groundwater resources of the Jacaré Guaçu River Basin (JGRB) are crucial water sources for the central-eastern region of the state of São Paulo. Over the years, there have been significant changes in its land use, with areas previously used for pasture and, to a lesser extent, native vegetation, converted to sugarcane plantations. This transformation in land use has affected the hydrological, sedimentological, and nutrient dynamics of the basin, impacting the provision and conservation of WES. Additionally, climate change may also impact these services due to projected reductions in rainfall and higher temperatures by the end of the century in São Paulo. The JGRB is an important case study because it is already experiencing the effects of land use changes, and climate change may exacerbate these impacts on WES. Moreover, being a rural basin allows for sustainable land management, aligning with one of the objectives of this thesis, which is to identify priority areas for ecological conservation and restoration to enhance WES provision (Chapter 4).

This research was conducted to assess the individual and combined effects of climate and land use changes on WES in the JGRB, located in the state of São Paulo, southeastern Brazil. The hypothesis involved understanding how implementing green land use scenarios can improve WES supply and mitigate adverse effects of climate change. The study was structured into six chapters, each addressing specific yet complementary aspects of the research. The first chapter corresponds to this general introduction, followed by the research objectives and scientific hypothesis. The second chapter canvassed the literature to identify key areas of knowledge and understand relevant concepts of the WES-based approach. This chapter also discussed the potential and challenges of this approach applied to water resources planning and management. The third chapter focused on analyzing the performance of the biophysical models of WES used in this study, involving their calibration and validation. The fourth chapter was developed to create a methodology for identifying priority areas for ecological conservation and restoration in the study area. This chapter aimed to provide insights for watershed land use planning, evaluating how the implementation of green scenarios could increase WES supply. The fifth chapter complements the analysis by exploring the individual and combined effects of climate and land use changes on WES. In this chapter, the potential of green land use scenarios, based on the reintroduction of native vegetation, was investigated to expand the supply of WES and mitigate the adverse impacts of climate change. The sixth chapter presents the general conclusions of the research.

This study sought to understand not only the processes related to WES provision but also to propose guidelines for land use management to promote them in the face of climate and land use changes. The contributions and insights of this research are valuable for policymakers, researchers, and public managers interested in integrated water resources management.

1.2. Research Objectives

The study's overall objective was to assess the individual and combined effects of climate and land use changes on WES, specifically erosion control, water supply, and water purification, in the JGRB. To achieve this, the following specific objectives were established:

1) Evaluate the performance of InVEST biophysical models in simulating WES indicators.

2) Evaluate the effects of past climate and land use changes on WES.
3) Propose a methodology to identify priority areas for conservation and ecological restoration of WES.
4) Assess the individual and combined effects of future climate and land use changes on WES.
5) Evaluate if green scenarios, based on increasing native vegetation, can enhance WES provision and mitigate adverse effects of climate change.

1.3. Scientific hypothesis

This study is based on the hypothesis that increasing green areas through native vegetation restoration projects regulates the biophysical processes associated with water, nutrient, and sediment cycles at the watershed scale. It is hypothesized that restoring native vegetation in key areas enhances the resilience of natural ecosystems, making it a highly effective strategy to expand the provision of water ecosystem services and mitigate the adverse effects of climate change on these services.

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Chapter 2

WATER ECOSYSTEM SERVICES: POTENTIAL AND CHALLENGE FOR WATER RESOURCE MANAGEMENT

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ANJINHO, P.S et al. Water Ecosystem Services: Potential and Challenge for Water Resource Management. **Novel Perspectives of Geography, Environment and Earth Sciences Vol. 7**, p. 30-68, 2023. DOI: 10.9734/bpi/npgees/v7/18550D

ABSTRACT

Ecosystem services are goods and services provided by ecosystems for human well-being. This study canvasses the literature to identify knowledge areas and understand concepts relevant to addressing water ecosystem services. The potentialities and challenges of this approach applied to the planning and management of water resources were also discussed. The study addressed relevant topics such as ecosystem services, eco-hydrological processes, climate change, land use, ecosystem-based adaptation, biophysical modeling, economic valuation, and integrated water resources management. The ecosystem services-based approach has practical applications in water resource management; however, this study has identified knowledge gaps that should be addressed to ensure its effectiveness. Further research is in order to: 1) understand the synergic effects of multiple water resource drivers, 2) identify the ecohydrological processes of natural ecosystems and how restoration can enhance water ecosystem services and mitigate climate change, 3) expand knowledge of and validation in the use of biophysical models, 4) intensify the integration of biophysical assessment and economic valuation, and 5) include all dimensions of ecosystem service values to increase user and stakeholder participation in water resource management.

Keywords: Ecohydrological processes. Ecosystem services. Ecosystem services valuation. Integrated water resource management. Water ecosystem services.

2.1. Introduction

Population growth associated with economic and technological development has affected the environment. Alterations in the structure and functions of natural ecosystems and climate change have endangered biodiversity and ecosystem services, particularly freshwater ones (VÖRÖSMARTY et al.,2013; PHAM et al., 2019). Ecosystem services are goods and services provided by ecosystems that enhance human well-being (COSTANZA et al., 2017). The concept arose from the need to understand the functions of ecosystems and assess their anthropic vulnerabilities and served as a tool to reconcile socio-economic development and environmental conservation. Initial references were noted in Ehrlich and Ehrlich (1981) and Ehrlich and Mooney (1983), but the concept attained worldwide recognition in 2005 through publications of the Millennium Ecosystem Assessment (MEA, 2005). Subsequent studies have enhanced our understanding of ecosystems and their services, enabling biophysical quantification and mapping of areas with the greatest need for and availability of ecosystem services, computation of economic valuation, analysis of trends, and designation of indicators to assess the ecological status of ecosystems and their services (GRIZZETTI et al., 2016), measures crucial to policymakers and decision-makers (GREEN et al., 2015).

This study focuses on water ecosystem services (WES), also known as hydrological ecosystem services or freshwater ecosystem services (BRAUMAN et al., 2007; GREEN et al., 2015; AZNAR-SÁNCHEZ et al., 2019). These services are provided by aquatic and terrestrial ecosystems and can be determined for a water body or river basin (HERING et al., 2015; GRIZZETTI et al., 2016; MAES et al., 2016). Water ecosystem services such as erosion control, water supply, and purification are vital to human well-being and economic development. Due to the involvement of such multidisciplinary factors as ecology, hydrology, economics, environmental policies, and land use, numerous studies have employed its context (MARTIN-ORTEGA et al.,2013; VIGIAK et al., 2016; LA NOTTE et al., 2017; YAN et al., 2018). Although some studies examine theoretical questions on ecosystem services (DAILY, 1997; MEA, 2005; DE GROOT et al., 2010; COSTANZA et al., 2017), in regard to WES, most focus on such applications as biophysical modeling and economic valuation (HACKBART et al., 2017). Of the studies reviewed, only Brauman et al. (2007) provide a systematic theoretical basis that addresses the main concepts related to WES, and Cook and Spray (2012) reviewed the literature to understand the relationship between WES and integrated water resources management. While not review studies, Grizzetti et al. (2016) addresses theoretical concepts and present a systematic structure to assess WES, and Liu et al. (2013) proposed an ecosystem service framework to support integrated water resource management. Most analyze the evolution and state of WES research (HACKBART et al., 2017; AZNAR-SÁNCHEZ et al., 2019) or examine biophysical modeling (VIGERSTOL; AUKEMA, 2011; HALLOUIN et al., 2018) and impacts on WES (JIN et al., 2015; PHAM et al., 2019). Research on WES has grown exponentially over the past decade, but few review studies present the state-of-the-art (AZNAR-SÁNCHEZ et al., 2019), which is critical to disseminating scientific knowledge and guiding researchers.

Therefore, this study extends our comprehension of the theoretical and conceptual foundations that undergird its WES approach and describes the potentials and challenges of an ecosystem service-based approach applied to water resource planning and management. As research on WES is multidisciplinary, and knowledge is often fragmented, it identifies and discusses nine themes that synergistically provide a background for understanding its WES-based approach. To this end, SCOPUS and Web of Science databases were searched to find relevant, quality studies on these themes. The research focused on freshwater ecosystem services, generated from interaction among river basin ecosystems. The intent is not to provide a systematic, quantitative review, but rather to describe current scientific knowledge on WES and explore its application to water resource planning and management. Studies are cited to provide scientific background to the discussion, and themes are structured based on analysis of studies, in particular, Brauman et al. (2015), Grizzetti et al. (2016), and Sun et al. (2017).

This study is structured as follows. Section 2.2 provides an overview, addressing ecosystem structure and functions, as well as their services and classifications. Section 2.3 contextualizes WES and discusses the main themes related to a WES-based approach. Section 2.3.1 describes ecohydrological processes, showing how vegetation affects material and energy cycles and, consequently, WES. Section 2.3.2 presents the principal drivers that can affect the flow and WES availability. Section 2.3.3 discusses the role of natural ecosystems in regulating ecohydrological processes and their potential to mitigate the effects of environmental changes. Sections 2.3.4 and 2.3.5 consider biophysical modeling and economic valuation of WES, citing case studies. Section 2.3.6 highlights the potential of the ecosystem services-based approach to water resource management, and section 2.3.7 presents its challenges and limitations. Finally, section 2.4 summarizes the study results and provides recommendations for further research.

2.2. Contextualizing ecosystem services

Ecosystems can be defined as a set of biotic and abiotic factors that interact in the environment forming a fundamental ecological unit (TANSLEY, 1935). An ecosystem is a spatial unit in which dynamic interactions occur between biodiversity and physical environment. They can be natural, such as estuaries, lakes, rivers, and forests, or modified by humans, such as urban and rural areas (VILLAMAGNA et al., 2013), and vary in scale, from local to global (CBD, 2010). Diverse factors can affect ecosystems, including such natural catastrophes as floods and forest fires, and anthropic activities, which constitute the primary contributor to natural ecosystem degradation (MEA, 2005). Changes in biophysical characteristics can compromise the structure and function of natural ecosystems, impacting their supply of goods and services (ROCKSTRÖM et al., 2009; DIETZ, 2017), with adverse effects on forest and water resources, climate change, and biodiversity (OSTROM, 2009). Such negative impacts particularly harm the poor as they rely most on ecosystem services (MEA, 2005).

The structure and function of natural ecosystems have changed more rapidly in the latter half of the twentieth century than at any previous time. Some 60% of the services analyzed in the Millennium Ecosystem Assessment, including water and air purification, climate regulation, and fishing have been degraded or used unsustainably (MEA, 2005). Thus, it is vital to integrate ecological and anthropogenic systems to harmonize socio-economic development and environmental conservation (STEFFEN et al., 2015) through strategies that incorporate ecosystem services, emphasizing their importance to human well-being and provision of resources vital to economic development (COSTANZA et al., 2017). Ecosystems services are any benefits, direct or indirect, that humans obtain from ecosystem functions (MEA, 2005; COSTANZA et al., 2017), which are understood as the constant interactions among the biotic and abiotic factors that form the structure of ecosystems and include energy transfer, nutrient cycling, and climate regulation (DALY; FARLEY, 2004). These functions describe the biophysical relations of ecosystems, and when they produce direct or indirect benefits, are considered ecosystem services (BRAAT, 2013). This perspective has been criticized for its utilitarian view of environmental systems, which focused on the economy while overlooking intrinsic values

(FÜRST, 2015). It should be noted that ecosystem functions are not always directly related to ecosystem services and that a service can be generated from one or more ecosystem functions, while a function can result in one or more services.

To enhance understanding of ecosystem services, Haines-Young and Potschin (2010) proposed a cascade model, since modified by De Groot et al. (2010). The model links functions, services, benefits, and values (Figure 2.1). Benefits can be economic, social, health, and intrinsic (HAINES-YOUNG; POTSCHIN, 2010), and ecosystem services can be classified as intermediate and final (POTSCHIN; HAINES-YOUNG, 2011), a crucial distinction in regard to economic valuation as it precludes double counting (FISHER et al., 2009).

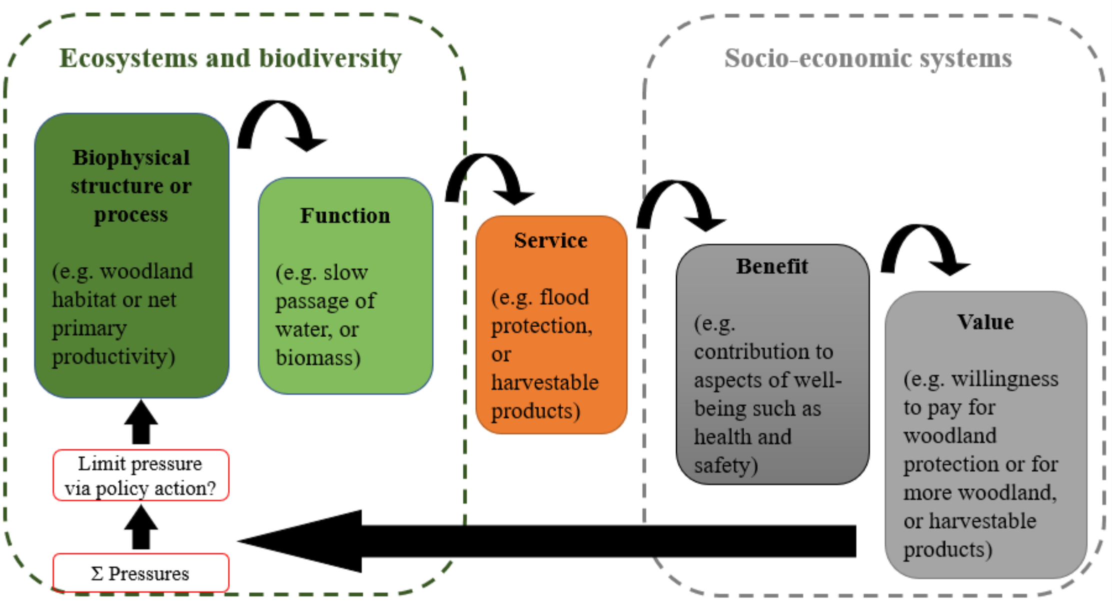

Figure 2.1. Ecosystem service cascade model (adapted from Potschin and Haines-Young, 2011).

Numerous studies have systematized the concept of ecosystem services (COSTANZA et al., 1997; MEA, 2005; WALLACE, 2007; FISHER et al., 2009). The most diffuse classification was undertaken by the Millennium Ecosystem Assessment, which classified ecosystem services as 1) provisioning (providing natural goods, such as water, wood, and energy), 2) regulating (controlling ecosystem processes, such as climate, water purification, and flooding), 3) cultural (denoting intangible benefits, including educational, spiritual, and recreational) and 4) supporting (designating basic processes, such as nutrient cycling, soil formation, and primary production) (MEA, 2005). A more recent and simpler classification that should be noted is the European Environment Agency's Common International Classification of Ecosystem Services

(CICES), which standardizes the concept and facilitates mapping, quantification, and valuation. CICES is based on the approach in MEA (MEA, 2005), enhanced through a structured literature review (HAINES-YOUNG; POTSCHIN, 2018). Supporting services are not included in CICES, as they are deemed part of the structure and function of ecosystems. It should be borne in mind that although several analogous classification systems have been proposed (COSTANZA et al., 2017), the adoption of a classification system depends on the characteristics of each study. It is essential to consider the ecological, social, and political aspects in which ecosystem services are being examined, as the use of an inappropriate classification system can compromise research results (FISHER et al., 2009).

Understanding the structure and function of ecosystems, as well as the services they provide is a critical prerequisite to formulating sound socio-economic policies. The first major initiative highlighting the importance of integrating ecosystem services and development occurred in 1995 at a meeting of leading researchers conducted by Pew Scholars in Conservation and the Environment (COSTANZA et al., 2017). The event gave rise to Nature's Services: Societal Dependence on Natural Ecosystems (DAILY, 1997). Other major initiatives include the Millennium Ecosystem Assessment (MEA, 2005), The Economics of Ecosystems and Biodiversity (TEEB) (TEEB, 2010), and the Intergovernmental Science-Policy Platform on Biodiversity and Ecosystem Services (IPBES).

Coordinated by the United Nations Environment Program and carried out between 2001 and 2005, MEA was a collaborative effort that involved more than 2,000 authors and reviewers. Its benchmark study provided the first global assessment of the state of ecosystems and enhanced understanding of their role in human well-being and future trends, including principal causes of their degradation and strategies to conserve them (MEA, 2005). Through MEA, it was possible to establish the scientific basis required to disseminate an ecosystem services-based approach worldwide. Thus, it was following MEA that the ecosystem service concept began to be widely discussed in the literature in the context of sustainable development, with a significant increase in mid-2003 (FISHER et al., 2009).

TEEB resulted from an agreement among environmental ministers of the G8+5 nations, meeting in Potsdam, Germany, in 2007. The initiative’s primary objective was to demonstrate the economic benefits of ecosystem services and biodiversity and the adverse impact of their degradation (TEEB, 2010). Conducted between 2008 and 2010 through the collaboration of more than 500 researchers, TEEB presented its results in six reports at the tenth Conference of the Parties to the United Nations Convention of Biological Diversity, in Nagoya, Japan.

Created in 2012, IPBES is an independent intergovernmental body with members from 126 nations and four United Nations bodies (United Nations Environment Program, Food, and Agricultural Organization, United Nations Development Program, and United Nations Educational. Scientific, and Cultural Organization (COSTANZA et al., 2017). Its primary objective is to disseminate information on the state of biodiversity, ecosystems, and associated services to inform decision-making.

Critical challenges in incorporating an ecosystem services-based approach in conservation include clarifying concepts and determining precise assessment methods. Many questions remain to be properly understood to assess the sustainability of ecosystems, including their capacity to provide services, as well as service flow and demand and natural and anthropic pressures (VILLAMAGNA et al., 2013). In addition to such methodological challenges, the lack of appropriate institutional structures and the need for greater transparency must be addressed (COSTANZA et al., 2017).

2.3. Contextualizing water ecosystem services

Water runs through all environments and interacts with other ecosystems. Water ecosystem services are generated by aquatic ecosystems, such as oceans, lakes, rivers, and streams, and their interaction with terrestrial ecosystems (HERING et al., 2015; GRIZZETTI et al., 2016). These services are directly linked to the hydrological cycle, which, in turn, is related to other ecosystem processes, such as nutrient and sediment flow, climate regulation, soil formation, and primary production (SUN et al., 2017). To facilitate understanding of WES, Brauman et al. (2017) proposes the following classifications: 1) extraction, that is, the capacity of aquatic ecosystems to provide water for multiple uses (agriculture, livestock, and urban), 2) in situ uses (electricity generation, transportation, recreation, and fish farming), 3) mitigation of water damage via regulatory functions (flood mitigation, water purification, and erosion control), 4) cultural services (aesthetic, spiritual, and tourism uses), and 5) supporting services (creating habitats for aquatic communities).

Grizzetti et al. (2016) noted two approaches to WES organization and analysis, one related to the typology of aquatic ecosystems and services by rivers, lakes, aquifers, wetlands, estuaries, swamps, and so forth (MAES et al., 2016) and the other related to the ecohydrological processes of river basins (BRAUMAN et al., 2007). Interactions between vegetation, climate, and hydrology at various spatial and temporal scales determine the ecohydrological processes and, consequently, WES. The following section presents an overview of how these interactions occur, highlighting the critical role vegetation plays in ecosystem energy and material flows.

2.3.1. Ecohydrological processes and water ecosystem services

Ecohydrology integrates ecology and hydrology to create a comprehensive approach to addressing environmental problems (ZALEWSKI, 2015). Ecohydrological processes are crucial to understanding WES availability and flow. All ecosystems within a river basin can provide WES, varying according to the basin's climate, fauna, flora, drainage area, and other characteristics (ALLAN, 2004). Vegetation is one of the chief components of ecosystems and is often regarded as the ecosystem itself due to its importance in ecosystem functions. The composition and configuration of vegetation impact ecohydrological processes that, in turn, affect WES quantity, quality, location, and flow (BRAUMAN et al., 2007). The effects of vegetation on ecohydrological processes can be described from studies of the energy, water, carbon, and nutrient cycles (phosphorus and nitrogen) (SUN et al., 2010).

The influence of vegetation on energy flow arises from the capacity of different plant species to capture and disseminate solar energy (MAES et al., 2011). The effects of ecosystems on climate biophysical factors are discussed within the scientific community and require further research to compile, examine, and evaluate the evidence. Research indicates that surface roughness, albedo, and evapotranspiration are the biophysical factors most affected by vegetation changes that can alter the surface and air temperature (MAES et al., 2011; ALKAMA; CESCATTI, 2016) and that their effects on surface temperature vary according to scale, latitude, seasonality, and regional climatic characteristics (HESSLEROVÁ et al., 2013; LI et al., 2015; ELLISON et al., 2017). On local and regional scales, forests have a greater capacity to cool the surface than other types of cover (HESSLEROVÁ et al., 2013; SYKTUS MCALPINE, 2016). In tropical regions, forests cool the temperature as a result of high rates of evapotranspiration (JACKSON et al., 2008). Although tropical forests have greater absorption of shortwave solar radiation due to their low surface albedo, this heat absorption is compensated by the latent heat released through evapotranspiration, yielding a liquid cooling of the surface (BAN-WEISS et al., 2011). The higher humidity generated in tropical forests facilitates the development of clouds that reflect incident solar energy into space, cooling the local climate (JACKSON et al., 2008). In the middle latitudes, forests cool the surface moderately as a result of the greater heating provided by surface albedo compared to the cooling caused by evapotranspiration (LI et al., 2015). At high latitudes, boreal forests heat the surface due to a decrease in albedo compared to snowy surfaces (ELLISON et al., 2017).

Water and matter flows are conducted by solar energy, with water being the principal agent integrating natural processes (RIPL, 2003). As with energy flow, water dynamics are guided by the type of vegetation that, in conjunction with other elements, affects water flow (BRAUMAN et al., 2007; ELLISON et al., 2017). Vegetation's influence on water flow can be determined by analyzing the hydrological cycle. Vegetation intercepts raindrops that fall on the surface, softening their impact on soil (BRAUMAN et al., 2007), while retaining precipitation that can subsequently be evaporated. The interception of rain by its canopy tends to reduce infiltration and water yield in river basins (BROWN et al., 2005). The amount of water intercepted by vegetation varies according to the characteristics of plant species and rainfall. Frequently overlooked in hydrological studies, interception can be a significant factor in water balance in vegetated watersheds. A study of Brazilian forests found that 7.2% to 22.6% of the rain in the Amazon rainforest is intercepted by vegetation, while in the Atlantic Forest, the spectrum is 8.4% to 20.6% (GIGLIO; KOBIYAMA, 2013). Organic matter and vegetation roots prevent soil particles from compacting, decreasing surface water flow and increasing soil porosity, which enhances hydraulic conductivity, infiltration, and water retention (WILCOX et al., 2003). Changes in vegetation type are a determining factor that influences soil's hydraulic properties. A Kenya study by Owuor et al. (2018) found that water infiltration is approximately twice as high in soil with native vegetation as in agricultural soil. The reduction in infiltration induced by land use changes can result in increased runoff and material transport to water bodies, which is propitious to flooding. Forests play a critical role in water flow between air and land. Although forests protect soil from solar radiation, reducing evaporation, these ecosystems transmit a considerable quantity of water to the atmosphere through transpiration (BALBINOT et al., 2008). Evapotranspiration affects a river basin's water balance, reducing availability according to the vegetation's structure and age, enabling vegetation to recharge atmospheric moisture and redistribute precipitation, which may impact other locations (ELLISON et al., 2017). Plants with deep roots have greater access to soil moisture (CALDER, 1998), while younger plants consume more water for growth (DELZON; LOUSTAU, 2005), impacting the rate of water transfer to the atmosphere. In the Atlantic Forest, in the State of São Paulo, Brazil, the average annual evapotranspiration of secondary forests varies from 44.8% to 78.6% in relation to total annual precipitation (CICCO, 2009).

Carbon and nutrient cycles are inherently linked to hydrological processes characterizing water availability and flow, such as evapotranspiration, soil water storage, and runoff (GAO et al., 2013). These processes control the biogeochemical cycles in aquatic and terrestrial ecosystems, mediating carbon and nutrient exchange (MANZONI; PORPORATO, 2011).

The atmosphere, oceans, and terrestrial ecosystems serve as our principal carbon reservoirs. Terrestrial ecosystems exchange carbon with the atmosphere through photosynthesis, autotrophic and heterotrophic respiration, and other natural causes, such as fires that oxidize organic matter. The carbon in terrestrial ecosystems (living biomass and soil) is about three times greater than the CO2 in the atmosphere (FALKOWSKI et al., 2000). As a result of different physiological characteristics, changes in vegetation can affect carbon storage and flow in the soil and atmosphere. Forests store more carbon per area than any other cover, with tropical forests having the greatest potential for carbon storage (PAN et al., 2011). The carbon stock of primary tropical forests is estimated at 141-159 PgC (MCKEY et al., 2020), and researchers are assessing the potential of land management and restoration to mitigate global warming effects (GRISCOM et al., 2017; FARGIONE et al., 2018). Converting natural to agricultural land use depletes organic carbon in soil by up to 60% in temperate regions and 75% in tropical ones (LAL, 2004). Changes in the soil's organic carbon, in turn, reduce primary productivity and degrade soil and water quality. Terrestrial organic and inorganic carbon is stored, processed, and transported by freshwater ecosystems (rivers, lakes, and reservoirs) in the form of particles or dissolved carbon (HAMON, 2020). Regnier et al. (2013) estimated that land use changes, soil erosion, and other anthropogenic pressures can increase the flow of carbon to inland waters by up to 1 PgC yr^{-1} since pre-industrial times, primarily because of carbon exports.

The nutrient cycle occurs through interaction between the biota and the environment. Each ecosystem has its characteristics that affect nutrient flow (JOHNSON;

TURNER, 2019). Nutrients become available in ecosystems from external geochemical and internal biological cycles. The former refers to inflow from atmospheric deposition, rock weathering, biological fixation, and artificial fertilization and outflow from soil leaching, volatilization, erosion, river flow, and gas emissions, while the latter references nutrient flow from the interaction between soil and vegetation (SELLE, 2006). In native forests, the dynamic internal balance of nutrients occurs primarily through interaction between deposition and absorption. Minerals in the environment are absorbed by forests for the growth and maintenance of plants that, in turn, are sources of nutrients for other organisms. The residual organic matter generated by the biota is broken down into simpler substances by decomposing organisms, causing nutrients to return to the soil (BANI et al., 2018). Precipitation and runoff from trees are other means of transferring nutrients to the soil (ARCOVA; CICCO, 1987). Climate, plant species, forest state, and soil fertility are key factors that impact nutrient cycling in forest ecosystems (VIRTUOSIC; SANFORD, 1986). The conversion of natural areas, rich in biodiversity, into agricultural ecosystems, characterized by monocultures and pastures, alters the basic mechanisms that regulate nutrient recycling (LUIZÃO, 2007). Artificial fertilization of agricultural land increases nitrogen and phosphorus to levels that exceed plants' absorption capacity, causing excess nutrients to be leached into watercourses (VITOUSEK et al., 2009). About 70% of global agricultural land evidence a phosphorus surplus (MACDONALD et al., 2011), and studies have found that anthropic effects have tripled global phosphorus mobilization on the land-water continuum and substantially increased the accumulation of phosphorus in soil (YUAN et al., 2018). In addition to introducing nutrients, vegetation changes alter water and energy flow (ELLISON et al., 2017), as well as the ecosystem substrate (SHOROHO; KAPITSA, 2014), affecting soil's biological activity and the decomposition rate of organic matter (BANI et al., 2018).

2.3.2. Challenges to water ecosystem services

Understanding the ecological status of aquatic ecosystems requires comprehensive knowledge about their functions, which involve interactions among multiple anthropogenic uses and the ecosystem's environment and biodiversity. Impacts on these ecosystems and their services can arise from natural or anthropic origins, with the latter primarily responsible for their degradation (MEA, 2005). Grizzetti et al. (2016) proposed a structure to facilitate understanding of links among drivers, pressures, and ecosystem status and services (Figure 2.2). Multiple pressures can adversely impact the status of aquatic ecosystems in regard to water quantity, quality, hydromorphology, and biodiversity. Accordingly, the availability of water ecosystem services depends on the status of the ecosystem, which, in turn, depends largely on anthropic factors. Numerous pressures can impact ecosystem status, such as the construction of dams for energy and irrigation and of other river works, the introduction of exotic species, and water pollution (POIKANE et al., 2020). Several studies have cited climate change and land use as the principal drivers that can affect the WES (COUTURE et al., 2018; BUCAK et al., 2018; BAI et al., 2019; DE MELLO et al., 2020).

Land use is a relevant factor as the degree of anthropic activity reflects the level of socioeconomic development, which increasingly demands land for agriculture, livestock, industry, urban growth, and other needs (JIN et al., 2015). Of the world's 130,000,000 km² of the continental area not covered by ice, more than 70% is used for anthropic activities (IPCC, 2019). The effects of land use on water ecosystem services are well documented (YANG et al., 2018; FERREIRA et al., 2019; KHAN et al., 2019; SRICHAICHANA et al., 2019). Hasan et al. (2020) performed a literature review to summarize current knowledge on the effects of land use on ecosystem services. As they have demonstrated, land use change can critically affect the quantity and value of ecosystem services and has created conflicts regarding the allocation of scarce water resources. Such changes can alter ecohydrological processes and modify material and energy flows (SUN et al., 2017), affecting the status of the aquatic ecosystem from quantitative, qualitative, biological, and hydromorphological perspectives (GRIZZETTI et al., 2016).

Land use affects hydrological processes, in particular, evapotranspiration (ELISSON et al., 2012), which can reduce local water quantity as forested river basins produce less water than those with less forest cover (JACKSON et al., 2000; ANDRÉASSIAN et al., 2004; MOLINA et al., 2012; KUNDU et al., 2017; DE BARRO FERRAZ et al., 2019). On regional and global scales, however, evapotranspiration plays a key role with vegetation, particularly forests, acting as biotic pumps, redistributing precipitation to other locations and fostering a positive water balance (ELLISON et al., 2017). In the Amazon, recycling of local precipitation varies between 35% and 80%, influencing the water balance of adjacent regions as so-called "flying rivers" transport moisture produced by the forest to river basins in Brazil and South America (MARENGO et al., 2018). It is estimated that 70% of the water resources in the River Plate basin depend on moisture from the Amazon rainforest (VAN DER ENT et al., 2010). D'Almeida et al. (2007) note that large-scale prediction models indicate that deforestation decreases precipitation and reduces runoff, while on the local scale, the reduction in evapotranspiration provides increases runoff. Converting natural environments, such as forests and wetlands, to anthropic use can affect evapotranspiration and, consequently, precipitation and water availability (ELLISON et al., 2012).

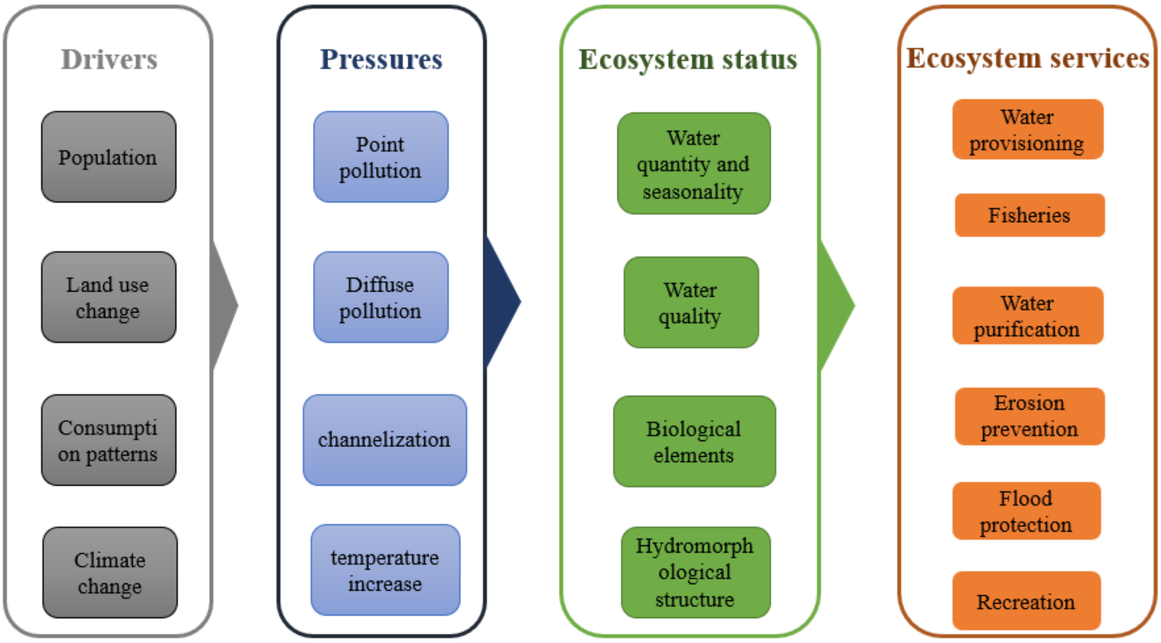

Figure 2.2. Links among drivers, pressures, and ecosystem status and services (adapted from GRIZZETTI et al., 2016).

Water quality is affected by the introduction of pollutants and sediments generated by anthropic activities spread across the river basin (ANJINHO et al., 2021). The effects of land use on water quality depend on its interaction with such factors as climate, hydrology, pedology, geomorphology, landscape configuration, and composition (XIAO et al., 2016; DE MELLO et al., 2020). Types of land use impact water quality in diverse ways. Agricultural activities, for example, pollute water through sediments and nutrients leached into water bodies (LE MOAL et al., 2019). Enrichment of nutrient concentration in aquatic ecosystems causes eutrophication, which deteriorates water quality and biodiversity (GUIGNARD et al., 2017; BISWAS et al., 2018), while pastures are another source of pollutants (DE MELLO et al., 2020). Urbanization degrades water quality through the introduction of domestic and industrial sewage and the draining of impermeable land (BISWAS et al., 2018; ZHAO et al., 2018). On the other hand, heavily forested river basins purify water, reducing treatment costs (CUNHA et al., 2016; DE MELLO et al., 2018).

Hydromorphology is affected by the anthropic use of aquatic habitats, such as riparian vegetation and flood plains, that fragments their connectivity (ALLAN, 2004; MERENLENDE; MATELLA, 2013), creating pressure on their ecosystems through channeling and narrowing of channels, damming, proliferation of exotic species, and loss of habitat and pollutant processing capacity (SWEENEY et al., 2004; POIKANE et al., 2019). Nearly half the global volume of rivers is moderate to severely impacted by flow regulation, fragmentation, or both (GRILL et al., 2015). Hydromorphological changes are a prevalent type of recurrent pressure on European aquatic ecosystems, second only to nutrient enrichment (POIKANe et al., 2019). It is estimated that 40% of Europe's water bodies are affected by hydromorphological changes (POIKANE et al., 2020).

Aquatic biodiversity can be impacted by changes in quantitative, qualitative, and hydromorphological attributes. Several factors can decrease biodiversity, with land use one of the most significant (CAZZOLLA, 2016). Anthropized basins generally have less biodiversity than forested ones (BAYRAMOGLU et al., 2020). Van Soesbergen et al. (2019) analyzed the effects of land use on the biodiversity of rivers in Africa's Lake Victoria drainage basin and found that converting natural land to agricultural use resulted in the loss of 20% of the richness of freshwater species, and for livestock the value found was 30%. Analysis of 289 European streams at the headwaters of the Elbe, Danube, and Main rivers confirmed that land use changes affect the composition of fish communities (BIERSCHENK et al., 2019).

A pressing challenge affecting ecosystems worldwide is climate change. Researchers at the Intergovernmental Panel on Climate Change (IPCC) indicate that the climate has tended to heat up throughout the century as a consequence of greenhouse gases emitted into the atmosphere through natural and anthropic processes. It is estimated that from 1850-1900 to 2006-2015, the average global air temperature increased by 1.53º C, and the average global surface temperature (land and ocean) increased by 0.87º C (IPCC, 2019). Should these effects intensify, significant climatic changes will occur, altering, for instance, rainfall volume and distribution.

Climate plays a crucial role in the hydrological cycle and ecological status of aquatic ecosystems, affecting WES availability and flow (BAI et al., 2019). Changes in temperature and precipitation can trigger cataclysmic events, such as floods and droughts, incurring environmental and socioeconomic losses (IPCC, 2019). The frequency and intensity of droughts, for example, have increased over the past half-century (BELL et al., 2018). In the metropolitan region of São Paulo, the historically low rainfall between 2013 and 2014 led to periods of drought, impairing the water supply needed for agricultural production and energy generation (FERREIRA et al., 2019). In 2009, four years after a severe drought and forest fires, the Amazon rainforest, one of the most preserved ecosystems in the world, was struck by floods and landslides that caused the death of 19 people and drove 186,000 from their homes (MARENGO et al., 2012).

Hydrological changes induced by climate affect soil properties, such as the dynamics of organic matter, water retention, and erosion (BREVIK, 2012). Heavy rainfall increases soil's susceptibility to erosion, which adversely affects food production (BAKKER et al., 2007). Eroded particles can also carry contaminants adsorbed to the sediment, which pollute waters and have adverse effects on ecosystems and human health (HAHN et al., 2019). Increased runoff from precipitation favors greater nitrogen export as a result of soil leaching (ØYGARDEN et al., 2014), and higher temperatures can also impact it due to increased mineralization of organic matter in the runoff (ØYGARDEN et al., 2014). Trolle et al. (2015) found that high temperatures associated with greater nutrient export increase phytoplankton biomass, including toxin-producing cyanobacteria.

Temperature warming and changes in hydrological and biogeochemical cycles affect biodiversity (WOODWARD et al., 2010; PORTER et al., 2013). A meta-analysis of 143 studies determined that more than 80% of the analyzed species were affected by temperature changes, indicating that the effects of global warming are already perceptible in flora and fauna (ROOT et al., 2003). Freshwater ecosystems, which support about 10% of all known species, including one-third of vertebrates (STRAYER; DUDGEON, 2010) are imperiled by climate change, particularly in the tropics, which host numerous endemic species (CUMBERLIDGE et al., 2009). It is estimated that more than 27% of the 29,500 freshwater species on the IUCN red list are endangered by extinction (TICKNER et al., 2020). Climate change affects freshwater biodiversity primarily through warming temperatures and changes in flow that, with other stressors, synergistically impact ecosystem functions (DUDGEON et al., 2007; REID et al., 2018; DUDGEON, 2019).

2.3.3. The role of natural ecosystems in addressing global challenges

Natural ecosystems are critical to regulating ecohydrological processes, and researchers are examining their potential to mitigate climate changes while enhancing the capacity of ecosystem habitats and services to conserve biodiversity. A recent IPCC report highlights the importance of combating deforestation and implementing restoration in mitigating global warming (IPCC, 2019). Forests operate as sinks that sequester considerable amounts of carbon from the atmosphere (PAN et al., 2011; FARGIONE et al., 2018; MACKEY et al., 2020). Such natural measures as environmental restoration, reforestation, and land use management could reduce CO_2 emissions by an estimated 23.8 $PgCO_2e\ y^{-1}$, using 2030 as a reference point, and constitute a fundamental strategy to maintain warming of the global average temperature below 2ºC (GRISCOM et al., 2017).

Forest restoration can contribute to ecosystem service conservation as it can intensify the hydrological cycle and regulate humidity (ELLISON et al., 2017). However, care must be taken in such projects. Trees use water to maintain their physiological processes, but the quantity can cause water deficits and compromise other users. Greeff (2010) has reported water problems in forest plantations in arid regions of Africa. Accordingly, restoration projects must take into account the composition and configuration of vegetation (DE BARROS FERRAZ et al., 2014), preferably using native species adapted to the region's natural characteristics, which often use less water than eucalyptus plantations (DE BARROS FERRAZ et al., 2019). In the case of planted forests, forest management practices are a key factor in water availability (DE BARROS FERRAZ et al., 2013; GARCIA et al., 2018).

The ecohydrological functions of native forests vary according to the quantity, quality, and configuration of fragments (DE BARROS FERRAZ et al., 2014). Natural ecosystems, such as riparian forests, wetlands, and flood zones, enhance water quantity and quality and provide biodiverse habitats. Hilltop forests intercept rain and regulate water flow, while facilitating infiltration and recharging of aquifers, which helps control water availability downstream (TAMBOSI et al., 2015). Hillside forests increase soil stability and reduce runoff due to interception of precipitation and litter accumulation, protecting the surface and controlling water flow and soil erosion (DUAN et al., 2016; XIA et al., 2019). Riparian forests regulate ecohydrological processes responsible for providing diverse ecosystem services (DUFOUR et al., 2019). An overview of these services is presented by Riis et al. (2020). WES-related examples include nutrient removal, flow regulation, climate regulation, erosion control, water purification, and biodiverse habitats. Due to their characteristics, researchers have designated riverside ecosystems as hotspots for adapting to climate change (CAPON et al., 2013). Wetlands are recognized for their ecosystem functions and biodiversity (GARDNER; FINLAYSON, 2018), providing such services as water purification, climate regulation, nutrient cycling, hydrological cycle regulation, and habitats (PACINI et al., 2018; XU et al., 2020).

In addition to improving the WES supply and mitigating global warming, the restoration of natural ecosystems or green infrastructure has been recommended as an adaptive strategy for climate change adaptation (SUSSAMS et al., 2015; DA SILVA; WHEELER, 2017). The concept of ecosystem-based adaptation refers to the integrated use of ecosystem services and biodiversity to maintain ecosystem resilience and facilitate adaption to the adverse effects of climate change (CBD, 2010). WES payment initiatives are a prime example of ecosystem-based adaptation measures (MARTIN-ORTEGA et al., 2013). Remunerating ecosystem service providers could encourage environmental restoration to enhance land use and adapt to climate change (TAFFARELLO et al., 2017).

2.3.4. Mapping and biophysical modeling of water ecosystem services

The mapping of ecosystem services consists of their spatialization to identify where and to what extent ecosystems contribute to human well-being. Maps provide biophysical and monetary information that enables analysis of the economic costs and tradeoffs of ecosystem changes (GRIZZETTI et al., 2016) and extends understanding of service supply, demand, and flow on different spatial and temporal scales, informing the formulation of guidelines for natural resource planning and management (BAGSTAD et al., 2013; CROSSMAN et al., 2013).

The growing interest in research on ecosystem services has been driven, in part, by the development of methods and tools to quantify and map them (BAGSTAD et al., 2013). Increased use of Geographic Information Systems (GIS), in conjunction with spatial data acquisition and analysis technology, has led to the emergence of models and tools to quantify ecosystem services (SCHÄGNER et al., 2013). Current tools range from basic approaches, which use land use data as proxies to complex models that consider physical processes in modeling ecosystems (PALOMO et al., 2017). A pioneer study on mapping ecosystem services, Costanza et al. (1997) mapped the economic value of 17 services in 16 global biomes. Subsequent research has explored innovative assessment methods and tools (HACKBART et al., 2017).

Methods used to map ecosystem services on a landscape scale can be categorized as: 1) direct mapping, which provides comprehensive spatial data on their distribution, 2) empirical models, which are based on point data estimated through such methods as regression analysis, 3) simulation and process models, which simulate ecosystem functions, generally using data for calibration and validation, 4) logical models, which map ecosystem services through a set of indicators, using decision rules, 5) extrapolation methods, which parameterize ecosystem properties, principally, land use, to determine service supply levels based on summarized spatial values, and 6) data integration methods, which synthesize pre-existing space products to map ecosystem services, customarily via a rules-based approach (ENGLUND et al., 2017).

Methodologies generally use ecosystem service indicators that describe the state and trends of ecosystems. Different indicators are used to evaluate specific services, and a service can be examined through one or more biophysical or socioeconomic indicators (CHEN et al., 2019). The biophysical assessment focuses on determining ecosystem service structure, function, and flow, on the left side of the cascade model (HAINES-YOUNG; POTSCHIN, 2010), while the socioeconomic assessment looks at benefits and values, on the right side (see Figure 2.1). Benefits are generally measured in monetary terms. In some cases, however, they can be expressed in biophysical units (VIHERVAARA et al., 2017).

Biophysical indicators can be obtained directly through field observation or indirectly through the interpretation of data, such as that provided by remote sensors, which were not necessarily installed to evaluate ecosystem services (EIGENBROD et al., 2010; VIHERVAARA et al., 2017). The selection of indicators depends on the characteristics of each study. Examples include land use, vegetation, climate, hydrology, and water pollution (DE GROOT et al., 2010; EGOH et al., 2012). The use of spatially explicit indicators is essential to operationalize and implement the ecosystem services concept and enable sustainability assessment and territorial planning. The Ecosystem Services Supply Index is a synoptic indicator of the level of supporting and regulating ecosystem services related to carbon and water dynamic that has been used to diagnose, plan, and monitor processes by scientists, governmental and judicial authorities, and nongovernmental organizations, among others, to inform interventions and empower vulnerable stakeholders (STAIANO et al., 2021).

Biophysical tools capable of representing ecosystem structure and function through mathematical computation can be used in an integrated manner to fill spatial and temporal gaps in direct and indirect measurements (PALOMO et al., 2017). Such tools enable analysis of ecosystem service availability, demand, and flow under diverse socioeconomic conditions and assessment of the effects of multiple pressures on ecosystems and their services (VILLAMAGNA et al., 2013; COSTANZA et al., 2017).

Several models examined in the literature can be used to generate scientific knowledge and solve practical problems related to natural resource management (BAGSTAD et al., 2013; CHEN et al., 2019). Duarte et al. (2016) demonstrated the importance of mapping ecosystem services in determining priority areas for conservation, while Outeiro et al. (2019) indicated that conflicts that may arise among services in a given region. Their study described how tourism on the Brazilian island of Fernando de Noronha can compromise local fishing. The models can also be used to assess the impact of regulatory change on ecosystem services, informing the formulation of environmental protection standards (GARRASTAZÚ et al., 2015), and how climate and land use can alter carbon balance (PAVANI et al., 2018).

Hydrological models are crucial tools in the biophysical assessment of WES (BRAUMAN et al., 2007; GRIZZETTI et al., 2016). Many, such as Soil and Water Assessment Tools (SWAT) (ARNOLD et al., 2012), Integrated Valuation of Ecosystem Services and Tradeoffs (InVEST) (SHARP et al., 2018), Artificial Intelligence for Ecosystem Services (Villa et al., 2014), and Geospatial Regression Equation for European Nutrient Losses (GREEN) (GRIZZETTI et al., 2015), can be used to simulate WES in river basins. Using hydrological models, it is possible to represent the spatial and temporal dynamics of river basins, enabling analysis of the relationship among ecosystem status, services, and pressures (GRIZZETTI et al., 2015). Understanding these relations facilitates the development of sustainable scenarios that mitigates the impact on water resources and services.

Indicators used to assess WES can be directly related to water bodies, such as the surface occupied by lakes and reservoirs, or they can involve interaction among terrestrial and aquatic ecosystems, such as the expansion of riparian vegetation and wetlands with the set used dependent on the study’s objectives. Grizzetti et al. (2016) proposed a set of 206 indicators most frequently used in the literature, classified as capacity, which refers to the ecosystem’s potential to provide services; flow, which refers to the current use of its services; and benefit, which reflects human well-being and the value system. WES biophysical indicators describe the state of water resources in terms of quantity, quality, and aquatic biodiversity. Examples include nutrient load, quantity of native fish, water chemical status, river flow, and precipitation (MAES et al., 2016; HACKBART et al., 2017).

Hydrological models can be used to assess a variety of WES under different approaches. Li et al. (2019) used the hydrological model CLM-GBHM to assess Chinese flood regulatory services. The study simulated the relative effects of climate, vegetation, and reservoirs and highlighted the fundamental role forest restoration played in improving them (LI et al., 2019). Using the InVEST model, Yan et al. (2018) assessed the potential of wetlands to retain nitrogen in river basins, demonstrating the significance of the water purification these ecosystems offer. The same approach can be seen in a study by Vigiak et al. (2016) which used the SWAT model to assess the effects of riparian vegetation on sediment retention in Europe's Danube River basin. The study found that the sediment retention provided by riparian vegetation reduces sediment flow and contributes to the conservation of aquatic ecosystems.

2.3.5. Economic valuation of water ecosystem services

The ecosystem services-based approach can assign monetary value to goods and services provided by ecosystems, demonstrating their value in economic language that enables comparison of their benefits and analysis of their synergies and tradeoff to inform land use and conservation policies (NAIME et al., 2020). While discussion of methods used for the economic valuation of ecosystem services is ongoing, the principal objective of this valuation is to convey the value of ecosystem services to markets and create economic incentives for conserving nature (GÓMEZ-BAGGETHUN; RUIZ-PÉREZ, 2011). A history of such valuation can be found in Gómez-Baggethun et al. (2010).

An early study by Costanza et al. (1997) estimated the monetary value of 17 ecosystem services in 16 biomes. Their values ranged from $16 to 54 trillion a year, with an average of $33 trillion. Although subsequent studies developed new valuation methods, this pioneering study introduced an awareness exercise on the impact of ecosystem service loss.

Methods used to value ecosystem services can be classified as direct and indirect market valuation (FARBER et al., 2002). The former, which refers to their market exchange value (DE GROOT et al., 2002), is widely used in the valuation of provisioning services related to goods provided by ecosystems, such as food and wood. Naime et al.

(2020) used it to value the supply of forest products and forage for calves provided by tropical ecosystems on Mexico’s Pacific coast. The latter method is used in the absence of explicit markets when ecosystem services are quantified using techniques based on the concepts of Willingness to Pay (WTP) and Willingness to Accept (WTA) Compensation. The indirect market evaluation uses six main methods. In avoided cost, the monetary value of ecosystem services is calculated on the basis of the cost entailed in their absence, such as the cost that would be required to control and mitigate floods in the absence of vegetation (VÁZQUEZ-GONZÁLEZ et al., 2019). Replacement cost is used to estimate the value of ecosystem services by comparison with those of an equivalent anthropic service as when the water purification services provided by the floodplains are quantified by comparing the costs of using a treatment plant (HOPKINS et al., 2018). Income factor refers to approaches used to link ecosystem services to increased economic productivity as when the function of production in agriculture is used to assess the effects of ecosystem services on agricultural yields (SWINTON et al., 2007). Travel cost quantifies ecosystem services based on travel expenses, which may reflect their value, and is frequently used to value recreation and ecotourism services (SHRESTHA et al., 2002; LARSEN et al., 2020). Hedonic pricing assumes that service demand reflects the prices people are willing to pay for commercial goods, such as the value consumers accord urban green spaces in residential areas (LIEBELT et al., 2018). Contingent valuation is based on how much people are willing to pay for ecosystem services, generally using hypothetical situations to assess the price to be paid for service restoration. Loomis et al. (2000) used this method to estimate the monetary value of five ecosystem services (dilution of wastewater, natural water purification, erosion control, biodiverse habitats, and recreation) that would hypothetically be restored along 45 miles of the South Platt River in the United States. The study found that people were willing to pay up to $21 a month more on their water bills for restored services. Extrapolated to the population living along the river, the figure could reach $70 million.

Another method used in the economic valuation of ecosystem services is aggregating values, which transfers data from one location to another to aggregate values on larger spatial and temporal scales (COSTANZA et al., 2014). Costanza et al. (1997) used this approach through the benefit transfer method to quantify the monetary value of global ecosystem services. While simple, it can be used to assess the effects of land use and to increase awareness of the need to preserve ecosystems and their services (COSTANZA et al., 2014).

The selection of economic valuation methods depends on the objectives of the study and the services it will examine (FARBER et al., 2006). HACKBART et al. (2017) surveyed the biophysical, economic, and mixed methods used in WES valuation. Most studies (71%) used indirect approaches based on the type of ecosystem and its land uses. The most widely used economic indicators were market price and the costs of water treatment, vegetation recovery, and electricity, while water supply, power generation, and recreation were the services most evaluated.

Some studies integrate biophysical and economic methods to estimate WES monetary value, using the results of the biophysical model as input data. This mixed method is often used when hydrological processes interfere with water, energy, and biogeochemical cycles. La Notte et al. (2017) estimated the monetary value of European water purification services, using the GREEN biophysical method to quantify nitrogen retention in kg. year^{-1} and the replacement cost economic method to value WES, estimating the value at €459 billion for 2005. Brauman et al. (2015) estimated the monetary value of Hawaiian water supply services using hydrological modeling to quantify the effects of land use on water flow and avoided pumping costs to calculate economic value. Using the InVEST model, Nguyen et al. (2020) quantified the biophysical value of Vietnamese soil erosion control and valued the service accordingly using avoided cost, while Kadaverugu et al. (2020) used the InVEST model to quantify the biophysical and economic values of flood mitigation provided by India's green areas.

2.3.6. Potential of the ecosystem services-based approach in the management of water resources

The use of the ecosystem services-based approach to managing natural resources and addressing environmental crises is being increasingly encouraged. Indubitably, it creates a new way of thinking about ecosystems, enhancing knowledge about their state, vulnerability, and resilience.

The primary objective of water resource management is to maintain the effective functioning of aquatic ecosystems to ensure the water quantity and quality required to meet present and future demand. The rapid emergence of global pressures on water security poses significant challenges to water resource management (GRIZZETTI et al., 2017; Vörösmarty et al., 2018). In many countries, water resource planning is carried out on a river basin scale, which involves the wide array of research, policies, and actions required to ensure the sustainability needed to meet water use needs.

A principal challenge in water resource management is to understand complex hydrological processes and their interaction with anthropic activities. The environmental effects of the latter have altered matter and energy flow, which, in turn, impacts the health of ecosystems and their capacity to provide goods and services for human well-being and economic development (MEA, 2005). While WES are affected by a series of factors that involve interaction among physical, biological, and anthropic factors, climate and land use changes are the primary present and anticipated threats to their integrity, and understanding how they affect ecosystems is essential to formulating sustainable water policies (BUCAK et al., 2018; BAI et al., 2019). The ecosystem services-based approach systematically examines the complexity of river basins, linking ecosystem status, services, and pressures and enabling the assessment of additive, synergistic, and antagonistic effects of anthropic activities on ecosystem services and their economic value (GRIZZETTI et al., 2016; BAI et al., 2019).

Numerous initiatives with an ecosystem services-based approach have emerged to enhance water resource management. In Brazil's Atlantic Forest biome, 16 initiatives incorporate the concept (TAFARELLO et al., 2017). The initiatives were carried out through the National Water Agency of Brazil's Water Producer program, which provides payments for ecosystem services to encourage rural landowners to adopt soil management and forest conservation practices that improve water availability (ANA, 2012; RUGGIERO et al., 2019).Such initiatives promote not only the conservation of water resources but of entire ecosystems, thus enhancing the availability of other services, such as soil quality, carbon stock, and biodiverse habitats (BENAYAS et al., 2009). Other Latin American countries have also implemented payment programs for water ecosystem services (MARTIN-ORTEGA et al., 2013).

The European Union's Managing Aquatic ecosystems and Water Resources under multiple Stress (MARS) Project is a prime example of the potential of an ecosystem services-based approach to planning and managing water resources (HERING et al., 2015). Conducted on water body, river basin, and European scales, its primary objective was to understand the effects of multiple pressures on European aquatic ecosystems and their services, and its results will support the implementation of river basin restoration policies and the review of such water policies as the Water Framework Directive.

A significant characteristic of water ecosystem services is that they are disseminated throughout the river basin; thus, downstream users suffer from adverse effects on upstream ecosystems. An ecosystem services-based approach enables quantifying diverse WES values, increasing awareness and informing the debate among stakeholders in water resource management and the negotiation of tradeoffs (BRAUMAN et al., 2007). The approach could be incorporated into planning river basins and other sectors that interface with WES. In Brazil, water resource planning is generally carried out on the basis of the relations between water supply and demand, and water quality and neglects to take into account future effects of climate and land use changes.

Well-calibrated and validated biophysical models are vital to understanding ecohydrological processes and the effects of the principal drivers of change in river basins. They enable quantifying WES biophysical values and assessing future scenarios in the river basin, identifying those most sustainable for water resources. Studies have highlighted the effects of landscape planning on the provision of WES (DE BARROS FERRAZ et al., 2014; DING et al., 2016; CLÉMENT et al., 2017; CUNHA et al., 2019). Biophysical models facilitate the assessment of the impact of landscape patterns to identify those most beneficial to the region's ecosystems as well as the effectiveness of environmental restoration strategies and payments for water ecosystem services. Thus understanding how landscape ecosystems interact and function is crucial to water resource management. TAFFARELLO et al (2016), for instance, found an inverse correlation between water production and forest cover, which conflicts with the initiative of Brazil’s Water Producer project to increase water availability in local river basins (ANA, 2012).

Insofar as water resource management entails resolving conflicting stakeholder interests, identifying synergies, and negotiating of tradeoffs, economic valuation is critical to demonstrating the value of WES to decision-makers. Awareness of the economic value of ecosystem services, in addition to their biophysical significance, can justify the preservation or restoration of a specific ecosystem (GRIZZETTI et al., 2016), and spatial and temporal analysis of WES values should guide land use planning to ensure sustainable and economically viable water resource management.

2.3.7. Challenges and limitations of the ecosystem service-based approach

The ecosystem services-based approach to water resource management requires an integrated analysis of ecosystem status and pressures and a biophysical and economic assessment of its services to advance conservation and human well-being (GRIZZETTI et al., 2016). As evidenced in the research reviewed in this study, however, challenges and limitations hinder its more extensive use and require further research. Accordingly, the principal challenges and limitations follow.

A clear understanding of ecohydrological processes is critical to assessing the synergistic effects of multiple pressures on ecosystem services. Awareness of how terrestrial ecosystems impact matter and energy flow is also crucial to managing sustainable water resources. Research has demonstrated the key role of natural ecosystems in mitigating the effects of climate change and land use, with their restoration constituting a promising strategy for adapting to climate change (CAPON et al., 2013; SUSSAMS et al., 2015; DA SILVA; WHEELER, 2017; TAFFARELLO et al., 2017). Nevertheless, additional research to identify the panoply of their benefits and the most effective services to reduce the degradation of aquatic ecosystems and mitigate the effects of anthropic activities should be undertaken (FELD et al., 2011. As recommended by Ellison et al. (2017), the effects of vegetation beyond the limits of river basins should be kept in mind as ecohydrological functions of forests, such as redistribution of rainfall, transcend its boundaries, necessitating integrated, articulate management at the regional level.

The emergence of mathematical models and technologies for the acquisition, analysis, and processing of spatial data has enhanced our understanding of ecosystem functions, enabling the quantification of their biophysical value. However, challenges remain, and greater knowledge and validation of biophysical modeling methods are needed (CROSSMAN et al., 2013). While many tools are described in the literature, it is worth noting that all models have limitations and uncertainties that must be properly assessed. A primary challenge in assessing ecosystem services is to validate simulated results with data observed in the field, as nonvalidated data cannot be deemed representative (HACKBART et al., 2017). Analysis of 347 studies by Englund, Berndes, and Cederberg (2017) indicated that only 12% were validated with empirical data. The dearth of data, particularly in underdeveloped countries, makes it difficult to assess ecosystem services (CROSSMAN, 2013). New methods are required to quantify additional services, as not all can be quantified and mapped, with provision and regulation services being the most recurrent (BURKHARD; MAES, 2017). Improving hydrological models is crucial to enhancing the understanding of ecohydrological processes in river basins. More complex hydrological models, such as SWAT, are able to model a wide range of hydrological functions on a daily scale across sub-basins (ARNOLD et al., 2014), but require detailed data inputs, which are often unavailable, and users adept in hydrology and modeling (VIGERSTOL; AUKEMA, 2011). Incorporating additional ecohydrological processes into the models, while maintaining operational simplicity constitutes a significant challenge (GUSWA et al., 2014).

To better understand interactions among terrestrial and aquatic ecosystems, it is necessary to couple hydrological models on a river basin scale with models on a water body scale, such as models of water ecology, quality, and hydraulics (BREWER et al., 2018). Analyzing the functions of aquatic ecosystems enhances understanding of how terrestrial stressors can affect the water body and its ecological status. Approaches such as the MARS project assess ecosystem services on watershed, water body, and European scales (HERING et al., 2015).

A classic problem plaguing the economic valuation of ecosystem services is the risk of double counting, which occurs when a service is generated by another service and both are counted (DE GROOT et al., 2002). This problem arises from the myriad classifications and definitions of ecosystem services (FISHER et al., 2009). Ojea et al. (2012) described this problem in their analysis of studies on the economic valuation of WES provided by forests, using two classifications, finding risk of double counting as a result of ambiguous and overlapping service definitions. Other challenges arise from uncertainties in biophysical valuation and in structural and parametric factors associated with monetary quantification, including the number of services, benefits, and economic valuation metrics used in the valuation (BOITHIAS et al., 2016). Therefore, it is important to identify the functions and services to be evaluated, as well as the most appropriate classification methods.

Many studies analyze biophysical and economic values of water ecosystem services in a fragmented manner, and methods that provide greater integration are needed (KEELER et al., 2012), as proposed by Grizzetti et al. (2016). A literature review by Hackbart et al. (2017) found that only 12% of the studies examined evaluated the biophysical and economic values of WES, according to an analysis of supplementary data published by the authors. Ecosystem service models such as InVEST incorporate biophysical and economic assessment methods, but their use is restricted to only some WES, and it is necessary to incorporate a greater number to inform cost-benefit analyses and identify tradeoffs. Indeed, all costs and benefits for human well-being that changes in the status of ecosystems occasion should be accounted for. In their analysis of services related to water quality, Keller et al. (2012) conclude that water quality can generate final ecosystem services for diverse beneficiaries. Their study integrates biophysical and economic models, land use management, and procedures to avoid double counting.

Finally, it is essential to involve all stakeholders in discussions related to WES decision-making, as conflicts may arise (GRIZZETTI et al., 2016) as values pertaining to ecosystem services extend beyond economic perspectives, such as inherent, fundamental, eudemonistic, and instrumental values (JAX et al., 2013). Notwithstanding the preceding, a literature review by Hackbart et al. (2017) found community participation was noted in only 22% of the analyzed articles.

2.4. Conclusion

This study reviewed the scientific literature on water ecosystem services to provide information and guidance to researchers and others concerned with water resource management. Its analysis identifies and describes the principal concepts that underlie the ecosystem services-based approach with an emphasis on water ecosystem services generated by the interaction between terrestrial and aquatic ecosystems in the river basins. It also identifies and discusses the potentials, challenges, and limitations of the ecosystem services-based approach in the context of water resource management.

Understanding the ecohydrological processes resulting from the interaction between hydrological and ecological factors and their relation to human well-being and anthropic activities is key to understanding matter and energy flow, which influence WES availability and flow. The ecosystem services-based approach proposed by Grizzetti et al. (2016) takes into account drivers, pressures, and ecosystem status and services and integrates hydrological processes, WES, and human well-being, enabling an assessment of biophysical worth and the calculation of the economic value of ecosystem services.

Natural ecosystems, such as forests, riparian vegetation, wetlands, and flood plains, play a critical role in regulating ecohydrological processes fundamental to their health and services. Depending on their characteristics, composition, and configuration, they provide a range of ecosystem services of significant value to socioeconomic development and biodiversity. Well-designed ecosystem restoration can maximize synergies among ecosystem services and reduce tradeoffs. In addition, natural ecosystems can mitigate the effects of climate change and inform adaptive strategies.

The mapping of WES through biophysical modeling and economic valuation can identify priority areas for ecosystem restoration and the relative monetary benefits of development strategies. Biophysical modeling enhances our understanding of ecohydrological processes and their relationship with multiple pressures and thus our identification of those most sustainable for water resources. Economic valuation can demonstrate the socio-economic worth of ecosystem services in terms relevant to stakeholders, in particular, decision-makers.

Water resources management requires a holistic approach to understanding how multiple stressors can impact water resources and harm current and future uses in the river basin. A WES-based approach takes into account both environmental conservation and human well-being. However, gaps that hinder its more extensive use must be addressed. Further research is needed to better understand the synergistic effects of multiple pressures on water ecosystem services and to analyze the costs and benefits of ecosystem restoration projects and to expand knowledge of the use of biophysical models that incorporate methods to validate simulated results with field data and developing analytical tools that incorporate an expanded set of ecohydrological processes at various scales. Further studies that link biophysical assessment and economic valuation are also needed, incorporating all dimensions of values for ecosystem services. Finally, it is necessary to ensure transparency and greater involvement of stakeholders, promoting integrated and participatory management of water resources.

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Chapter 3

EVALUATION OF INVEST'S WATER ECOSYSTEM SERVICE MODELS IN A BRAZILIAN SUBTROPICAL BASIN

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ABSTRACT

The biophysical modeling of water ecosystem services is crucial to understanding their availability, vulnerabilities, and fluxes. Among the most popular models, the Integrated Valuation of Ecosystem Services and Trade-offs (InVEST) models stand out. While many studies have used them, few have assessed their performance. This study evaluates the performance of InVEST's Seasonal Water Yield, Nutrient Delivery Ratio, and Sediment Delivery Ratio models in a subtropical basin in southeastern Brazil on temporal and spatial scales, using 39 years of streamflow data, 29 for total phosphorus and total nitrogen, and 19 for total suspended solids. Statistical indicators R^2, PBIAS, and NSE, were also calculated. The performance of the models varied according to the type of simulated WES and analysis scales used, with the Seasonal Water Yield model demonstrating the best performance and effectively representing the spatial and temporal variability of the average annual streamflow. All models performed well in simulating long-term mean values when compared to observed data. While one should bear in mind the study's limitations, the results indicate that the models perform well in terms of relative magnitude, although their application in studies involving water-resource management and decision making is limited.

Keywords: Water ecosystem services. InVEST model. Water yield. Sediment export. Nutrient export.

3.1. Introduction

A water ecosystem services (WES)-based approach, incorporating an integrated analysis among multiple pressures, ecological statuses, and ecosystem services has been identified as an effective tool to plan and manage water resources, as it links environmental conservation with socioeconomic development (GRIZZETTI et al., 2016). Such an approach enables an assessment of how anthropic activities affect ecosystem composition and functioning, impacting WES, including water supply services for human use, irrigation, and energy generation, as well as regulation services associated with flood mitigation, erosion control, and water purification (BRAUMAN et al., 2007).

A pillar of this approach is biophysical modeling, which quantifies WES from mathematical equations in computational environments (PALOMO et al., 2017). Biophysical models facilitate the understanding of ecohydrological processes in hydrographic basins and the assessment and forecasting of multiple pressures (GRIZZETTI et al., 2016). Well-calibrated, validated models have numerous applications in water management, such as quantifying the effects of land use and climate change (BUCAK et al., 2018; Bai et al., 2019; Ferreira et al., 2019), assessing flood risk (KADAVERUGU et al., 2021), and designing and evaluating forest restoration programs (FELD et al., 2011; Li et al., 2019; LARA et al., 2021; SOUZA et al., 2021), in addition to generating and transferring historical data for unmonitored basins, which is critical for hydrological studies (HRACHOWITZ et al., 2013). Such applications can help formulate and evaluate environmental conservation policies that support sound decision making in water resource management and land-use planning (BENRA et al., 2021).

Over the past few decades, free models to map ecosystem services have emerged (VILLA et al., 2009; BOUMANS et al., 2015; SHARP et al., 2020), ranging from simple approaches based on land-use data or habitat-based proxies to complex models that quantify physical processes in ecosystems (PALOMO et al., 2017). Traditional hydrological models such as the Soil and Water Assessment Tool (SWAT) (ARNOLD et al., 2012), Variable Infiltration Capacity model (LIANG et al., 1994), and the Regional Hydro-Ecological Simulation System (TAGUE; BAND, 2004) can be used to map and quantify WES. While they can accurately represent ecohydrological processes critical to a broad spectrum of ecosystem services, such as drinking water and recreation (KEELER et al., 2012; GRIZZETTI et al., 2016), their application is limited in regions with a dearth of data since their extensive parameters require detailed data about the study area as well as users with expertise in hydrology and modeling for calibration and validation (VIGERSTOL; AUKEMA, 2011; HRACHOWITZ et al., 2013).

Among simpler alternative models such as Artificial Intelligence for Ecosystem Services (VILLA et al., 2009), Integrated Valuation of Ecosystem Services and Tradeoffs (InVEST) (SHARP et al., 2020), and the Multiscale Integrated Model of Ecosystem Services (BOUMANS et al., 2015), the InVEST's models stand out and are frequently used to quantify and map WES. InVEST works with hydrological simplifications at the watershed scale that enable the simulation of such services as annual and seasonal water yield, water purification, and erosion control (SHARP et al., 2020). InVEST's models have been applied in diverse WES contexts and locations, including assessing the effects of mitigation policies in Europe (JORDA-CAPDEVILA et al., 2019), climate change and land use in WES in the United States (BAI et al., 2019), and ecological restoration in China (YANG et al., 2018). Although these models are applied globally, there are few studies that investigate their performance in comparison with empirical values (TERRADO et al., 2014; HAMEL et al., 2015; REDHEAD et al., 2016; REDHEAD et al., 2018; HAMEL et al., 2020; HUITING et al., 2020; BENRA et al., 2021). Of these, only Lu et al. (2020) analyzed the temporal performance of the Seasonal Water Yield (SWY) model, while the vast majority evaluated the spatial performance of InVEST models using long-term average values.

Assessing the performance of ecohydrological models is crucial to understanding the significance of parameters and input data to the reliability of their results, which inform decision-making and policy formulation (HACKBART et al., 2017). In addition, such assessments can aid developers seeking to enhance the effectiveness and efficiency of such tools (REDHEAD et al., 2016) and users looking to understand their potential and limitations in watersheds (WILLCOK et al., 2016), since their performance may vary according to regional climatic and hydrogeological characteristics.

A limited number of studies address the use of InVEST's WES models in Brazil (MANHÃES et al., 2016; SAAD et al., 2018; RESENDE et al., 2019; ROSÁRIO et al., 2019; GOMES et al., 2020; HAMEL et al., 2020b; SAAD et al., 2021), but none analyze their performances, comparing them with observed data. This study sought to calibrate and validate InVEST's SWY, Nutrient Delivery Ratio (NDR), and Sediment Delivery Ratio (SDR) models, considering their ability to simulate WES spatial and temporal variability. The study investigates the hypothesis that InVEST's WES models can effectively represent the observed annual values of streamflow, exported sediment, total nitrogen (TN), and exported total phosphorus (TP) in a subtropical watershed located in southeastern Brazil. The specific objectives were to assess the models' sensitivity to variation in calibration parameters, calibrate and validate the models, and evaluate the performance of the models. It is hoped that the results of this study can clarify the strengths and limitations of InVEST WES models to assist those using these tools to formulate policies for the conservation of water resources.

3.2. Materials and methods

3.2.1. Study area

The study was carried out in the Jacaré-Guaçu River Basin, in the central-eastern portion of the state of São Paulo, between the geographical coordinates 21º37'00" S and 22º22'00" S and 47º43'00" W and 48º56'00" W (Figure 3.1). The drainage area is nearly 4,172.12 km^2, covering the municipalities of Araraquara, Boa Esperança do Sul, Gavião Peixoto, Ibaté, Ibitinga, Itirapina, Nova Europa, Ribeirão Bonito, São Carlos, and Tabatinga, and is a sub-basin of the water resources management unit of the State of São Paulo (UGRHI 13), viz., the Tietê-Jacaré Hydrographic Basin. The Jacaré-Guaçu River is a direct tributary of the Tietê River, the largest watercourse in the state of São Paulo, and a source of water for UGRHI 13. It is formed by the junction of the Lobo and Feijão streams, which originate in the Itaqueri mountain range and Cuscuzeiro, covering 155 km until reaching the Ibitinga reservoir in the mid-course of the Tietê River (CBH-TJ, 2016). The basin includes small reservoirs that produce energy, such as the Lobo and Santana plants, and others that supply small rural properties.

The Jacaré-Guaçu River Basin lies between the CWA and CWB climatic zones, with dry winters and humid summers (KÖPPEN, 1918). Average annual precipitation is approximately 1400 mm, with a rainy season between October and March (Figure 3.2), which accounts for an average 80% of the total annual precipitation. Average monthly temperatures in the region range from 17.4º C in June to 23.7º C in February.

The topographic elevation varies from 372.0 m to 1024.0 m above sea level. The basin has a predominantly flat relief, composed of smoothly undulating hills (around 80%), arising from weathering of the Botucatu and Pirambóia formations, with low drainage density. The high slopes are mainly concentrated in areas of undulating and steep relief, near the sources of the Jacaré-Guaçu River and the drainages in the central portion of the basin.

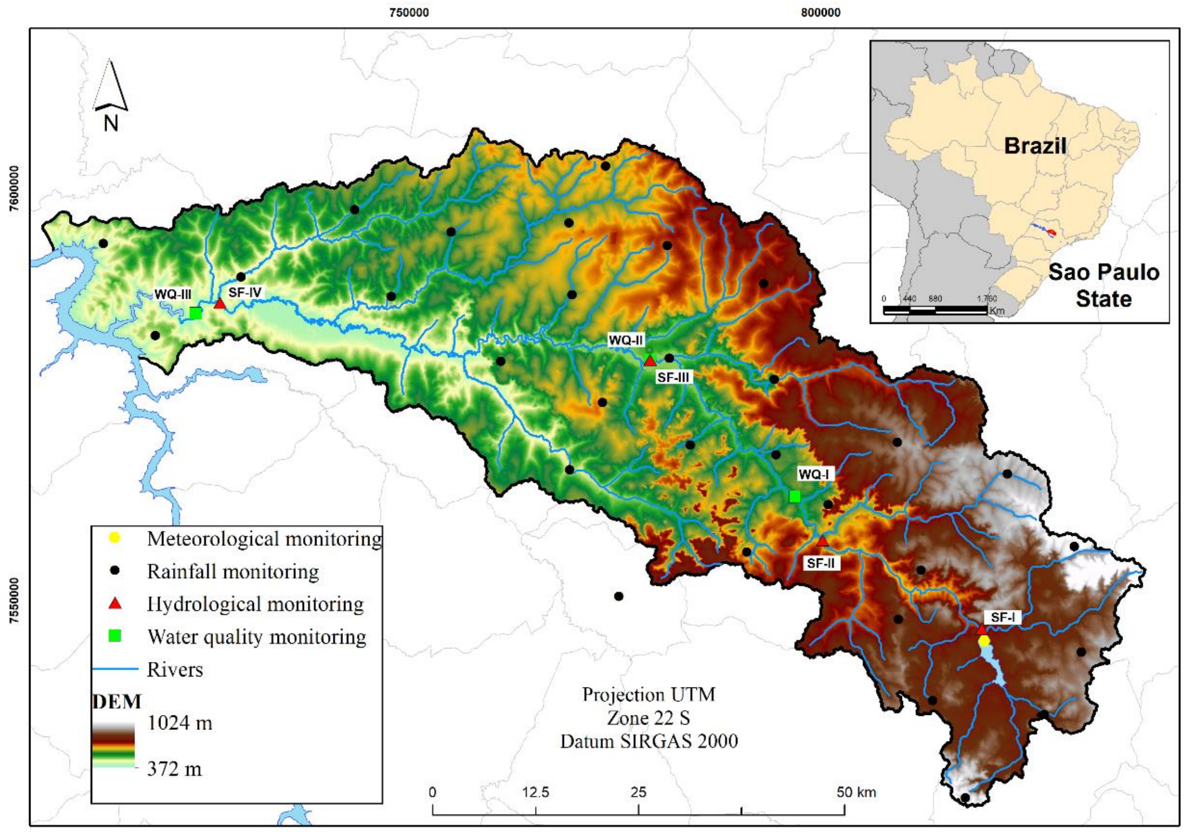

Figure 3.1. Location of Jacaré-Guaçu River Basin with principal watercourses, digital elevation model (DEM), meteorological, rainfall, hydrological and water quality monitoring sites.

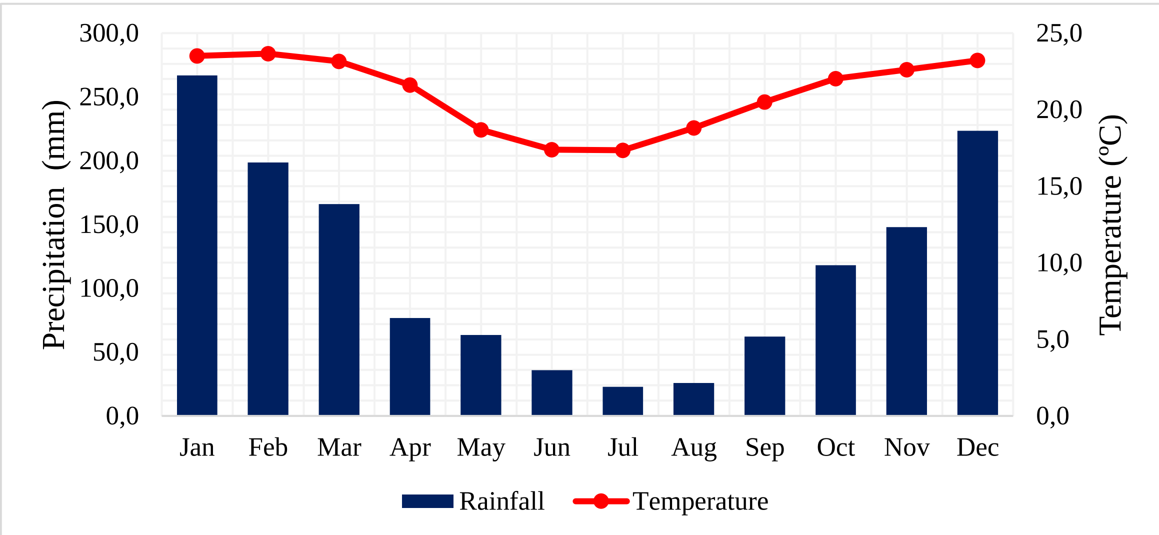

Figure 3.2. Distribution of the Jacaré-Guaçu, River Basin's average monthly precipitation and temperature (1981-2019). Graph generated based on data from Brazil's National Water and Sanitation Agency.

The basin is on the Guarani Aquifer System (GAS), formed by Aeolian sandstones from the Jurassic (Botucatu Formation) and fluvio-eolic Triassic (Pirambóia Formation) periods, which form underground water reservoirs. GAS is one of the world's largest underground freshwater reservoirs, with 1,200,000 km2 covering Brazil, Argentina, Paraguay, and Uruguay (COSTA et al., 2019). Aquifer recharge occurs in approximately 10% of the upwelling areas of the Botucatu and Pirambóia formations (LUCA; WENDLAND, 2016). The basin is an important GAS recharge area, where the aquifer is unconfined. At the basin, the aquifer covers an extensive area (~1640 km2) ranging from the region of Itirapina, at the head of the basin, to Ibitinga, close to its outlet. In addition to GAS, the Bauru and Serra Geral aquifers are found in the basin (CBH-TJ, 2016).

The basin features 10 types of soils: Red-Yellow Argisol, Haplic Gleysol, Red-Yellow Latosol, Red Latosol, Haplic Luvisol, Litholic Neosol, Quartzarenic Neosol, Red Nitosol, Haplic Organosol, and Haplic Planosol. Latosols constitute the predominant class and cover 60% of the basin, followed by Red-Yellow Argisols (14.77%) and Quartzarenic Neosols (12.77%) (ROSSI, 2017).

The basin's native vegetation is composed of grassland and forest, represented by remnants of Brazilian Cerrado (Savanna), riparian, and semi-deciduous forests (CBH-TJ, 2016). Intense changes have been observed in the landscape as a result of expanded agricultural activities, in particular, sugarcane cultivation, that have significantly reduced natural vegetation (TREVISAN et al., 2021). At present, natural areas occupy only 17% of the basin (MAPBIOMAS, 2021). The reduction of the basin's natural areas, such as wetlands and riparian forests adversely impacts the region's biodiversity and ecosystem services.

3.2.2. Database

The SWY, NDR, and SDR models were used with data from monitoring stations and high spatial resolution cartographic data. ALOS-PALSAR images with a spatial resolution of 12.5 m, freely available at the Alaska Satellite Facility (ASF, 2021), were used to determine DEM. Land-use data from 1985 to 2019 with a spatial resolution of 30 m were obtained from the Brazilian Annual Land Use and Land Cover Mapping Project (5th collection) (MAPBIOMAS, 2021). Meteorological data were attained directly from the climatological station of the Center for Water Resources and Environmental Studies of the School of Engineering of São Carlos. Precipitation data from the monitoring stations of the NationalWater and Sanitation Agency (ANA) (ANA, 2021) and data estimated by the Climate Hazards Group Infrared Precipitation with Stations of high resolution (0.05º) obtained via Google Earth Engine were also used. Daily and monthly streamflow data were obtained from ANA and the Department of Water and Energy of the State of São Paulo (DAEE) (ANA, 2021; DAEE, 2021). Data on total solids (TS), dissolved solids (DS), and TN and TP concentrations were acquired from the Environmental Company of the State of São Paulo (CETESB, 2021). Data characterizing the basin's soils were extracted from the pedological map of the state of São Paulo, at a scale of 1:100,000 (ROSSI, 2017).

3.2.3. Water Ecosystem Service Models

InVEST's ecosystem services models are free, open-source software used to evaluate a broad range of ecosystem services (SHARP et al., 2020). They are spatially explicit, that is, they use maps as input data and produce them as output data. The operating structures of each model used in this study are detailed below. Further information can be found in Sharp et al. (2020). The biophysical tables and all parameters required to run InVEST's WES models are available in the supplementary biophysical tables (Tables S 3.1 and S 3.2 in appendix A).

3.2.3.1. Seasonal Water Yield Model

The SWY model was used to quantify annual water production in the basin. The algorithm enables quantifying annual base flow (BF) and annual and monthly surface runoff (QF) for each pixel. The sum of BF and QF characterizes the basin's annual streamflow. Monthly QF is calculated based on a modified approach of the Natural Resource Conservation Service (NRCS) curve number method (NRCS, 1996), which determines it from monthly rainfall and the number of rainfall events (Equation 3.1).

$$QF_{i,m} = n_m\left(\left(a_{i,m} - S_i\right)\exp\left(-\frac{0.2S_i}{a_{i,m}}\right) + \frac{S_i^2}{a_{i,m}}\exp\left(\frac{0.8S_i}{a_{i,m}}\right)E_i\left(\frac{S_i}{a_{i,m}}\right)\right) \times \left(25.4\left[\frac{mm}{in}\right]\right) \tag{3.1}$$

$$a_{i,m} = \frac{P_{i,m}}{n_m}/25.4 \tag{3.2}$$

where $P_{i,m}$ is the monthly precipitation in pixel i for month m (mm); nm is the number of rain events in pixel i in month m; ai,m is the mean rain depth on a rainy day at pixel i in month m (Equation 2); S_i = 1000/CN_i - 10; CN_i is the curve number (Table S 3.1 in appendix A) for pixel i; and E_i is the exponential integral function. The value 25.4 is an inch to millimeter conversion parameter. The annual QF_i is the sum of the monthly values $QF_{i,m}$ (mm).

The local recharge for each pixel is calculated from the local water balance (Equation 3.3). The local recharge value is determined on an annual scale, using monthly values. The portion of available monthly rainfall that is not runoff over the surface is divided between local recharge and evapotranspiration. For a given pixel, the partitioning is affected by upgradient recharge, and parameters α and β influence the availability of groundwater for evapotranspiration (Equation 3.4).

$$L_i = P_i - QF_i - AET_i \tag{3.3}$$

$$AET_{i,m} = \min\left(PET_{i,m};\ P_{i,m} - QF_{i,m} + \alpha_m \beta L_{Sum.avail;i}\right) \tag{3.4}$$

$$PET_{i,m} = K_{c,i,m} \,.\, ET_{0,i,m} \tag{3.5}$$

where L_i is the local recharge for pixel i (mm), P_i the annual precipitation for pixel i (mm), AET_i, the real annual evapotranspiration in pixel i (mm), $AET_{i,m}$, the real monthly evapotranspiration in pixel i (mm), $PET_{i,m}$, the monthly potential evapotranspiration at pixel i (mm), αm, the fraction of upslope annual recharge available in month m (default: 1/12), β_i, the fraction of the upslope subsidy available for downslope evapotranspiration (default: 1), $L_{Sum.avail,i}$, the sum of upslope subsurface water potentially available at pixel i, $Kc_{,i,m}$, the monthly crop coefficient for ground cover type (Table S 3.1 in appendix A) in pixel i, and $ET_{0,i,m}$, the reference evapotranspiration (Equation S 3.1 in appendix A) at pixel i for month m (mm).

The annual base flow index (B), which represents the portion of water that reaches the watercourse via groundwater, is calculated based on local recharge values. Negative values indicate that the pixel does not contribute to BF, and B is assigned a value of zero. When the pixel contributes to BF, the value of B is calculated as a function of the amount of flux leaving the pixel and its relative contribution to BF reloading this pixel. For a pixel that is not adjacent to the stream channel, the cumulative base flow ($B_{sum,i}$) is proportional to the cumulative base flow that leaving the adjacent downslope pixels minus the cumulative base flow that was generated on that same downslope pixel.

$$B_{sum,i} = L_{sum,i}, \text{if j is a nonstream pixel} \tag{3.6}$$

$$\text{or } B_{sum,i} = L_{sum,i} \textstyle\sum_{j \in \{\text{cells to which cell i pours}\}} \text{pij}, \text{if j is a stream pixel} \tag{3.7}$$

$$B_i = \max\left(B_{sum,i} \cdot \frac{L_i}{L_{sum,i}}, 0\right) \tag{3.8}$$

where $L_{sum,i}$ is the cumulative upstream recharge, p_{ij}, the proportion of flow from cell i to j, and the base flow Bi can be directly derived from the proportion of the cumulative base flow leaving cell i, with respect to the recharge available to the upstream cumulative recharge.

3.2.3.2. Sediment Delivery Ratio Model

InVEST's SDR model was used to quantify the contribution of sediments to watercourses. The model was derived from studies by Borselli et al. (2008), and is based on the quantification of the annual rate of soil loss per pixel and the sediment delivery rate (SDR), which represents the proportion of soil loss that is transported and deposited in watercourses. The model does not consider in-stream processes, assuming that all sediment that reaches the watercourse is transported to the outlet of the hydrographic basin.

In the SDR model, the quantification of the annual soil loss per pixel (ton $ha^{-1}.year^{-1}$) is estimated using the Revised Universal Soil Loss Equation (RUSLE) (Equation 3.9). The determination of the RUSLE parameters is presented in the supplementary material.

$$USLE_i = R_i.\ K_i.\ LS_i.\ C_i.\ P_i \tag{3.9}$$

where R_i is the rainfall erosivity in pixel i ($MJ \cdot mm \cdot ha^{-1} \cdot h^{-1}$) (Equation S 3.2 in appendix A); K_i, the soil erodibility at pixel i ($ton \cdot ha \cdot h \cdot MJ^{-1} \cdot ha^{-1} \cdot mm^{-1}$) (MANNINGEL et al., 2002), LS_i, the slope length-gradient factor at pixel i (dimensional) (Equation S 3.3 in appendix A), C_i, the cover-management factor in pixel i (Table S 3.2 in appendix A), and P_i, the support practice factor in pixel i (Table S 3.2 in appendix A).

The sediment delivery rate is calculated as a function of the hydrological connectivity of the basin (Equation 3.10). For its determination, it is first necessary to calculate the Hydrological Connectivity Index (IC) (Equation 3.11), which describes the hydrological connection between the sources of sediments in the landscape and the watercourses. The higher the pixel's IC value, the greater is the probability of sediment reaching the watercourse. The IC is based on the relationship between the characteristics of the area upstream of each pixel (Dup), such as land cover, slope, and drainage area

(Equation 3.12), and the characteristics of the flow path between the pixel and the watercourse (Ddn), such as distance, land cover, and slope (Equation 3.13).

$$\mathrm{SDR_i} = \frac{\mathrm{SDR_{max}}}{1 + \exp\left(\frac{\mathrm{IC_0} - \mathrm{IC_i}}{\mathrm{k_b}}\right)} \tag{3.10}$$

where SDRmax is the maximum theoretical SDR, set to a mean value of 0.8 (VIGIAK, 2012), and IC_0 and kb are calibration parameters.

$$\mathrm{IC} = \log_{10}\left(\frac{\mathrm{D_{up}}}{\mathrm{D_{dn}}}\right) \tag{3.11}$$

$$\mathrm{D_{up}} = \bar{\mathrm{C}}\bar{\mathrm{S}}\sqrt{\mathrm{A}} \tag{3.12}$$

$$\mathrm{D_{dn}} = \sum_{\mathrm{i}} \frac{\mathrm{d_i}}{\mathrm{C_i\,S_i}} \tag{3.13}$$

where $\bar{C}$ is the average of the factor C of the upstream catchment area; $\bar{S}$ the mean of the upstream slope gradient (m. m^{-1}), A, the upstream contribution area (m^2), di, the length of the flow path along according to the steepest downslope direction (m), C_i, the C factor for each pixel, and S_i the pixel slope gradient.

Calculation of the exported sediment load per pixel in ton ha^{-1}. $year^{-1}$ is given by Equation 3.14. The basin's total sediment export is calculated by the sum of all pixels constituting the watershed.

$$\mathrm{E_i} = \mathrm{USLE_i} \times \mathrm{SDR_i} \tag{3.14}$$

3.2.3.3. Nutrient Delivery Ratio Model

The NDR model was used to quantify annual TN and TP cargo exports. The model maps the nutrient sources along the watershed and their transport to watercourses, enabling quantification of the nutrient retention services provided by vegetation. The model is based on a simple mass balance approach, representing steady-state nutrient flux through empirical relationships. The mass balance is determined based on the nutrient loadings and retention properties of pixels belonging to the same runoff. The algorithm first calculates the annual nutrient load and then the NDR, which corresponds to the proportion of nutrients that reach the watercourse.

Nutrient loads in each pixel are calculated using average TN and TP export coefficients, which vary according to the watershed's land use. In this study, the coefficients of the Mathematical Model of Correlation between Land Use and Water Quality (MQUAL), version 1.5 (SMA, 2010) were used. The nutrient loads associated with each land use class were corrected as recommended by Sharp et al. (2020) (Equation S 3.4 in appendix A). The adjusted values of the nutrient export coefficients are presented in Table S 3.2 in appendix A.

Then the model modifies the pixels' nutrient loads based on the basin's surface runoff potential (Equation 3. 15). The model enables analysis of nutrient loads associated with sediments and dissolved, which are transported through the surface and underground flow, respectively. This study considered only the surface transport of nutrients.

$$\text{modified.load}_{xi} = \text{load}_{xi} \times \text{RPI}_{xi} \tag{3.15}$$

$$\text{RPI}_{xi} = \frac{\text{RP}_i}{\text{RP}_{av}} \tag{3.16}$$

where modified.loadxi is the modified load of nutrients in each pixel, loadxi, the nutrient load on each pixel, RPIxi, the runoff potential index at pixel i, RPi, the runoff value of pixel i; and RPav, the average value of runoff in the watershed. In practice, the RP values are defined through InVEST's SWY model or through spatialized precipitation data. This study used average annual precipitation data as a proxy to determine the basin's surface runoff potential.

After quantifying nutrient loads, the model simulates their transport to the watercourse using the NDR factor (Equation 3. 17), calculated for each pixel based on the IC and retention properties of pixels that belong to the same flow path, a similar approach to the SDR concept (SHARP et al., 2020).

$$\text{NDR}_i = \text{NDR}_{0,i}\left(1 + \left(\frac{\text{IC}_i - \text{IC}_0}{k}\right)\right)^{-1} \tag{3.17}$$

where $NDR_{0,i}$ is the nutrient proportion not retained by downstream pixels (see SHARP et (2020), for further details), IC_i, the hydrological connectivity index, and IC_0 and k are calibration parameters.

The nutrient load exported per pixel in (kg ha^{-1} $yr^{-}1$) is calculated according to Equation 3.18. The total nutrient export is calculated by the sum of all pixels in the watershed. InVEST's nutrient export model only considers nonpoint sources, it was necessary to incorporate TN and TP point sources. Determination of the basin's point pollution is presented in greater detail in the supplementary material.

$$X_{expi} = \text{modified.load}_{xi} \times NDR_i \tag{3.18}$$

3.2.4. Sensitivity analysis

Sensitivity analysis was conducted by varying the models' calibration parameters. For the SWY model, the approach of Hamel et al. (2020), in which the α and β parameters were changed one at a time to verify their BF sensitivity was adopted. With the default value of α = 1/12, the values of β were varied from 0 to 1 in increments of 0.2. The same procedure was performed for α, in which the default value of β = 1 was maintained and the values of α = 1/6 and α = 1/3 were used to analyze their BF response. For the SDR model, parameters kb and IC_0 (default values: 2 and 0.5, respectively) were modified to assess their influence on annual sediment export. The kb and IC_0 values were changed from 0.5 to 3 in 0.5 and from 0.25 to 1 in 0.25 increments, respectively. For the NDR model, the parameter k was varied, using the same approach as the SDR model and the parameter critical flow length, that is, the minimum metric distance required for a fragment of a certain type of soil use to retain nutrients maximally. As input data for the NDR model, the critical flow length does not have a default value. The default value of 150 meters was considered and the sensitivity of this parameter was set to values of 30, 90, 150, 300, and 500. For all models, the threshold flow accumulation value was set to 1000, the value that best represents the drainage mapped in the basin at a scale of 1:250,000 (IBGE, 2021).

3.2.5. Model calibration and validation

This study calibrated and validated the InVEST models to determine the values of the calibration parameters that best represent WES's spatial and temporal variability. Calibration and temporal validation were performed comparing simulated and observed annual mean values. As the basin's monitoring stations are sparse, viz., four for streamflow measurement and three for water quality, it was not feasible to use each station's long-term average values to calculate spatial assessment. Accordingly, to represent spatial variability, the study used all values of the historical series sampled in the basin. WES-specific values were used to normalize the data and eliminate the drainage area effect.

The SWY model was calibrated and validated for the basin's four sub-basins (SF-I, SF-II, SF-III, and SF-IV), using observed daily and monthly streamflow data (ANA, 2021; DAEE, 2021). The historical series of all sub-basins had faults that varied according to the monitoring station. To fill in the gaps and standardize the 39-year time scale for all stations, the study used a flow regionalization method based on area proportionality, which assumes the existence of a proportional linear relationship between drainage area and flow, a method validated for the region in Anjinho et al. (2021). The average annual streamflow (QF + BF) results in mm. $year^{-1}$ simulated by the SWY model were converted to $m^3. s^{-1}$ and compared with observed values. The calibration period was 1981 to 2010 and the validation period, 2011 to 2019.

The SDR and NDR models were calibrated and validated for three sub-basins (WQ-I, WQ-II, and WQ-III), using data from bimonthly measurements of TS, DS, TN, and TP concentrations. Total suspended solids (TSS) data were obtained indirectly by subtracting TS – DS. Of all the monitoring stations, only WQ-II presents streamflow measurements along with water quality parameters. Thus for the other sub-basins, the instantaneous streamflow were estimated through regionalization based on the proportionality of the area, using streamflow data from nearby monitoring stations (ANA, 2021). The annual loads of SST, TN, and TP were estimated based on the concentrations of water quality parameters (mg. L^{-1}) and flow ($m^3. s^{-1}$). Historical series of 9 years for sub-basin WQ-I and 19 years for sub-basin WQ-II (12 and 7 years for calibration and validation, respectively) were obtained for both variables. For sub-basin WQ-III, 20 years (12 and 8 years for calibration and validation, respectively) were obtained for TSS, and 30 years (22 and 8 years for calibration and validation, respectively) for TN and TP. Due to the dearth of sampling (merely 6 measurements per year) and the data's seasonality, the observed loads of TSS, TN, and TP were processed to represent average annual values. For TN and TP, the outliers were removed using the relation lower outlier = Q1 – (1.5 * IQR) and higher outlier = Q3 + (1.5 * IQR), where Q1 is quartile 1, Q3, quartile 3, and IQR, interquartile variation (IQR = Q3 – Q1). For TSS, in which a greater effect of seasonality was observed, only the values that were between Q1 to Q3 were considered.

3.2.6. Model performance analysis

The performance of the models was evaluated by comparison with data observed in the monitoring stations, considering annual average values. The analysis was conducted to evaluate WES temporal and spatial performance. Three statistical indicators were used: the Nash and Sutcliffe coefficient (NASH; SUTCLIFFE, 1970), percentage bias (PBIAS), and the coefficient of determination (R^2). The classification suggested by Rauf et al. (2018) was used to interpret the results (Table 3.1).

Table 3.1. Classification of statistical performance indicators.

Classes	NSE	R²	PBIAS
Very good	0.75 > NSE ≤ 1.00	0.85 > R² ≤ 1.00	<|5|
Good	0.65 > NSE ≤ 0.75	0.70 > R² ≤ 0.85	|5| - |10|
Satisfactory	0.50 > NSE ≤ 0.65	0.60 > R² ≤ 0.70	|10| - |15|
Acceptable	0.40 > NSE ≤ 0.50	0.40 > R² ≤ 0.60	
Unsatisfactory	NSE ≤ 0.40	≤ 0.40	≥ |15|

3.3. Results

3.3.1. WES models sensitivity analysis

The sensitivity analysis of the SWY model parameters indicated that β is the most sensitive and has the greatest influence on BF variation (Figure 3.3). Increased β values decreased BF in all sub-basins, primarily, in the range of values that varies between $0 \leq \beta < 0.4$. Compared to the default values, reduction in the value of β to 0.2 increases BF 26% on average, with the greatest variation (39%) in sub-basin SF-IV. For α, however, the trends varied. BF decreased by an average of 3% to α = 1/6 and increased by an average of 5% to α = 1/3, chiefly in sub-basin SF-IV, where the average increase was approximately 10%.

Sediment export in the SDR model showed greater sensitivity for parameter kb, whose increase is associated with greater sediment export to all sub-basins (Figure 3.3). For kb = 0.5, the exported sediment value is on average 100% lower than the default value, and for kb = 3, the value is on average 107% higher. In absolute values (t. yr^{-1}), the highest sensitivity occurs between $0.5 \leq kb \leq 1$, where the sediment exported for k = 1 is 34 times greater. Values between $1.5 \leq kb \leq 2.5$ tend to vary sediment export by approximately -50% and +50%, respectively. Changes in IC_0 values showed lower sensitivity and opposite behavior compared to kb variations. The increase in IC_0 values is related to a lower sediment export. On average, an increase of 0.25 in IC_0 values tends to decrease the value of exported sediment by 11%. Compared to the default value, the value of $IC_0 = 1$ provided an increase of 20% of the sediment exported to all sub-basins, while the value of $IC_0 = 0.25$ decreased by 12%.

The sensitivity of the parameters k and critical flow length showed the same behavior for TP and TN (Figure 3.3). In general, nutrient exports were more sensitive to changes in critical flow length values. This study considered the value of 150 m as the default for this parameter, decreasing this value to 30 m provided a reduction of approximately 12% in the value of exported nutrients, while the value of 500 m increased by almost 25%. The parameter k was more sensitive between $0.5 \leq k \leq 1$ and its effect is more expressive in the decrease of nutrient export than in the increase. Relative to the default value ($k = 2$), decreasing to $k = 0.5$ decreased nutrient export by 15%, while changing to $k = 3$ showed a slight increase of almost 3%.

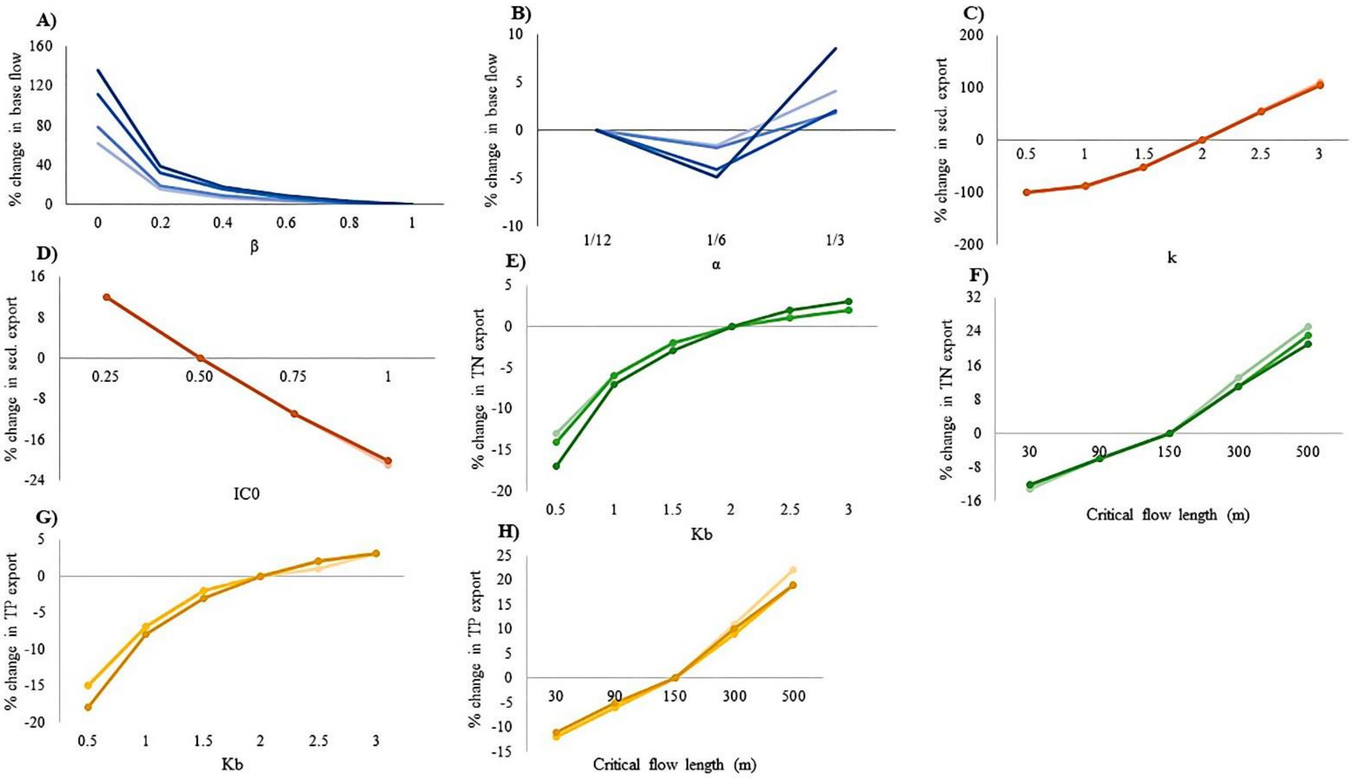

Figure 3.3. InVEST WES model sensitivity: (A) parameter β (SWY), (B) parameter α (SWY), (C) parameter k (SDR), (D) parameter IC0 (SDR), (E) parameter k (NDR-TN), (F) critical flow length parameter (NDR-TN), (G) parameter k (NDR-TP), and (H) critical flow length parameter (NDR-TP).

3.3.2. Calibration and validation of water ecosystem services temporal variability

The SWY, SDR, and NDR models perform differently in the spatial and temporal scales. Figures 3.4, 3.5, and 3.6 show the simulated and observed WES values over time and the models' adjusted parameter values. Table 3.2 presents performance indicators.

The best calibration and validation performance was observed for the SWY model. A visual comparison of the simulated and observed annual streamflow indicates a good fit for all sub-basins (Figure 3.4). Although the best performance involved values close to the long-term annual averages, the model was able to represent streamflow variation over time. R^2 indicated an acceptable performance for the calibration period, but NSE was unsatisfactory for all sub-basins. PBIAS indicated that the SWY model underestimated annual streamflow in sub-basins SF-I and SF-IV and overestimated it in sub-basins SF-II and SF-III, with very good and good performance, respectively. For the validation period, R^2 values indicated satisfactory to acceptable performances. NSE values indicated satisfactory performance and PBIAS values presented different values for each sub-basin, with unsatisfactory performance observed in sub-basin SF-II and very good performance in sub-basin SF-III.

Table 3.2. InVEST WES model performance in light of temporal variability (* inversely proportional relationships, negative slope).

			Calibration			Validation		
Monitoring Station	**Model**	**Indicator**	**R^2**	**PBIAS (%)**	**NSE**	**R^2**	**PBIAS (%)**	**NSE**
SF-I	SWY	Streamflow	0.4	−0.6	−0.6	0.5	8.1	0.6
SF-II	SWY	Streamflow	0.5	6.6	−0.6	0.8	30.3	0.6
SF-III	SWY	Streamflow	0.5	8.8	−4.6	0.7	0.9	0.5
SF-IV	SWY	Streamflow	0.6	−3.4	−2	0.7	−8.5	0.6
WQ-I	SDR	Exported sediment	0.3	0.2	0.2	-	-	-
WQ-II	SDR	Exported sediment	0	0.6	−0.1	0.2	−14.6	−0.1
WQ-III	SDR	Exported sediment	0	6.6	−0.3	0.1 *	5.6	−0.4
WQ-I	NDR	Exported TP	0.2	50	−4.5	-	-	-
WQ-II	NDR	Exported TP	0.6 *	−23	−1.1	0.4	1.7	0.2
WQ-III	NDR	Exported TP	0.3	−10	0.1	0.3 *	2.2	−0.3
WQ-I	NDR	Exported TN	0.3	−18.6	−0.8	−	−	−
WQ-II	NDR	Exported TN	0.4 *	2	−0.2	0.4 *	12.3	−0.6
WQ-III	NDR	Exported TN	0.1	27	−1.5	0.6 *	44	−3.4

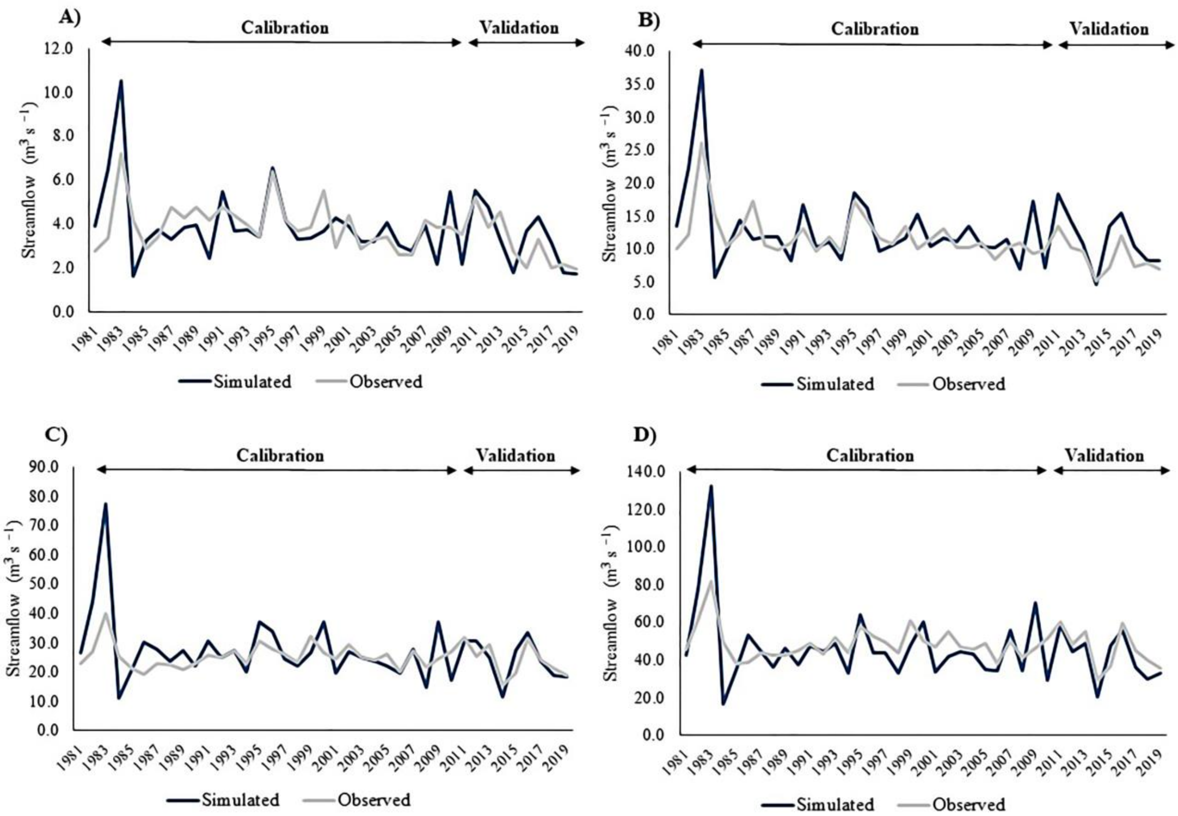

Figure 3.4. Comparison of simulated and observed data for annual streamflow for the calibration and validation period: (A) sub-basin SF-I, (B) sub-basin SF-II, (C) sub-basin SF-III, (D) and sub-basin SF-IV, with simulated values considering adjusted parameters $\beta = 0.2$, $\alpha = 1/12$, and $\gamma = 1$.

The SDR model effectively represented years with values close to the long-term average, but did not perform well in representing the annual variability of exported sediment (Figure 3.5). The results indicated large discrepancies for specific years, but those between the observed and simulated values were not systemic. NSE and R^2 values for the calibration and validation period reflected the SDR model's limited capacity to represent the annual variability of exported sediment, indicating inconsistent performance (Table 2). PBIAS values showed that the SDR model overestimated the sediment load exported annually in the calibration period, with very good performance in sub-basins WQ-I and WQ-II and good performance for sub-basin WQ-III. PBIAS found varying trends in the sub-basins for the validation period, underestimating the sediment load exported in sub-basin WQ-II and overestimating it in sub-basin WQ-III, with satisfactory and good performance, respectively (Table 3.2).

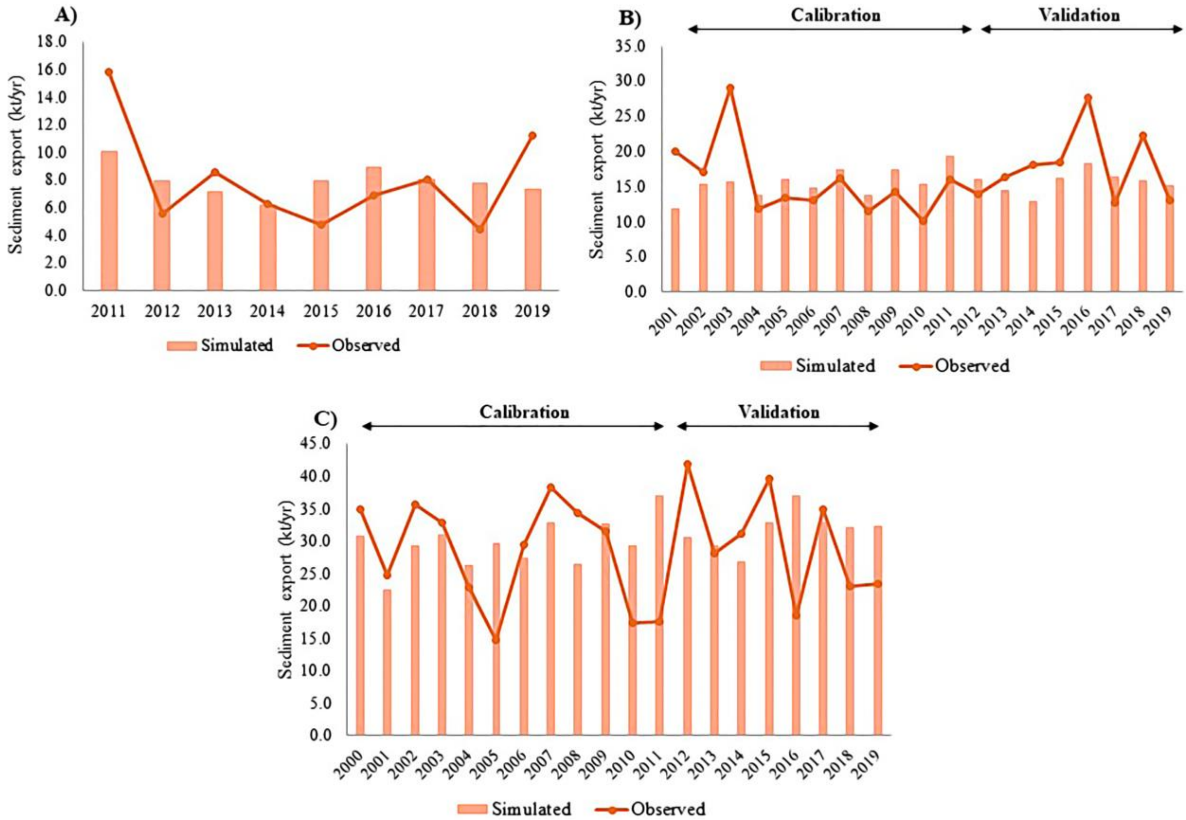

Figure 3.5. Comparison of simulated and observed exported sediment during the calibration and validation period: (A) sub-basin WQ-I, (B) WQ-II, and (C) WQ-III, with simulated values considering adjusted parameters k = 0.8 e IC0 = 0.45.

Nutrients simulated by the NDR model present higher performance for values close to the long-term mean of the observed data. However, unlike the SWY and SDR models, the NDR model is unable to represent the annual variability of nutrient loads (Figure 3.6). For TP and TN, values tend to remain close to the average, showing a slight variation over time. Concerning the NDR model's performance, the adjustment of the calibration parameters showed high variability among sub-basins. With regard to the values of the annual TP loads for the calibration and validation period, the R^2 and NSE indicators indicated unsatisfactory performance for all sub-basins (Table 3.2). Although R^2 was increased for sub-basin WQ-II (R^2 = 0.6) in the calibration period, the analysis found an inversely proportional relationship between the simulated and observed data, which indicates the model's inconsistent performance. PBIAS, however, indicated satisfactory performance in the calibration period for sub-basin WQ-III and very good performance for the validation period in sub-basins WQ-II and WQ-III (Table 3.2). The performance indicators obtained for modeled TN annual loads showed the same trend as for modeled TP annual loads. The PBIAS indicator indicated very good and satisfactory performances only in sub-basin WQ-II for the calibration and validation period, respectively (Table 3.2).

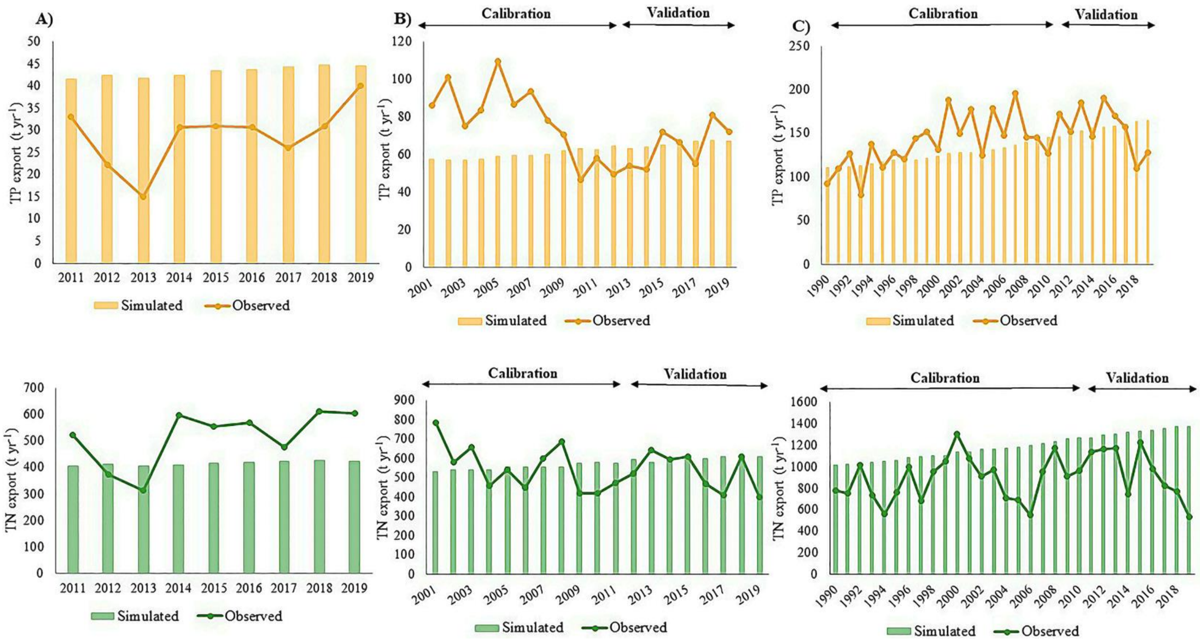

Figure 3.6. Comparison of simulated and observed exported nutrients for the calibration and validation period: (A) sub-basin WQ-I, (B) sub-basin WQ-II, and (C) sub-basin WQ-III.TP values (yellow graphs) were simulated considering parameters k = 2 and critical flow length = 30. TN values (green graph) were simulated considering parameters k = 0.2 and critical flow length = 30.

3.3.3. WES spatial performance analysis

SWY model results demonstrated a reasonable fit with the observed data (Table 3.3). R^2 indicated acceptable performance, and the PBIAS and NSE indicators demonstrated a very good and unsatisfactory performance, respectively. For the SDR, NDR-TN, and NDR-TP models, PBIAS indicated a performance ranging from satisfactory to very good, while the other indicators showed unsatisfactory performance.

Table 3.3. InVEST WES model performance considering spatial variability.

Model	R^2	PBIAS	NSE
SWY	0.47	3.50	−0.39
SDR	−0.10	−6.25	−0.13
NDR-TN	0.30	11.00	0.13
NDR-TP	0.00	−3.31	−0.23

The study’s results indicate that, in general, the models were able to simulate the long-term mean values observed in the sub-basins (Table 3.4). The largest discrepancy occurred in sub-basin WQ-I for the NDR-TP model, and the smallest discrepancy was observed in sub-basin SF-I for the SWY model.

Table 3.4. Long-term values of simulated and observed data of variables QF, BF, streamflow, exported sediment, TN, and TP.

Sub-Basin	Period	QF (m^3 s^{-1})	BF (m^3 s^{-1})	Simulated Streaflow (m^3 s^{-1})	Observed Streamflow (m^3 s^{-1})	Discrepancy (%)
SF-I	1981–2019	1.2	2.6	3.8	3.8	1
SF-II	1981–2019	3.1	9.4	12.5	11.3	11
SF-III	1981–2019	8.9	18.0	26.9	25.1	7
SF-IV	1981–2019	13.1	32.6	45.8	47.9	−5
Sub-basin	**Period**	**Simulated exported sediment (kt.yr^{-1})**	**Observed exported sediment (kt.yr^{-1})**			**Discrepancy (%)**
WQ-I	2011–2019	8.350	7.759			8
WQ-II	2001–2019	14.843	15.533			−4
WQ-IIII	2000–2019	27.557	31.757			−13
Sub-basin	**Period**	**Nonpoint TN load (t.yr^{1})**	**Point TN load (t.yr^{1})**	**Simulated TN (t.yr^{1})**	**Observed TN (t.yr^{1})**	**Discrepancy (%)**
WQ-I	2011–2019	136.4	280.4	416.8	512.0	−19
WQ-II	2001–2019	242.3	331.4	573.6	542.4	6
WQ-IIII	2000–2019	485.9	707.2	1193.0	900.0	32
Sub-basin	**Period**	**Nonpoint TP load (t.yr^{1})**	**Point TP load (t.yr^{1})**	**Simulated TP (t.yr^{1})**	**Observed TP (t.yr^{1})**	**Discrepancy (%)**
WQ-I	2011–2019	16.2	27.0	43.2	28.8	50
WQ-II	2001–2019	29.6	32.6	62.2	73.2	−15
WQ-IIII	2000–2019	63.0	71.7	134.8	143.9	−6

3.4. Discussion

3.4.1. WES sensitivity analysis

Unlike other studies that analyzed the sensitivity of calibration parameters and input data (BAGSTAD et al., 2018; REDHEAD et al., 2018; WANG et al., 2018), this study examined just the calibration parameters' sensitivity, choosing not to analyze the sensitivity of the input data because the vast bulk came from monitoring stations, which tend to have higher quality than other databases. When feasible, empirical values were also used for some input parameters, such as soil erodibility and crop and nutrient export coefficients, which best represent the characteristics of the studied area.

With regard to the SWY model, the study indicated the β parameter as the most sensitive, having a significant effect on flow routing and, consequently, on BF values. Hamel et al. (2020) also found greater sensitivity for β, with BF varying by nearly 50% in some sub-basins. For α = 1/12 and α = 1/6, the decreasing BF was similar to Hamel et al. (2020), but for alpha = 1/3, there was a BF increase (Figure 3.3), associated with the determination of $AET_{i,m}$, which is conditioned by PET or water availability, according to Equation (4). The parameters α and β are associated with the fraction of the annual recharge of pixels upstream (upslope) available for evapotranspiration of a pixel downstream (downslope) (SHARP et al., 2020). The configuration of alpha = 1/3 and beta = 1 (default value) renders the potential available water ($L_{sum.avail,i}$), very high, requiring the algorithm to use $PET_{i,m}$ to calculate $AET_{i,m}$ (Equation 3.4).

The sensitivity of the SDR model parameters k and IC_0 followed that of Hamel et al. (2015), as anticipated in light of the model's configuration (SHARP et al., 2020). Although both parameters characterize the relationship between the connectivity index and sediment delivery rate, the sensitivity of k was greater than that of IC_0, with higher values associated with a higher sediment delivery rate, as predicted by Vigiak et al. (2012), suggesting that k variations are more effective for data calibration and validation. The result of the sensitivity analysis of the IC_0 parameter appears more sensitive than that in Hamel et al. (2015), although it showed the same linear decrease in exported sediment.

For the NDR model, the sensitivity of the parameter k occurred as anticipated, given the relationship between nutrient export and k is generally exponential when k is less than nine and linear when it is greater (HAN et al., 2021). As noted in other studies (REDHEAD et al., 2018; HAN et al., 2021), the results of this research showed that the parameter k is most sensitive between the values of $0 \leq k \leq 1$, in which the projected curve presents sigmoidal behavior, that is, an expressive increase at the onset and a tendency to stabilize as k values increase. In this study, the effect of k in all sub-basins was similar as a result of basin's hydrogeological similarity. However, as demonstrated by Redhead et al. (2018), the response in k variations is specific to each location, and thus may differ from the results herein. Variations in critical flow length values indicate a directly proportional linear relationship with the exported nutrient load. This was also expected, since it is assumed that the greater the distance for a land-use fragment to reach its maximum retention capacity, the greater the probability of the nutrient load reaching the watershed (SHARP et al., 2020).

3.4.2. InVEST WES model performance

The study's sensitivity analysis increases our understanding of the effect of calibration parameters on the modeled results and how to optimize their representation of the observed data, which its performance analysis indicates the InVEST WES models are reasonably effective in simulating, albeit with high variability according to the model and analysis scale. Using the SWAT model and the Generalized Watershed Loading Function, Santos et al. (2020) modeled the streamflow and sediment and nutrient loads in the upper part of the basin with results analogous to those herein, with both indicating improved performance in simulating streamflow.

With regard to the InVEST WES models' calibration and temporal validation, the best performance was observed for the SWY model. Despite some indicators of unsatisfactory performance, particularly in the calibration period for NSE, the results show that the model was able to represent the temporal variability of the average annual streamflow in the sub-basins for the calibration and validation period (Figure 4 and Table 2). The effective performance of the SWY model may be associated with its high sensitivity to variations in precipitation, as noted in the literature (WANG et al., 2018; HUITING et al., 2021). Likewise, the inferior performance of the NDR and SDR models may be related to their lower sensitivity (REDHEAD et al., 2018; BENEZ-SECANHO; DWIVEDI, 2019; SAHALE et al., 2019). Insensitivity to precipitation in UK watersheds (REDHEAD et al., 2018) is inherent in the NDR model's configuration (Equation 3.16), where its sole effect is to modify the nutrient load's impact on surface runoff, based on an index that relates pixel precipitation to the basin's average rainfall. That is, the effect of precipitation is more closely associated with its configuration than with its intensity. In the SDR model, as opposed to the NDR, precipitation has a greater expressive influence on sediment export (Figure 5) because rainfall erosivity is key to triggering erosion (Equation 3.9). Some studies have indicated high sensitivity to erosivity in the

SDR model (HAMEL et al., 2015; SÁNCHEZ-CANALES et al., 2015). Although this study used annual rainfall and land-use data as model inputs, temporal variability was not well captured by the SDR and NDR models.

The spatial performance of InVEST's WES models is often evaluated using long-term average values. Due to the dearth of monitoring stations, this study included all values in the historical series sampled in the basin to calculate the statistical indicators and evaluate the spatial performance of the models. Although not detailed herein, it should be noted that an initial analysis was conducted, using WES values not normalized by the drainage area, which deemed the performance of all models good. However, as the study's objective was to examine the models' capacity to forecast WES behavior in the basin, taking into account the variability of land use patterns, specific WES values were used, and the models' spatial performances were significantly reduced (Table 3.3).

When compared with observed long-term mean values, the results were similar to those in the literature (TERRADO et al., 2014; HAMEL et al., 2015; REDHEAD et al., 2018; HAMEL et al., 2020; BENRA et al., 2021), indicating that the InVEST WES models yield good results in terms of relative magnitude. The SWY model performed best, with simulated long-term average flow deviations of less than 10% from observed values. These results confirm the findings of other studies that have shown reasonable performance for the SWY model (HAMEL et al., 2020; LU et al., 2020; BENRA et al., 2021). The long-term average loads of exported sediments simulated by the SDR model also showed limited discrepancies with observed values, corroborating studies that have featured its potential to simulate sediment dynamics (TERRADO et al., 2014; SÁNCHEZ-CANALES et al., 2015; HAMEL et al., 2015). The greatest deviations in NDR model simulations were found in sub-basins WQ-I and WQ-III, which overestimated TN and TP exports by 50% and 32%, respectively. Redhead et al. (2018) obtained similar results in UK watersheds, with the vast majority showing deviations from observed values for TN and TP of 65% and 44%, respectively.

In calibrating the models, it could be seen that that the values assigned to the calibration parameters generally reflected the hydrogeological characteristics of the basin, which is located in a flat region, in which some 80% of the relief is composed of smoothly undulating hills with low drainage density (ROSSI et al., 2017), with a slope around 8%. The basin's soils are primarily sandy and deep (~75%), as is characteristic of Brazil's Cerrado biome. Thus, the basin has a low potential to generate surface runoff and, consequently, to transport nutrients and of sediments to watercourses. The values assigned to the calibration parameters reflected these characteristics.

In the SWY model, the values $\beta = 0.2$ and $\alpha = 1/12$ presented the best relationship with observed values and increased the BF share of water yield, conditions that occur in regions with flat, smooth topography. Their determination is consistent for the basin as it is an important recharge area for the Guarani Aquifer, one of the largest underground freshwater reservoirs in the world (LUCAS; WENDLAND, 2016; COSTA et al., 2019). The values assigned to the SDR model parameters ($k = 0.8$ and $IC0 = 0.45$) also reflect the basin’s environmental characteristics, characterizing environments with low potential for sediment transport, although their soils are highly susceptible to erosion (COSTA et al., 2018; ANJINHO et al., 2021). The NDR model-TP was the only one in which the default value of the calibration parameter was maintained ($k = 2$), although the transport of nutrients was reduced through the critical flow length parameter.

3.4.3. InVEST WES model potentials and limitations

InVEST’s WES models present simple approaches and demand few input data compared to other physical-based hydrological models, such as SWAT. These characteristics facilitate decision-making in non-instrumented basins or regions where data is scarce, as demonstrated by Benra et al. (2021) and corroborated by this study. InVEST’s WES models enable spatial understanding since they are distributed at pixel scale, and the WES value in each pixel varies depending on its location, considering such key factors as land use, vegetation, relief, and soil types, which remain a major challenge for ecohydrological models (BROOKS et al., 2015; FAN et al., 2019). Such characteristics make these models important tools for environmental planning, enabling an analysis of the effects of diverse future scenarios, such as climate and land-use changes, the primary drivers of WES degradation (BUCAK et al., 2018; BAI et al., 2019). While WES model performance differs for each model and temporal and spatial scale, in general, the study results indicate the models’ capacity to represent long-term average values, and, in the case of the SWY model, to simulate annual average values, enabling a representation of the variability of extreme annual values (see 1983 in Figure 4).

Like any other model, InVEST’s WES models have advantages and limitations. Accordingly, further research to enhance them and increase their transparency is in order. As noted in the InVEST manual, the models use simple equations and limited parameters to estimate water ecosystems services (SHARP et al., 2020). An analysis of the results of this study confirm the limitations noted in the InVEST user manual and in other studies (HAMMEL et al., 2015, REDHEAD et al., 2018; SHARP et al., 2020). The principal limitation of the SWY model is its inability to accurately represent water flow, that is, surface runoff and base flow. The discrepancies arise from its simulation of surface runoff, based on an adaptation of the SCS curve number method, which disregards topographical effects, and of base flow, whose simplified routing equations can generate inconsistent results in terms of absolute numbers (SCORDO et al., 2018). It should also be noted the model fails to simulate the annual variability of water yield in the watershed. Although it enables evaluation of the monthly surface runoff, this limits its use to contexts that demand data on a more refined time scale, as in the simulation of reference streamflow to calculate water availability (NEVES et al., 2020).

The effect of simplification is even more significant in the SDR and NDR models, which are even more sensitive to input data. Uncertainties related to input parameters, such as R and K from RUSLE, and export and nutrient retention coefficients can have considerable impact on the models' simulations (HAMMEL et al., 2015; SHARP et al., 2020; HAN et al., 2021). In many regions, there is no information available on these empirically determined parameters, necessitating the use of data from other locations, which may have quite different climatic and hydrogeological characteristics.

Other limitations associated with the generalization of complex physical processes relate to nutrient and sediment dynamics. In the SDR model, sediment yield is solely determined by RUSLE, disregarding such sources as the gully, stream bank, and mass erosion, which are useful in comparing simulations with observations (HAMMEL et al., 2015). The determination of TN and TP loads in the NDR model disregards the cycle of each nutrient, quantifying both loads in the same way through the relationship between land-use and export coefficients, a considerable abstraction given that their environmental dynamics are quite different (WASSEN et al., 2013). Neither the SDR nor NDR model take into account the dynamics of nutrients and sediments in watercourses, assuming that the entire load that enters the watercourses is exported to the watershed. The NDR model does not take into account point loads, which can adversely impact urbanized basins, especially in areas where basic sanitation is deficient. In the basin, for example, where urban areas represent only 4% of the area, points contribute, on average, up to 60% of the total loads.

3.4.4. Potential, uncertainties, and limitations

Unlike most studies that analyzed the spatial performance of InVEST's WES models, considering long-term average values (TERRADO et al., 2014; HAMEL et al., 2015; REDHEAD et al., 2016; REDHEAD et al., 2018; HAMEL et al., 2020; BENRA et al., 2021), this study analyzes their performance, considering WES spatial and temporal variability. Of the studies reviewed, only Lu et al. (2020) analyzed the temporal performance of the SWY model using Pearson's correlation, albeit using a brief historical series of observed flow data. This study uses historic series of land-use and meteorological data measured at monitoring stations to simulate the temporal variability of WES, considering climate and land use, which exert significant influence on WES dynamics in hydrographic basins.

The principal uncertainties pertaining to the study's calibration method pertain to the use of historical series of observed data. The daily and monthly streamflow data, for example, had numerous flaws, and several stations lacked data for the complete series (1981–2019). With regard to TN, TP, and TSS water quality data, it should be noted that CETESB samples are only taken every two months. In addition, many CETESB monitoring stations do not perform streamflow measurements at the points where water quality samples are taken, which makes determining nutrient and sediment loads needed for comparison with model results problematic. An attempt was made to circumvent flow data deficiencies using hydrological regionalization, and the effects of limited annual sampling and, consequently, the seasonality of the water quality data, were reduced by removing outliers (see Section 2.5), since bi-monthly measurements do not represent the annual TN, TP, and TSS averages. Thus, despite strenuous efforts to calibrate and validate the WES models, uncertainties and limitations remain.

In addition to such challenges with observed data, there are uncertainties related to the empirical parameters used in the models. The study sought to use regional data for all parameters, since they best represent the environmental characteristics of the basin studied (see supplementary material). However, for some parameters, such as CN and nutrient retention efficiency coefficients, for example, it was not feasible to use empirical values, which can contribute to uncertainty in model results. For the NDR model, uncertainties include quantification of TN and TP point loads, estimated from on the per capita load of domestic sewage, using export coefficients, population data, and nutrient removal coefficients, and the values are uncertain due to the scarcity of data on basic sanitation in the basin's municipalities.

3.5. Conclusion

This study investigated the performance of InVEST 3.9.0 WES models, analyzing their ability to represent the spatial and temporal variability of observed values. The results show a high variability in their performances, according to the type of water ecosystem services simulated and scales of analysis. The best performance was observed for the SWY model, which effectively represented the spatial and temporal variability of the average annual streamflow in the analyzed sub-basins. The SDR and NDR models were unable to represent the temporal variability of the exported loads of sediments and nutrients. The inferior performance of these models may be associated with lower sensitivity to precipitation variability. The NDR model, in particular, appears insensitive to annual variations in precipitation, which impact the annual load of nutrients exported in the basin.

The spatial performance considering specific WES values was low for most statistical indicators. In general, with the exception of some sub-basins, all models showed good performance in simulating long-term mean values, which corroborates the results of other studies.

Properly calibrating models' parameters is essential to enhancing their performance, and the values the study assigned to them reflected the basin's hydrogeological characteristics. Uncertainties regarding the methodology used for calibration and validation relate to the quality of the historical series of observed data of daily and monthly streamflow and inadequate water quality sampling data, as well as the failure to measure streamflow data. While the study attempted to circumvent such obstacles, uncertainties remain, and the results should be interpreted with circumspection. Furthermore, some findings may be solely empirical, as the study area lacks broad hydrogeological variability.

Despite the uncertainties and empirical nature of this study, its results and discussions should aid researchers and other users of InVEST models to inform and make decisions and formulate policies. To minimize uncertainties and enhance results, the use of the complete historical series of streamflow and, particularly of water quality parameters is recommended to better reflect the basin's hydrological characteristics and correspond to simulated data. In as much as the performance of the models may vary according to the hydrogeological nature of the region in which they are being applied, further research in varied basins in diverse regions should be conducted to complement the findings detailed herein.

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3.7. APPENDIX A - Supplementary information

The biophysical data to run the WES models are presented in tables S 3.1 and S 3.2.

Table 3.1. Biophysical table for the SWY model.

Land use	Monthly kc values												CN values by hydrological group			
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**A**	**B**	**D**	**D**
Forest Formation	1	1	1	1	1	1	1	1	1	1	1	1	36	60	73	79
Forest Plantation	1	1	1	1	1	1	1	1	1	1	1	1	36	60	73	79
Grassland	0.85	0.85	0.85	0.85	0.85	0.85	0.85	0.85	0.85	0.85	0.85	0.85	39	61	74	80
Mosaic of Agriculture and Pasture	0.8	0.8	0.8	0.8	0.8	0.8	0.8	0.8	0.8	0.8	0.8	0.8	67	78	85	89
Other non Forest Formations	0.85	0.85	0.85	0.85	0.85	0.85	0.85	0.85	0.85	0.85	0.85	0.85	39	61	74	80
Other Non Vegetated Areas	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	77	86	91	94
Other Temporary Crops	0.8	0.8	0.8	0.8	0.8	0.8	0.8	0.8	0.8	0.8	0.8	0.8	67	78	85	89
Pasture	0.75	0.75	0.75	0.75	0.75	0.75	0.75	0.75	0.75	0.75	0.75	0.75	49	69	79	84
Perennial Crop	0.69	0.69	0.69	0.5	0.5	0.29	0.29	0.29	0.5	0.69	0.69	0.69	65	75	82	86
River, Lake and Ocean	1	1	1	1	1	1	1	1	1	1	1	1	99	99	99	99
Savanna Formation	0.9	0.9	0.9	0.9	0.9	0.9	0.9	0.9	0.9	0.9	0.9	0.9	39	61	74	80
Soy bean	0.83	0.83	0.83	0.83	0.83	0.83	0.83	0.83	0.83	0.83	0.83	0.83	64	72	79	81
Sugar Cane	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.16	64	72	79	81
Urban Infrastructure	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	98	98	98	98

References to kc values: Allen et al. (1998), Marin and Angelocci (2011), Redhead et al. (2016) e Marin et al. (2019).

References to CN values: USDA (1986)

Table S 3.2. Biophysical tables for SDR and NDR models.

Land use	usle_c	usle_p	LULC_veg	load_p	load_n	eff_p	eff_n	crit_len_p	crit_len_n
Forest Formation	0.0004	0.8	1	0.93	14.6	0.85	0.85	30	30
Forest Plantation	0.047	1	1	0.47	7.3	0.7	0.7	30	30
Grassland	0.01	0.8	1	0.25	4.58	0.6	0.6	30	30
Mosaic of Agriculture and Pasture	0.05	0.5	1	0.36	6.58	0.5	0.5	30	30
Other non Forest Formations	0.02	0.8	1	0.25	4.58	0.6	0.6	30	30
Other Non Vegetated Areas	1	1	0	0.13	4.89	0.05	0.05	30	30
Other Temporary Crops	0.11	0.5	1	1.68	14.36	0.25	0.25	30	30
Pasture	0.05	0.5	1	0.36	6.58	0.5	0.5	30	30
Perennial Crop	0.135	0.5	1	1.68	14.36	0.25	0.25	30	30
River, Lake and Ocean	0	0	0	0	0	0.01	0.01	30	30
Savanna Formation	0.01	0.8	1	0.4	7.32	0.75	0.75	30	30
Soy bean	0.1437	0.5	1	1.68	14.36	0.25	0.25	30	30
Sugar Cane	0.1124	0.5	1	1.68	14.36	0.25	0.25	30	30
Urban Infrastructure	0.02	1	0	0.12	4.7	0.01	0.01	30	30

References to USLE C factor: Berto et al. (2001), Oliveira et al. (2015), Silva et al. (2015), Batista et al. (2017) e Gomes et al. (2019).

References to USLE P fator: Bertoni na Lombardi Neto (1990) e Cunha et al. (2017).

References for TN and TP loads: SMA (2010).

References to eff_n e eff_p: Resende et al. (2019), Bai et al (2019), Maranhães et al (2016).

References to cri_len: empirically determined value.

Evapotranspiration was determined using the Camargo method (Camargo et al., 1999), following the equation:

$$ET_0 = K \times Q_0 \times T_{ef} \quad \text{(S 3.1)}$$

Where ETo is the potential evapotranspiration in mm day^{-1}, Q_o is the extraterrestrial incident solar radiation in mm day^{-1}, T_{ef} is the effective average daily temperature in °C (Tef = 0.36 (3 Tmax – Tmin)), K is the adjustment factor, 0.01, for Ta (average annual temperature) up to 23.5 °C.

The rainfall erosivity factor (R) was calculated using equation S 3.2, which was proposed to the Campinas region by Lombardi Neto e Moldenhauer (1992). This is local is the closest to the study area. The annual erosivity factor (R) is the sum of the monthly values of the erosion index (EI).

$$EI = 68{,}730 \times \left(\frac{p^2}{P}\right)^{0{,}841} \quad \text{(S 3.2)}$$

Where EI is the average monthly EI ($MJ \cdot mm \cdot ha^{-1} \cdot h^{-1}$), p is the monthly average rainfall (mm) and P is the annual average rainfall (mm).

The soil erodibility factor (K) was determined based on the study by Manningel et al. (2002), in which the authors determined the K values to the state of Sao Paulo soils.

The LS factor was calculated using the Desmet and Govers (1996) method for two-dimensional surfaces, as described by equation S 3.3

$$LS_i = S_i \frac{(A_{i-in} + D^2)^{m+1} - A_{i-in}^{m+1}}{D^{m+2} \times x_i^m \times (22{,}33)^m} \quad \text{(S 3.3)}$$

Where Si is the slope factor for the pixel i, $A_{i\text{-}in}$ is the contributing area (m²) at the inlet of a grid cell which is computed from the Multiple-Flow Direction method, D is the grid cell linear dimension (m), m is the RUSLE length exponent factor, and x_i is the mean of aspect weighted by proportional outflow from grid cell determined by a Multiple-Flow Direction algorithm.

The nutrient loads associated with each land use class were corrected using Equation S 3.4.

$$\text{Load to land} = \frac{\text{Export from land}}{1 - \text{retention efficiency}} \tag{S 3.4}$$

The point loads of TN and TP were quantified based on the per capita production of domestic sewage, according to the export coefficients established by MQUAL 1.5 (TN = 2.41 kg person^{-1} and TP = 0.29 kg person^{-1}). Population data from the SIDRA IBGE database were used to determine nutrient loads. Population projections (Equation S 3.5) were performed to fill in the historical data series (1990 – 2019). Removal coefficients were considered for attenuation of nutrient loads (VON SPERLING, 2005), which varies according to each treatment system located in the BHJG.

$$P_t = P_0 + k_a \,.\, (t - t_0) \tag{S 3.5}$$

Where, P_t is the estimated population at time t, P_0 is the population at time t_0 and k_a is the population growth rate ($dp/dt = k_a$).

Chapter 4

ENHANCING WATER ECOSYSTEM SERVICES USING ENVIRONMENTAL ZONING IN LAND USE PLANNING

A version of this chapter is under review in the SustainabilityJournal.

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ABSTRACT

Land use and land cover (LULC) changes alter the structure and functioning of natural ecosystems, impacting the potential and flow of ecosystem services. Ecological restoration projects aiming to enhance native vegetation have proven effective in mitigating the impacts of LULC changes on ecosystem services. A key element in implementing these projects has been to identify priority areas for restoration, considering that resources allocated to such projects are often limited. This study proposes a novel methodological framework to identify priority areas for restoration and guide LULC planning to increase the provision of water ecosystem services (WES) in a watershed in southeastern Brazil. For doing so, biophysical models and multicriteria analysis were combined to identify priority areas for ecological restoration, propose environmental zoning for the study area, and quantify the effects of LULC changes and of a planned LULC scenario (implemented environmental zoning) on WES indicators. Previous LULC changes from 1985 to 2019 have resulted in a nearly 20% increase in annual surface runoff, a 50% increase in sediment export, a 22% increase in total nitrogen (TN) export, and a 53% increase in total phosphorus (TP) export. Simultaneously, they reduced the provision of WES (baseflow -27%, TN retention -10%, TP retention -16%), except for sediment retention, which increased by 35% during the analyzed period. The planned LULC scenario was successful in increasing the provision of WES while reducing surface runoff and nutrient and sediment exports. The methodology employed in this study proved to be effective in guiding LULC planning for improving WES. The obtained

results provide a scientific foundation for guiding the implementation of WES conservation policies in the studied watershed. This method is perceived as applicable at other watersheds.

Keywords: Water management. Ecological restoration. Land use and land cover. Modelling. InVEST model.

4.1. Introduction

LULC changes impact the ecohydrological processes responsible for maintaining the planet's major biogeochemical cycles, which, in turn, affect WES (ELLISON et al., 2017; SUN et al., 2017). Vegetation influences water and energy flows due to the capacity of different plant species to capture and redistribute energy and water in the environment (ELLISON et al., 2017). Therefore, nutrient and sediment cycles are also affected as they are inherently connected to the hydrological and energy cycles (MANZONI; PORPORATO, 2011; GAO et al., 2013). In addition to the direct impacts on habitats and biodiversity (PEREIRA, 2020), studies have shown that LULC changes can affect the WES (YOHANNES et al., 2021), including water yield (HU et al., 2021; DANESHI et al., 2021; GUO et al., 2023; WANG et al., 2023), water purification, erosion control, and flood regulation (UWIMANA et al., 2018; YANG et al., 2018; LEI et al., 2021; BENDITO et al., 2023). Although LULC may enhance the supply of some ecosystem services, such as food and timber, the degradation of these WES may impact human well-being and public health in the long term, causing water scarcity for human consumption, irrigation losses, and energy generation-related issues (BRAUMAN et al., 2007; GRIZZETTI et al., 2016). These issues are strategic factors for water and energy security. Thus, understanding the effects of different LULCs on WES is crucial for the development of watershed planning and management policies.

Ecological restoration projects are being developed and implemented worldwide with the purpose of increasing ecosystem resilience, the provision of ecosystem services, and promoting biodiversity conservation (BENAYAS et al., 2009; SHIMAMOTO et al., 2018; FIEDLER et al., 2021; CARDOSO et al., 2022; LI et al., 2023). Initiatives such as the Bonn Challenge (DAVE et al., 2019) and 1t.org (https://www.1t.org/) aim to restore millions of hectares of land by 2030. Ecological restoration is a practice that seeks to recover degraded or destroyed ecosystems, restoring their structure and ecosystem processes (TAMBOSI et al., 2015). Evidence shows that ecological restoration using native vegetation can have significant benefits in regulating water flows, reducing floods, and stabilizing water flow during dry periods (CALDER; AYLWARD, 2009; LARA et al., 2021; SERRA-LLOBET et al., 2022). Furthermore, ecological restoration contributes to improve soil and water quality, reducing erosion processes, and retaining sediments and nutrients flowing from the upstream areas of watersheds (FELD et al., 2018; SHIMAMOTO et al., 2018; QI et al., 2019; HUA et al., 2022).

Although essential for environmental conservation, ecological restoration aimed at improving WES must be properly planned and executed. Resources for projects of this nature are often scarce, thus requiring the identification of priority areas for restoration and efficient allocation of resources (DUARTE et al., 2016; VALENTE et al., 2021; ZHU et al., 2022). One way to identify priority areas for restoration is through effective environmental zoning methods that consider the characteristics and potential of the territory (SANTOS et al., 2021). Environmental zoning is a LULC planning tool that aims to promote sustainable territorial management, taking into account environmental and socioeconomic criteria (ANJINHO et al., 2022a). It can be applied at various territorial scales, including countries, states, municipalities, and watersheds. The adoption of guidelines for territorial management is crucial for the conservation of WES.

Many studies have been conducted to identify priority areas for the conservation and restoration of ecosystem services (DUARTE et al., 2016; COSTA et al., 2021; SILVA et al., 2023; ZHOU et al., 2023). In the context of WES, a part of the literature highlights the potential of multicriteria analysis to identify priority areas for forest restoration, aiming to increase the provision of these services. Valente et al. (2021) developed a decision support model based on multicriteria analysis to identify priority zones for forest restoration in the context of WES, adopting five criteria that were analyzed by experts through participatory techniques. Anjinho et al. (2022a) used multicriteria analysis and on-site assessment to develop an environmental zoning methodology aimed at increasing the provision of WES. Other studies have used biophysical models of ecosystem services, along with spatial analysis tools, to identify priority areas for ecological conservation and restoration (PENG et al., 2019; FAN et al., 2022; ZHU et al., 2022; POSSANTTI et al., 2023). The use of biophysical models, such as those available in the Integrated Valuation of Ecosystem Services and Tradeoffs (InVEST), is crucial for environmental zoning analyses as they allow for the quantification of the biophysical value of WES, identification of areas with higher service provision, as well as those with higher potential for degradation (WANG et al., 2022). Moreover, biophysical models enable the simulation of future scenarios and the identification of those that provide benefits to ecosystems and their associated services.

Despite the global relevance of ecological restoration practices in mitigating the impacts of human activities and climate change (CAPON et al., 2013; MELILLO et al., 2016), it is frequently not clear which ecological restoration strategy provides the greatest benefits for ecosystem services and habitats for biodiversity. This can be justified due to variations of the ecohydrological functions of native vegetation according to their composition and configuration in the landscape (FERRAZ et al., 2014; CUNHA et al., 2019; CAMPANHÃO et al., 2022), and the optimal strategy may vary depending on the specificities of each region and of the pressures felt therein. Some studies have used biophysical models to select priority areas for restoration (PENG et al., 2019; FAN et al., 2022; ZHU et al., 2022; POSSANTTI et al., 2023). The outcomes may allow deriving policy recommendations tailored to needs and draw efficient spatial development.

This study aims to enhance the provision of WES within a watershed located in southeastern Brazil providing evidence-based knowledge for the implementation of optimal ecological restoration strategies. The study explores the hypothesis that increasing green areas in strategic locations within the watershed can enhance the provision of WES and reduce surface runoff and nutrient and sediment exports. In doing so, a novel methodological framework is developed, combining multicriteria analysis and biophysical models to conduct environmental zoning and implement a planned LULC scenario of increasing the native vegetation areas in the studied watershed. Specific objectives of this work are: i) to quantify the LULC changes between 1985 and 2019; ii) to quantify the effects of LULC changes on eight indicators associated with WES: surface runoff, sediment export, nutrient export, sediment retention (erosion control services), nutrient retention (water purification), and baseflow (water supply); iii) to map the potential levels of WES degradation; iv) to propose an environmental zoning that promotes the increase of WES; and v) to evaluate the effects of a planned LULC scenario on indicators of WES.

4.2. Methodology

To meet the objectives of this study, a robust methodological framework that couples biophysical models and multicriteria analysis was developed. The LULC changes were analyzed within a Geographic Information System (GIS), using data from the Brazilian Annual Land Use and Coverage Mapping Project (5th collection) (MAPBIOMAS, 2021) for the years 1985 and 2019.

Biophysical models from the InVEST 3.12.0 package (NATURAL CAPITAL PROJECT, 2022) were used to quantify the indicators of surface runoff, sediment export, TN export, TP export, baseflow, sediment retention, TN retention, and TP retention, being the last four indicators direct of services of erosion control, water purification, and water supply. Therefore, this study considers only the last four as indicators of WES. As one of the objectives of this study was to quantify the effects of previous LULC changes on WES, LULC data from 1985 and 2019 were used as inputs in the biophysical models. For inputs that utilize meteorological data, such as precipitation, evapotranspiration, rain events, erosivity, and nutrient runoff proxy, long-term average values (1981 to 2019) were used for both years.

Multicriteria analysis was used to map the potential levels of WES degradation, using the outputs of InVEST's biophysical models. Then, environmental zoning was proposed for the study area, based on the integration of maps with levels of potential levels of WES degradation and of the LULC of 2019. The last step was to build a planned LULC scenario for the study area based on the proposed environmental zoning and evaluate its effects on the eight indicators used in this study, using the LULC configuration scenario as input on the biophysical models from InVEST. A detailed description of each methodological step is presented in the following subsections.

4.2.1. Study area

The Jacaré-Guaçu River Basin (JGRB) is located in the central-eastern region of the state of São Paulo, southeastern Brazil, and is part of Water Resources Management Unit number 13 (UGRHI 13), known as the Tietê Jacaré Basin (Figure 4.1) With a drainage area of approximately 4,172.12 km^2, the JGRB is composed of watercourses of different orders that contribute to the formation of the Jacaré-Guaçu River, which is the main watercourse of the JGRB and one of the surface water supply sources of UGRHI 13 (CBH-TJ, 2016). The region is characterized by flat relief, composed of smoothly undulating hills (around 80%), resulting from weathering of the Botucatu and Pirambóia formations, with low drainage density (ANJINHO et al., 2022b). The altitude of the watershed ranges from 372.0 m to 1,024.0 m above sea level. The soils in the region are predominantly sandy, with emphasis on the Latosols that cover 60% of the area (ROSSI; KANASHIRO, 2017). The climate of the region falls within the CWA and CWB climatic zones, characterized by dry winters and wet summers (PEEL et al., 2007). The JGRB is located in a transitional area between the Cerrado and Atlantic Forest biomes, mainly featuring Seasonal Semideciduous Forest and Savanna vegetation types (CBH-TJ, 2016).

JGRB represents an adequate case study since its water resources, such as rivers, streams, reservoirs, and groundwater, are essential for serving multiple water uses that are important for regional socio-economic development (CBH-TJ, 2016). Additionally, the area is environmentally significant due to the presence of important ecosystems for biodiversity conservation, such as remnants of Cerrado and Atlantic Forest (IF, 2006; SANTOS et al., 2023). Over the years, there has been an intense transformation of LULC in the watershed, resulting in the decline of natural ecosystems and the expansion of agricultural areas (TREVISAN et al., 2021). These LULC changes have affected the hydro-sedimentology of the watershed, altering the flows of water, nutrients, and sediments (SANTOS et al., 2018; ANACHE et al., 2019; ANJINHO et al., 2021a), while increasing the risk of degradation of water resources, including underground aquifers (COSTA et al., 2019).

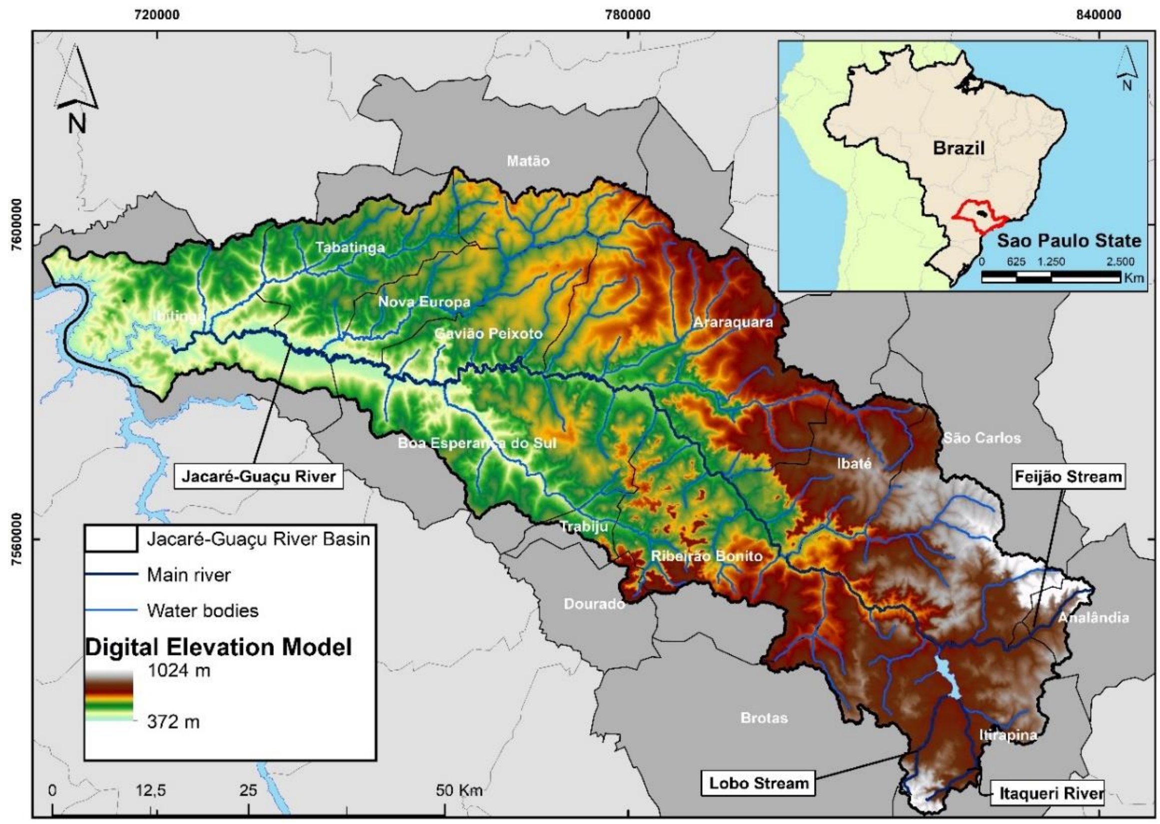

Figure 4.1. Location of Jacaré-Guaçu River Basin with Digital Elevation Model.

4.2.2. Analysis of land use and land cover changes

Data from the MAPBIOMAS project were used to characterize the LULC of JGRB. In total, thirteen LULC classes were identified: i) sugarcane; ii) planted forest; iii) grassland; iv) forest; v) savanna; vi) urban infrastructure; vii) perennial crops; viii) agriculture-pasture mosaic; ix) other non-forest natural formations; x) other temporary crops; xi) pasture; xii) river, lake and ocean; and xiii) soybean. However, for result visualization, the thirteen LULC classes were regrouped into six categories: i) agriculture (sugarcane, perennial crops, other temporary crops, and soybean), ii) water (river, lake, and ocean), iii) urban area (urban infrastructure), iv) planted forest (planted forest), v) pasture (pasture and agriculture-pasture mosaic), and vi) natural vegetation (grassland, forest, savanna, other non-forest natural formations).

The LULC transition matrix was used to quantify the changes that occurred between 1985 and 2019. This method allows for determining the quantity and direction of LULC changes, highlighting both the modified areas and the classes that remained unchanged during the analyzed period.

4.2.3. Biophysical modelling and quantification of the effects of land use and land cover

The InVEST biophysical models were run for the years 1985 and 2019, using previously calibrated parameters from the study conducted by Anjinho et al. (2022b). The parameters of the models were calibrated and validated on an annual scale using data on streamflow (39 years) and concentration of TN, TP (29 years), and total suspended solids (19 years) obtained from the Water and Sanitation Agency, Department of Water and Energy of the State of São Paulo, and Environmental Company of the State of São Paulo. The technical description of the models and the input data used can be found in Anjinho et al. (2022b).

The Seasonal Water Yield (SWY) model was used to quantify the annual surface runoff (QF) and baseflow (BF) of JGRB. QF is calculated using a modified approach of the curve number method from the Natural Resources Conservation Service (NRCS) (NRCS, 1996), while BF is estimated based on local recharge values, which are determined from the local water balance between precipitation, QF, and evapotranspiration. JGRB's annual precipitation was generated based on data from rainfall monitoring stations. Evapotranspiration was calculated using meteorological data from a climatological station at the Center for Water Resources and Environmental Studies, University of São Paulo, using the method by Camargo et al. (1999). QF was calculated using the adapted SCS method (NATURAL CAPITAL PROJECT, 2022). More information about the models can be found in Anjinho et al. (2022b).

The Sediment Delivery Ratio (SDR) model was used to quantify the export and retention of sediment in JGRB. The model is based on the Revised Universal Soil Loss Equation (RUSLE) and the SDR parameter to quantify the export and retention of sediment in each pixel of the watershed. The export of sediment represents the amount of sediment eroded in the pixels that effectively reach the watercourse, calculated by summing the product of production (RUSLE) and SDR. As suggested in the user manual (NATURAL CAPITAL PROJECT, 2022), the "Avoided export" model output was used as a proxy to quantify the sediment retention service in the watershed.

The Nutrient Delivery Ratio (NDR) model was used to quantify the export and retention of total nitrogen (TN) and total phosphorus (TP) in the study area. This model uses a simplified mass balance to map nutrient loads, without considering the nutrient cycle in detail as more complex models do. Similar to the SDR model, nutrient export in the NDR model is quantified by summing the product of nutrient loads in each pixel and their respective nutrient delivery ratio (NDR) values. The loads are quantified using average TN and TP export coefficients that vary according to the LULC in the watershed. The nutrient retention service was estimated by comparing nutrient exports from a hypothetical scenario (where all LULCs in the watershed were converted to agriculture) with the actual LULC conditions of 1985 and 2019, as suggested in the model manual (NATURAL CAPITAL PROJECT, 2022). The agricultural scenario was selected because it represents the LULC class with the highest TN and TP export coefficient values (SMA, 2010). The difference in nutrient exports between the agricultural scenario and the years 1985 and 2019 reflects the amount of nutrients that theoretically are not exported due to the analyzed LULC configuration.

The effects of LULC types on QF, sediment export, nutrient export, and WES were analyzed using the average values of these indicators for each LULC class, after being normalized on a scale from 0 to 1 using linear fuzzy logic (MARRO et al., 2010). The main objective of this analysis is to quantify the influence of each LULC type on these indicators.

4.2.4. Multicriteria and spatial analysis for the proposition of environmental zoning

Environmental zoning aiming to increase the provision of WES was developed through spatial analysis between potential levels of WES degradation and LULC in 2019, following a similar approach to the study by Anjinho et al. (2022a). To determine the potential levels of WES degradation, annual data for QF and annual exports of TN, TP, and sediments simulated for the year 2019 were considered. Areas with high degradation potential under anthropic influence (agriculture, planted forests, and pastures) were classified as priority areas for ecological restoration (Table 4.1). The restoration of these areas aims to reduce surface runoff, nutrient, and sediment export, and increase the provision of WES. Low and medium potential areas that are also under anthropic influence were designated as anthropic use zones (Table 4.1). These areas generally contribute little to surface runoff and nutrient/sediment export, making them suitable for human development. Urban areas were classified as consolidated use zones, considering the challenges of managing urban environments at a landscape scale (Table 4.1). The natural areas within the JGRB, including riparian forests, wetlands, Brazilian Cerrado, and Atlantic Forest, are crucial for conserving biodiversity and ecosystem services in the region (IF, 2006; SANTOS et al., 2023). Therefore, in environmental zoning, all natural areas, regardless of their potential level, have been categorized as conservation priorities (Table 4.1).

The study assumes that areas with higher runoff and export of sediments and nutrients tend to degrade the aquatic ecosystems. Nutrient enrichment leads to the eutrophication of aquatic ecosystems (LE MOAL et al., 2019; VIRIES, 2021), and increased erosion and sediment transport in the watershed can alter the natural characteristics of water bodies, pollute the waters due to the presence of pollutants adsorbed to the sediment, and contribute to the sedimentation of hydroelectric reservoirs (MIRANDA et al., 2014; ESTIGONI et al., 2017; MARTINEZ et al., 2023). Runoff was also included in this analysis because areas with higher runoff generation have the potential to increase soil erosion and, consequently, sediment and nutrient transport, as well as increase the risk of downstream flooding (DAS, 2019; DU et al., 2022; WANG et al., 2022).

The annual values of these three indicators were standardized on a scale of 0 to 1 using linear fuzzy logic (MARRO et al., 2010), and then a weighted linear combination was performed in a GIS to aggregate the three indicators, resulting in the map of potential WES degradation levels. An equal weight of 1 was assigned to the three indicators in the weighted linear combination. Subsequently, the values were reclassified into three classes: low, medium, and high.

Table 4.1. Criteria used for the development of environmental zoning.

Potential degradation levels	Land use and land cover	Environmental zoning
High	Anthropic use	Priority areas for restoration
low, and medium	Anthropic use	Anthropic use zone
Any potential degradation levels	Urban areas	Consolidated zone
Any potential degradation levels	Natural vegetation	Environmental conservation zone

4.2.5. Land use and land cover scenario building and quantification of its effects on biophysical indicators

The biophysical models from the InVEST 3.12.0 package (NATURAL CAPITAL PROJECT, 2022) were run again to assess the effects of the planned LULC scenario on QF, sediment and nutrient exports, and WES of JGRB. This scenario was developed based on the assumption that areas identified as priorities for ecological restoration were effectively restored. To achieve this, the 2019 LULC data and the proposed environmental zoning were spatially integrated on GIS. LULCs that coincided with priority areas for restoration were changed to equivalent natural vegetation, which includes Brazilian Cerrado and Atlantic Forest vegetation. The results were compared to the 2019 LULC values to quantify the effect of the changes.

4.3. Results

4.3.1. Land use and land cover changes between 1985 and 2019

The analysis of LULC dynamics revealed a change in landscape pattern between 1985 and 2019 (Figure 4.2). Agriculture was the main driver of change in JGRB, experiencing a growth of nearly 120% during the period (changes in terms of area (km²) can be viewed in Table S 4.1 in Appendix B). This expansion occurred mainly in areas that were previously designated as pastureland, and to a lesser extent, natural vegetation (Table S 4.2 in appendix B). Agriculture became the dominant LULC in JGRB in 2019, covering over 50% of its Area. Large percentage increases in urban areas and planted forests were also observed, although smaller in comparison to agriculture when analyzed in terms of area (km²). Urban expansion occurred primarily over pastureland, while planted forests occupied a larger proportion of areas that were previously covered by natural vegetation (Table S 4.2 in Appendix B). Despite their low representation in JGRB, it is important to highlight that urban areas and planted forests were the LULC types that exhibited the highest percentage growth during the analyzed period, with increases of 285% and 147% respectively.

In 1985, pastureland was the predominant LULC in JGRB and was distributed throughout its extent (Figure 4.2). Natural areas, represented by Atlantic Forest formations, Brazilian Cerrado grasslands, and savannas, were located near the headwaters of the Jacaré-Guaçú River and along the riverine regions, as well as in the form of small fragments within JGRB. Crops were situated along the right bank of the Jacaré-Guaçu River, occupying nearly a quarter of the watershed. In 2019, the LULC configuration changed. Pastureland is now fragmented in the landscape, while agriculture has the largest continuous areas in JGRB. Natural vegetation is restricted to the riverine regions; planted forests have expanded upstream in the watershed; and urban areas have developed during the analyzed period, increasing in their respective areas.

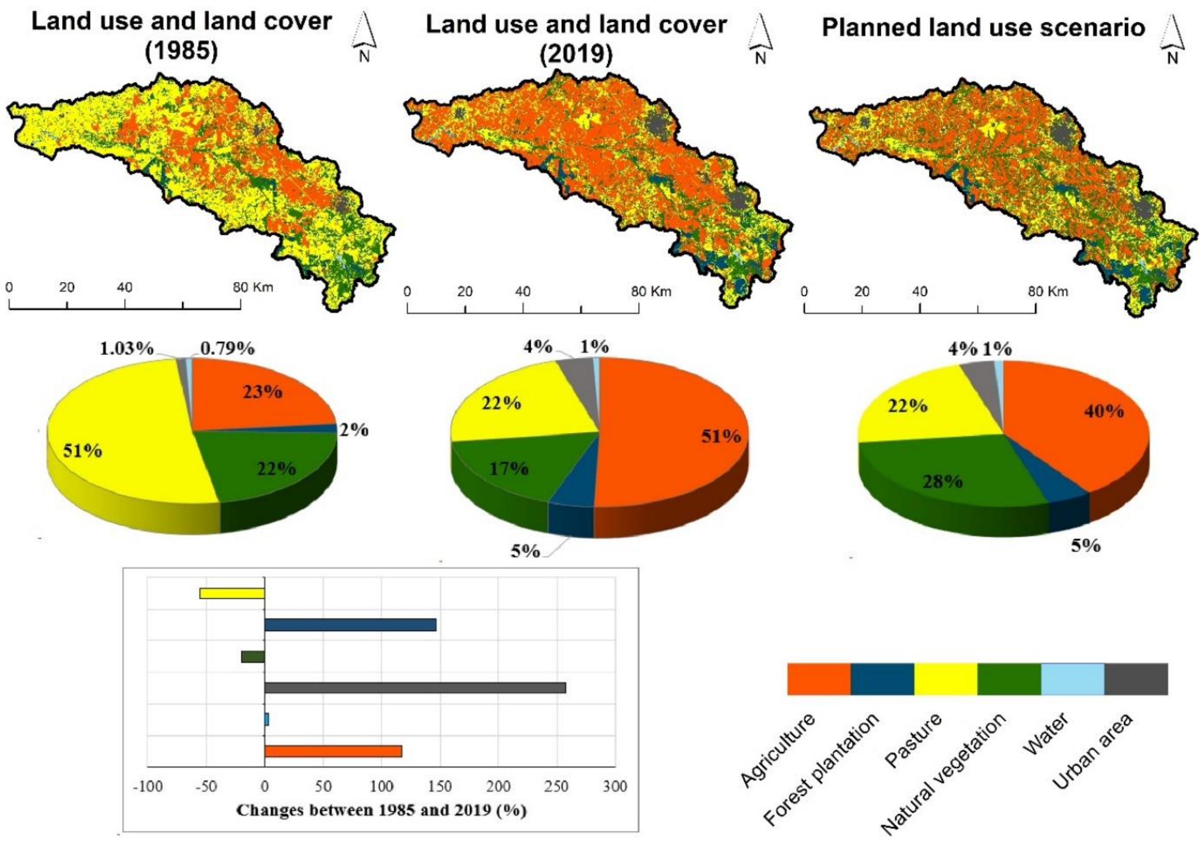

Figure 4.2. Land use and land cover dynamics and planned scenario for Jacaré-Guaçu River Basin.

4.3.2. Changes in surface runoff and exports of sediments and nutrients

The spatial pattern of the QF in the study watershed did not show significant changes between the analyzed years (Figure 4.3 and Fig. S 4.1 in Appendix B), but its average annual value increased by approximately 20% (Table 4.2). The highest percentage increases occurred in pasture and natural vegetation areas, while surface runoff values decreased in agricultural and urban areas. In terms of absolute values, surface runoff was more pronounced in urban areas, particularly where the cities of São Carlos, Araraquara, and Ibitinga are located. Urban areas and water were the LULC types that had the greatest influence on the QF of the watershed (Fig. S 4.2 in Appendix B).

The exported sediment in JGRB increased by approximately 50% between 1985 and 2019 (Table 4.2). The areas that experienced the greatest increases are located near the watercourses of the watershed, with more pronounced effects observed in the municipalities of Boa Esperança do Sul and Ribeirão Bonito, in the central part of the study area. (Figure 4.3). For both years, crops and pastures were the LULC classes that exhibited the highest sediment loads exported and also had the most significant effects (Table 4.2 and Fig. S 4.2 in Appendix B). In 2019, sediment loads exported by these two LULC classes accounted for nearly 95% of the total sediment load exported in JGRB. In terms of percentage, the highest increases during the period were observed in urban areas (2,113.76%) and planted forests (348.75%). However, it is important to note that urban areas exported the lowest sediment loads in both 1985 and 2019.

LULC changes also affected nutrient exports in JGRB. The areas with increased nutrient exports are scattered throughout the watershed, although for TN exports, they are more concentrated near the watercourses compared to TP (Figure 4.3). Despite the significant increase, a decrease in TN exports is observed on the right bank of the Jacaré-Guaçu River, particularly in the northeast region where the municipalities of Araraquara and Ibaté. Urban areas and planted forests showed the highest percentage changes in nutrient exports. In 2019, agricultural areas were responsible for exporting 70% of TN and 87% of TP, significantly influencing nutrient exports (Table 4.2 and Fig. S 4.2 in Appendix B).

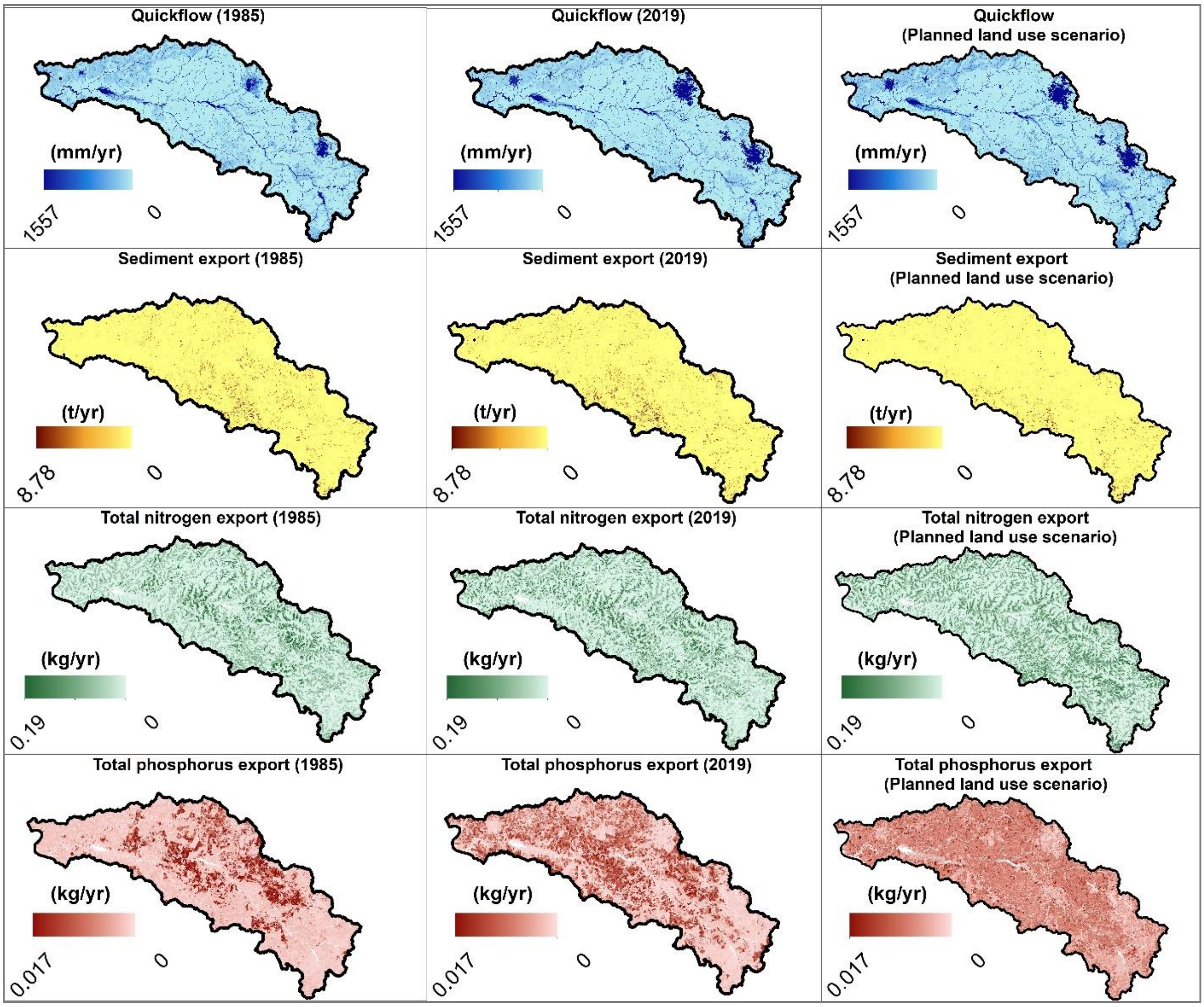

Figure 4.3. Spatial distribution of surface runoff and exports of sediments and nutrients in Jacaré-Guaçu River Basin.

Table 4.2. Simulated values of surface runoff, sediment exports, nutrient exports, baseflow, sediment retention and nutrient retention for 1985 to 2019.

Land use and land cover	**Quickflow (mm. yr^{-1})**			**Sediment export (t. yr^{-1})**			**Total nitrogen export (kg. yr^{-1})**			**Total phosphorus export (kg. yr^{-1})**		
	1985	**2019**	**Changes (%)**	**1985**	**2019**	**Changes (%)**	**1985**	**2019**	**Changes (%)**	**1985**	**2019**	**Changes (%)**
Agriculture	64	54	-16	10,768	27,524	156	225,573	399,446	77	36,811	73,270	99
Water	1,154	1,155	0	0	1	45	63	76	19	4	4	5
Urban area	1,011	1,004	-1	3	66	2,114	2,899	12,525	332	134	535	300
Natural vegetation	169	218	29	575	627	9	62,030	62,815	1.26	4,683	4,019	-14
Forest Plantation	26	28	7	353	1,586	349	2,615	7,505	187	350	1,023	192
Pasture	110	172	56	14,220	9,284	-35	178,233	89,523	-50	13,257	5,839	-56
JGRB	**128**	**154**	**20**	**25,920**	**39,087**	**51**	**471,413**	**571,889**	**21**	**55,239**	**84,690**	**53**
Land use and land cover	**Baseflow (mm. yr^{-1})**			**Sediment retention (t. yr^{-1})**			**Total nitrogen retention (kg. yr^{-1})**			**Total phosphorus retention (kg. yr^{-1})**		
	1985	**2019**	**Changes (%)**	**1985**	**2019**	**Changes (%)**	**1985**	**2019**	**Changes (%)**	**1985**	**2019**	**Changes (%)**
Agriculture	141	138	-3	1,805,134	4,519,504	150	166,773	361,429	117	34,290	77,523	126
Water	12	13	**3**	28,185	57,884	105	204	285	40	27	37	40
Urban area	195	192	-1	590	53,915	9038	1,732	6,799	292	156	533	241
Natural vegetation	219	199	-9	1,893,772	3,004,434	59	354,960	350,281	-1	58,633	47,882	-18
Forest Plantation	253	252	-0	123,829	503,007	306	20,259	51,429	154	5,616	13,840	146
Pasture	373	345	-7	5,174,698	4,031,867	-22	745,857	389,850	-48	140,843	61,892	-56
JGRB	**279**	**202**	**-27**	**9,026,207**	**12,170,611**	**35**	**1,289,786**	**1,160,074**	**-10**	**239,565**	**201,707**	**-16**

4.3.3. Changes in water ecosystem service indicators

The spatial pattern of BF in JGRB has changed over the years (Figure 4.4 and Fig S 4.1 in Appendix B). In 1985, high values, represented by dark blue, were observed in many parts of the watershed. However, in 2019, areas with higher BF values were restricted primarily near the sources of the Jacaré-Guaçu River, where the tributaries Ribeirão do Lobo, Ribeirão da Onça, Ribeirão Feijão, and the Itaqueri River are located, as well as scattered along the floodplain. The BF of the watershed decreased by approximately 30% during the period, with the most significant decreases observed in the natural vegetation and pasture classes (Table 4.2). Despite the decrease in BF value, pasture was the LULC type that had the greatest effect on BF, followed by planted forests (Fig S3 in Appendix B).

The spatial pattern of sediment retention service was similar for the analyzed years (Figure 4.4). Decreases in values were observed in small scattered fragments in JGRB (Fig S 4.1 in Appendix B). Sediment retention increased by 35% between 1985 and 2019 (Table 4.2). The most significant percentage of changes occurred in urban areas and planted forests. However, in absolute terms, the highest amounts of retained sediments in 2019 were found in agricultural areas (37%), pastures (33%), and natural vegetation (25%), which together accounted for 95% of the total sediment retention in JGRB. Natural vegetation and pasture had a greater effect on sediment retention service (Fig S 4.3 in Appendix B).

The nutrient retention service decreased between 1985 and 2019 (Table 4.2). The areas where reductions in TN and TP retention occurred are scattered in small fragments throughout JGRB, but more significantly for TP (Figure 4.4 and Fig S 4.1 in Appendix B). Similar to the sediment retention service, the largest changes were found in urban areas and planted forests. Agriculture, pasture, and natural vegetation are the LULC classes that presented the highest retained loads in 2019. Agriculture retained 31% of TN and 38% of TP, pasture retained 34% of TN and 31% of TP, and natural vegetation retained 30% of TN and 24% of TP. Natural vegetation and pasture had a greater effect on nutrient retention in the watershed. Planted forests also significantly influenced TP retention (Fig S3).

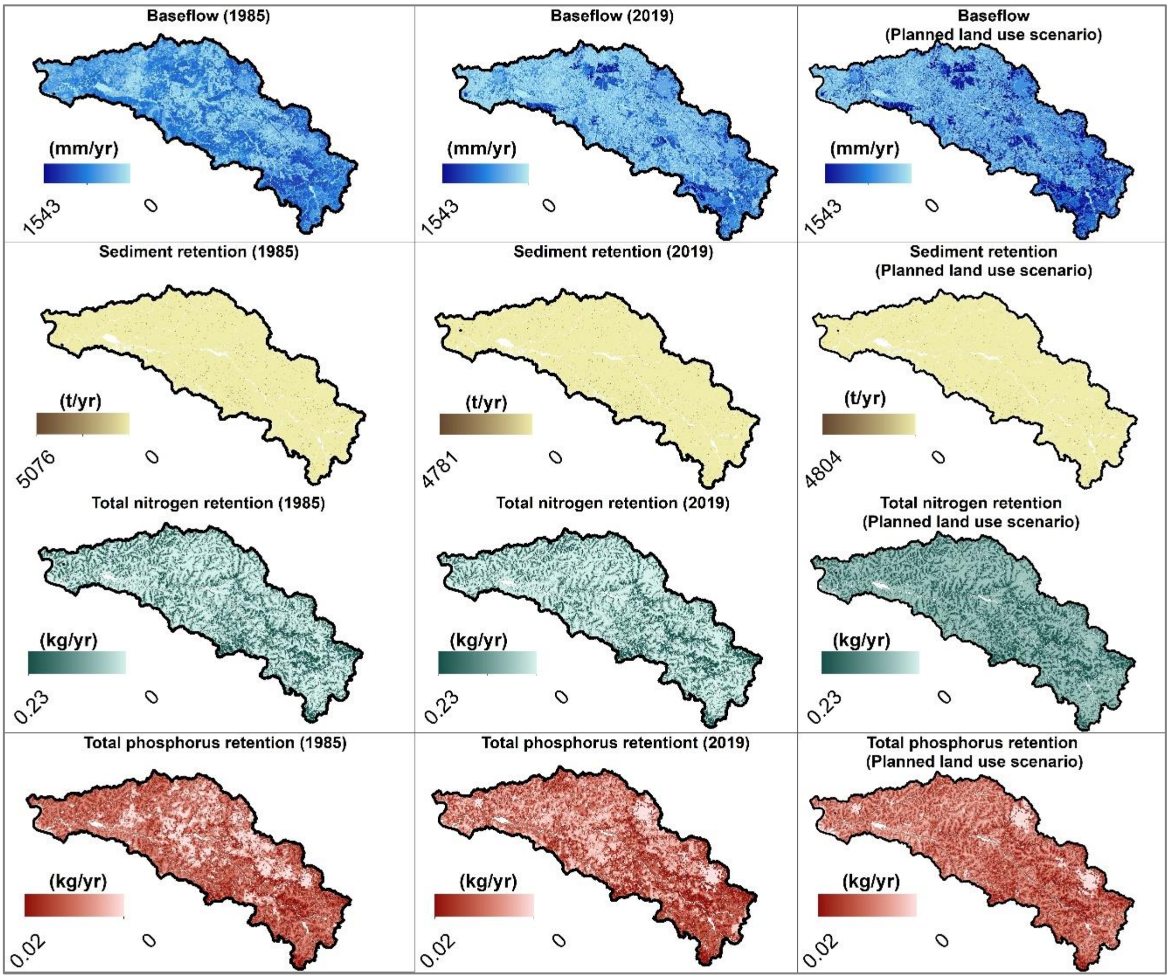

Figure 4.4. Spatial distribution of baseflow and sediment and nutrient retention in the Jacaré-Guaçú River Basin.

4.3.4. Proposal for environmental zoning aiming to increase the provision of water ecosystem services

The potential WES degradation levels and the proposed environmental zoning are presented in Figure 4.5, and the planned LULC scenario, generated based on the proposed environmental zoning, is depicted in Figure 4.2. The areas with the highest potential for WES degradation encompass 13% of JGRB and are fragmented across the landscape, where areas with high surface runoff and export of sediments and nutrients are located. The lowest potential degradation levels are observed upstream of JGRB and in many stretches along the Jacaré-Guaçu River, often associated with riparian forests and wetland areas.

The spatial analysis of potential WES degradation levels and LULC in 2019 resulted in the identification of five use zones, as illustrated in Figure 4.5. The anthropic use zone is the largest, occupying 67% of the area. The second largest zone corresponds to areas designated for environmental conservation, which refers to existing natural vegetation in JGRB. The zone designated for ecological restoration occupies 11% of the area and is concentrated in steeper areas near the watercourses of the watershed. The consolidated use zone refers to urbanized areas where it is not possible to relocate LULC

Based on the analysis of the environmental zoning, a planned LULC scenario was proposed for JGRB (Figure 4.2). Agriculture and natural vegetation are the two LULC classes that changed this new landscape configuration compared to the 2019 data. Agriculture remains the dominant class in the watershed, occupying 40% of the area. Natural vegetation is the second most representative class (28%) and is mainly located upstream of the watershed and near the Jacaré-Guaçu River and its tributaries. The remaining LULC classes did not show changes in their respective areas.

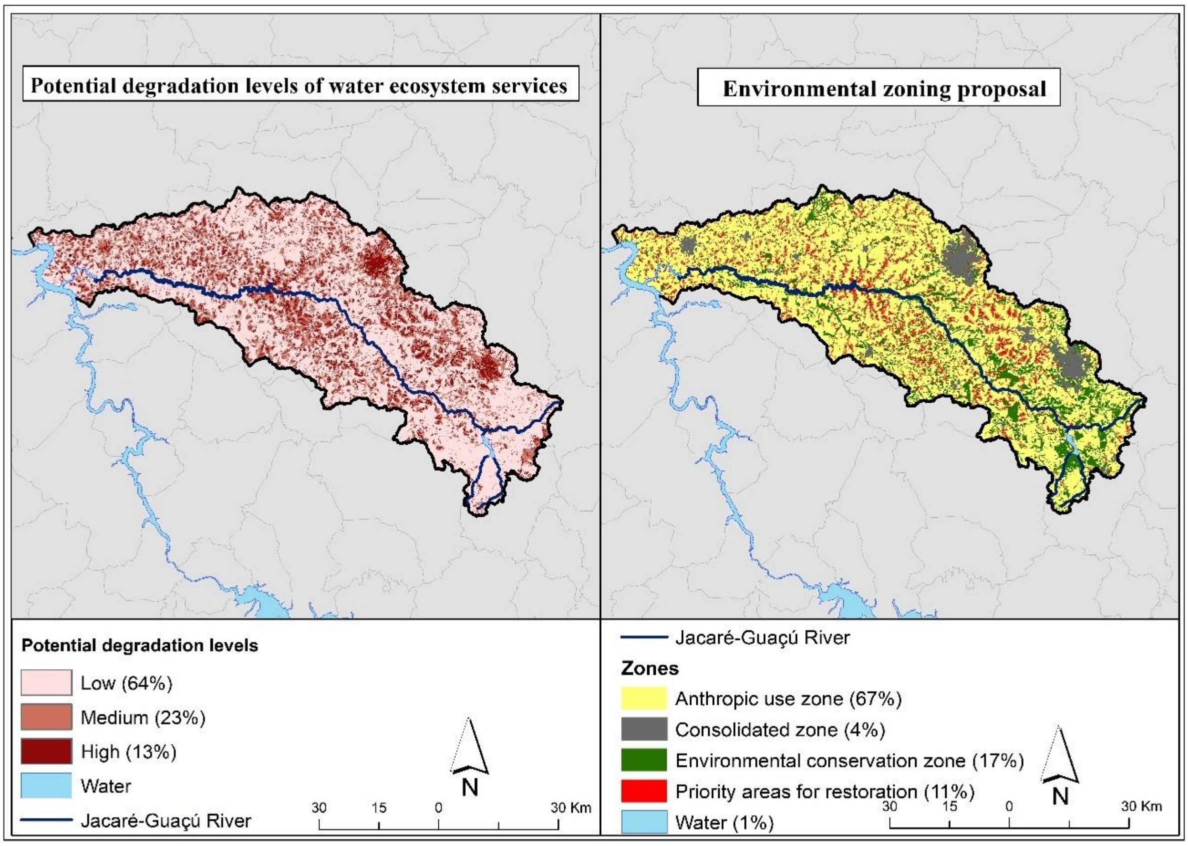

Figure 4.5. Potential degradation levels of water ecosystem services and proposed environmental zoning for the Jacaré-Guaçu River Basin.

4.3.5. Effects of the planned LULC scenario on surface runoff, sediment exports, nutrient exports, and water ecosystem services

The spatial distribution of QF, sediment exports, nutrient exports, and WES for the planned LULC scenario is presented in Figure 4.3 and Figure 4.4 and Table S 4.3 (in Appendix B) shows the simulated values. Overall, when compared to the 2019 LULC, it is observed that the planned LULC scenario resulted in a reduction in QF and sediment and nutrient exports, while also providing increases in BF and nutrient retention services (Figure 4.6). The QF showed a slight reduction of 2% with the changes in LULC. The largest reduction was observed for sediment exports (65%), followed by phosphorus (60%) and nitrogen (49%) exports. On the other hand, BF increased by around 4% and nutrient retention services increased by approximately 25%. The sediment retention service decreased by 27% in the new LULC configuration.

Just like in the years 1985 and 2019, water and urban areas were the LULC classes that most affected the QF of JGRB (Fig. S 4.2 in Appendix B). Pasture and planted forests had a greater effect on sediment exports, with the former also affecting nutrient exports along with natural vegetation. Agriculture had a more pronounced effect on phosphorus exports in the watershed. Regarding the BF, the LULC classes with the greatest influence were pasture and planted forests, while natural vegetation played a more significant role in sediment and nutrient retention (Fig. S 4.3 in Appendix B). Pasture also had a strong influence on sediment and nutrient retention and planted forests played a relevant role in phosphorus retention (Fig. S 4.3 in Appendix B).

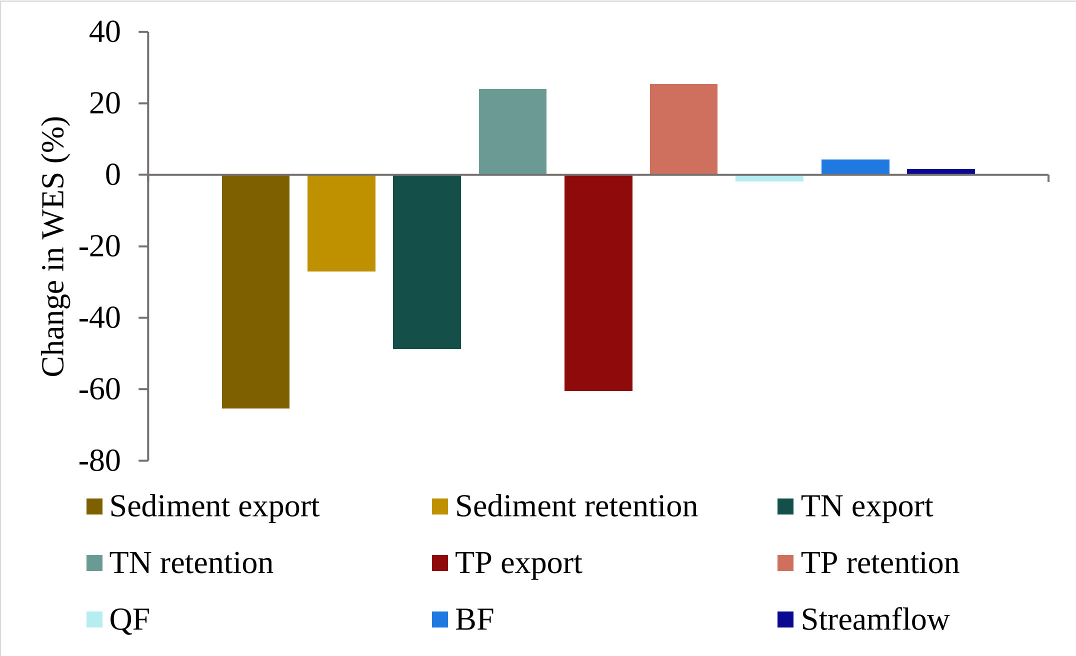

Figure 4.6. Percentage changes in surface runoff, sediment export, nutrient export, baseflow, sediment retention, and nutrient retention between the planned scenario and the 2019 land use and land cover.

4.4. Discussion

4.4.1. Analysis of the effects of LULC changes on surface runoff and the exports of sediments and nutrients

The study results revealed that the LULC pattern in JGRB has changed over the years. The main driver of change has been crops, which have significantly increased in the study area. This growth is associated with the economic model of the state of São Paulo, which has been largely dominated by the sugarcane industry in the past three decades, becoming one of the main agro-industrial centers in Brazil (IEA, 2018). These findings are consistent with other studies that have already indicated the expansion of this crop in the state of São Paulo, particularly over pasture areas (CHERUBIN et al., 2021; BUENO et al., 2022; OGURA et al., 2022). The area of natural vegetation also decreased during the analyzed period due to agricultural and planted forest expansion over areas of Atlantic Forest and Brazilian Cerrado, notably affecting the biodiversity and functions of these ecosystems (HUNKE et al., 2015; MORAES et al., 2017; COUTO-JUNIOR et al., 2019; DURÁN et al., 2020).

LULC changes in JGRB seem to be associated with higher sediment and nutrient exports in the year 2019. Previous studies conducted in the state of São Paulo also found similar results when forests and pastures were replaced by agriculture (TANIWAKI et al., 2017; COUTO-JUNIOR et al., 2019; SANTOS et al., 2020). In the Lobo stream watershed, which is one of the tributaries of the Jacaré Guaçu River, the main watercourse of the JGRB, Anjinho et al. (2021a) observed a greater influence of agriculture on annual nitrogen and phosphorus exports. The model hydrosedimentological established by Santos (2018) indicated higher sediment production during the wet months in a scenario that predicts an increase in urban and agricultural areas upstream of the JGRB. Sediment and nutrient exports were higher in areas with high hydrological connectivity, naturally predisposed to material transport, as predicted by InVEST's SDR models (NATURAL CAPITAL PROJECT, 2022).

Surface runoff proved to be less sensitive to LULC changes, which corroborates the previous model conducted by Santos (2018) that indicated a slight change in average monthly flow with LULC changes in the JGRB. The spatial pattern of the QF barely changed between 1985 and 2019, with small increases observed in urban areas due to soil sealing. Pasture and natural vegetation areas showed increases in average QF values during the analyzed period. With the expansion of sugarcane and other crops until 2019, natural vegetation and pasture became generally limited to regions of high hydrological connectivity, typically associated with steep slopes where human occupation is limited. This condition resulted in higher average QF values in these areas, which naturally tend to have high QF due to their physical characteristics, regardless of LULC type. Therefore, although this study found that pasture and natural vegetation had the highest QF values, excluding urban areas, it should be noted that QF would likely be even higher if these areas were occupied by sugarcane, especially during the first year of planting, as demonstrated by Youlton et al. (2016).

The low sensitivity of the QF to LULC changes may have contributed to mitigate the export of sediments and nutrients. Even though sediment and nutrient exports increased between 1985 and 2019, this increase could have been more significant if the physiographic characteristics of the watershed favored QF and, consequently, sediment and nutrient production and transport. The limited response of landscape changes on QF may be related to the physiographic characteristics of the JGRB. Overall, the JGRB is flat and composed of smoothly undulating hills resulting from weathering of the Botucatu and Pirambóia formations, with low drainage density (ANJINHO et al., 2022b). Additionally, the soils in the region are predominantly sandy, with Latosols covering 60% of the area (ROSSI; KANASHIRO, 2017). These characteristics reduce the intensity of surface runoff and the export of nutrients and sediments. These observations have been noted in other studies conducted in the region (ANJINHO et al., 2021; BUENO et al., 2022).

4.4.2. Analysis of the effects of LULC changes on water ecosystem services

The conversion of pasture and natural vegetation to agriculture in JGRB resulted in a decrease in all WES, except for sediment retention. Changes in the region's vegetation type may be associated with a decrease in JGRB's baseflow. JGRB's natural ecosystems, including wetlands, grasslands, savannas, and forests (IF, 2006; CBH-TJ, 2016; SANTOs et al., 2023), facilitate water infiltration and recharge of aquifers due to their deep-rooted vegetation that creates fissures in soil and allow greater penetration of water (LIMA et al., 2020), preserving the soil hydraulic characteristics (HUNKE et al., 2014). The reduction of pasture areas may have also affected the BF of the watershed. While Anache et al. (2019) observed higher impacts on soil hydrological patterns in pastures, at the hillslope scale, compared to sugarcane and Cerrado vegetation, the results of this study suggest a different effect in the JGRB. Pastures in JGRB primarily feature herbaceous species associated with extensive small-scale livestock production, located in low-slope areas, which naturally generate less surface runoff. These pastures may not be as impacted by grazing, allowing for better water infiltration. Additionally, the low-lying vegetation reduces evapotranspiration, increasing water availability and promoting vertical water movement in the soil (ANACHE et al., 2019).

The reduction in nutrient retention is directly related to the decrease in natural vegetation and pasture. Due to the specifics of the approach taken in this study, the results for this service were already expected, as the export coefficients used in this study assume higher nutrient export in agricultural areas compared to other LULC. Thus, the greater the difference in exported loads, the greater the contribution of the nutrient retention service. Other studies that used the NDR model also observed negative effects on water purification services with the reduction of natural areas (MEI et al., 2017; SCHIRPKE et al., 2017; DECSI et al., 2020; FANG et al., 2022).

A noteworthy finding of this study was the result of the sediment retention service, which increased with LULC changes. This increase may be associated with the higher sediment export resulting from the expansion of sugarcane in the JGRB. The "avoided export" output of the SDR model indicates vegetation's role in reducing erosion and retaining sediment from upstream areas. Consequently, the greater the sediment export upstream of a pixel, the greater its retention will be. Additionally, the physical characteristics of the JGRB also contribute to the increase in sediment retention. Although there may be sediment production due to the presence of erosion-prone soils, their transport in the watershed becomes limited due to the topography of the study area. In other words, the higher the production, the greater the retention.

4.4.3. Effects of environmental zoning on biophysical indicators

The environmental zoning proposed in this study indicates that 67% of JGRB consists of areas designated for anthropic use, which can be used for sugarcane production, the main economic activity in the region, or urban expansion. Another 4% represents consolidated areas where LULC changes are limited due to existing urban infrastructure. The conservation zone covers 17% of the area and includes fragments of Cerrado, riparian forests, gallery forests, and wetlands, which provide multiple ecosystem services (RIIS et al., 2020; RESENDE et al., 2021). Priority restoration areas are concentrated near watercourses and occupy 11% of the watershed. Our analysis linked the potential WES degradation levels with the socioeconomic characteristics of the watershed, represented in this study by LULC. Our goal was to identify a sustainable LULC scenario capable of increasing the provision of WES while promoting socioeconomic development. The results obtained were robust and feasible for implementation in the study area.

The study indicated that increasing natural vegetation by just 11% in strategic locations in JGRB can enhance the provision of WES, reduce surface runoff and the export of nutrients and sediments. These findings align with other studies in the literature that demonstrate the effects of ecological restoration on the provision of ecosystem services (BENAYAS et al., 2009; YANG et al., 2018; FERREIRA et al., 2019). In JGRB, the areas identified as priority restoration sites are associated with riparian zones, as they were deemed critical in terms of generating runoff and exporting sediments and nutrients. As discussed in previous studies, riparian zones play a crucial role in enhancing multiple ecosystem services, including nutrient removal, flow regulation, climate regulation, erosion control, water purification, and providing habitats for biodiversity (DUFOUR et al., 2019; RIIS et al., 2020). Additionally, they also play an important role in promoting landscape connectivity, acting as ecological corridors that offer refuge and facilitate gene flow among scattered patches of natural vegetation in the landscape (LUKE et al., 2019; HUERTA-RODRÍGUEZ et al., 2022).

In addition to ecological restoration, actions aimed at conserving existing fragments are also important, as the provision of ecosystem services can vary depending on the age of the vegetation, suggesting that public policies should promote the conservation of primary forest fragments, in addition to efforts focused on increasing forest cover (FERRAZ et al., 2014).

4.4.4. Methodological potentials, limitations, and uncertainties

The methodology employed in this study allowed for the spatial mapping of WES, identification of priority areas for conservation and ecological restoration, and evaluation of the effects of an alternative land-use scenario generated based on the proposed environmental zoning. The method is based on the use of free and simplified models, making it applicable in unmonitored watershed or those with limited available data, where the use of complex models is not feasible. Furthermore, the methodology is flexible and can be replicated in any rural region, allowing for adjustments in landscape composition and configuration. The advantage of this approach lies in its ability to quantify the impacts of planned land-use scenarios, in contrast to methods solely based on multicriteria analysis, as demonstrated by Valente et al. (2021) and Anjinho et al. (2022a).

Although the methodology proved to be effective for land-use planning aiming to increase the provision of WES, it is important to acknowledge its limitations and interpret the results with caution. The limitations discussed in this study focus on the results generated from the proposed methodology. Operational limitations of the InVEST models can be found in-Anjinho et al. (2022b).

One of the uncertainties related to the results of this study is associated with the outputs of the models used. The three hydrological models in InVEST operate at an annual scale, which prevents capturing the seasonal hydrological variability of the watershed. Surface runoff, sediment exports, and nutrient exports exhibit significant variations throughout the year, with peaks occurring mainly during the rainy season, which in the study area, takes place between October and March (ANJINHO et al., 2022b). Annual values mask and smooth out the seasonal effects of land-use changes on watershed hydrology, which can lead to misinterpretations when using them for decision-making. For example, studies in the literature demonstrate the effects of forests on water production, indicating that this type of vegetation can reduce the water yield of the watershed (SIQUEIRA et al., 2021), which would impact local water availability. However, when considering seasonal effects, it is observed that forests and other natural areas regulate water flow throughout the year

(TARIGAN et al., 2018), maintaining a minimum flow necessary to ensure water during dry periods. Additionally, seasonal exports of nutrients and sediments are also not captured by the models. In the JGRB, precipitation during the rainy months represents 80% of the total annual precipitation volume (ANJINHO et al., 2022b). Intense precipitation during this period promotes higher sediment and nutrient exports due to surface runoff and leaching from agricultural areas (NEVES et al., 2021). Therefore, additional studies at finer scales may be necessary to complement our findings and quantify the seasonal effects of land-use changes on WES in the study watershed.

The criteria adopted for environmental zoning (outputs from the InVEST WES models) may restrict more comprehensive land-use strategies aimed at providing multiple ecosystem services and promoting biodiversity. Although the areas proposed for restoration in this study may contribute to the provision of other ecosystem services, it is recommended to include in the analysis other services such as climate regulation, habitat provision, pollination, and recreation (ORSI et al., 2020) for a broader land-use planning. When it comes to biodiversity conservation, we know that many other characteristics are important and should be taken into consideration in identifying priority areas for conservation and ecological restoration, such as the quality, configuration, and connectivity of natural vegetation fragments in the landscape (FERRAZ et al., 2014). Although our results demonstrate the effectiveness of this approach for the four quantified WES in this study, we cannot assert whether additional ecological benefits will be effectively achieved with increased natural vegetation (REN et al., 2017), as they were not quantified in this paper.

4.5. Conclusion

The methodology of this study allowed quantifying the effects of land-use changes on surface runoff, nutrient exports, sedimentation, and WES, highlighting the importance of ecological restoration in mitigating these effects. The approach is straightforward and recommended for unmonitored watersheds or those with limited data availability. The method is flexible and can be replicated in rural regions that still allow modifications in land-use composition and configuration.

The results highlighted the negative impacts of agricultural expansion in the study area, particularly sugarcane cultivation, which had the greatest effect on annual sediment and nutrient exports. Due to the physical characteristics of the JGRB, land-use changes had a smaller impact on surface runoff, but the average annual value still increased by approximately 20% during the analyzed period. The conversion of pastures and natural vegetation to agriculture decreased the provision of WES, except for the sediment retention service.

Through the proposed environmental zoning, it was possible to identify priority areas for ecological restoration, which in this study are associated with riparian zones. The restoration of these areas has the potential to increase the provision of WES and reduce surface runoff, as well as nutrient and sediment exports in the JGRB. These findings provide valuable insights for decision-making and sustainable land-use planning. Our results offer a scientific basis for the implementation of legal instruments aimed at conserving and restoring natural ecosystems, such as the legally protected areas established in the Brazilian Forest Code and payments for environmental services programs.

4.6. References

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4.7. APPENDIX B - Supplementary information

Table S 4.1. Area of each land use class for the years 1985, 2019, and planned land use scenario

Land use	1985		2019		Planned land use scenario	
	km²	%	km²	%	km²	%
Agriculture	975	23%	2,112	51%	1,674	40%
Forest plantation	85	2%	209	5%	209	5%
Natural vegetation	901	22%	720	17%	1,164	28%
Pasture	2,136	51%	931	22%	925	22%
Urban area	43	1.03%	166	4%	166	4%
Water	33	0.79%	34	1%	34	1%
Total	4,172	100%	4,172	100%	4,172	100%

Table S 4.2. Land use and land cover conversion matrix from 1985 to 2019 (km²)

	2019						
1985	**Agriculture**	**Water**	**Urban area**	**Natural vegetation**	**Planted forests**	**Pasture**	**Total**
Agriculture	825.83	0.23	37.73	21.46	3.83	85.46	974.54
Water	0.04	31.59	0.02	0.87	0.03	0.36	32.91
Urban area	0.00	0.00	43.04	0.02	0.00	0.02	43.08
Natural vegetation	167.16	1.06	17.10	507.06	85.11	123.06	900.55
Planted forests	4.27	0.00	0.85	0.74	78.45	0.57	84.88
Pasture	1,114.42	0.95	67.24	189.48	41.88	721.70	2,135.66
Total	2,111.71	33.83	165.98	719.63	209.31	931.17	4,171.61

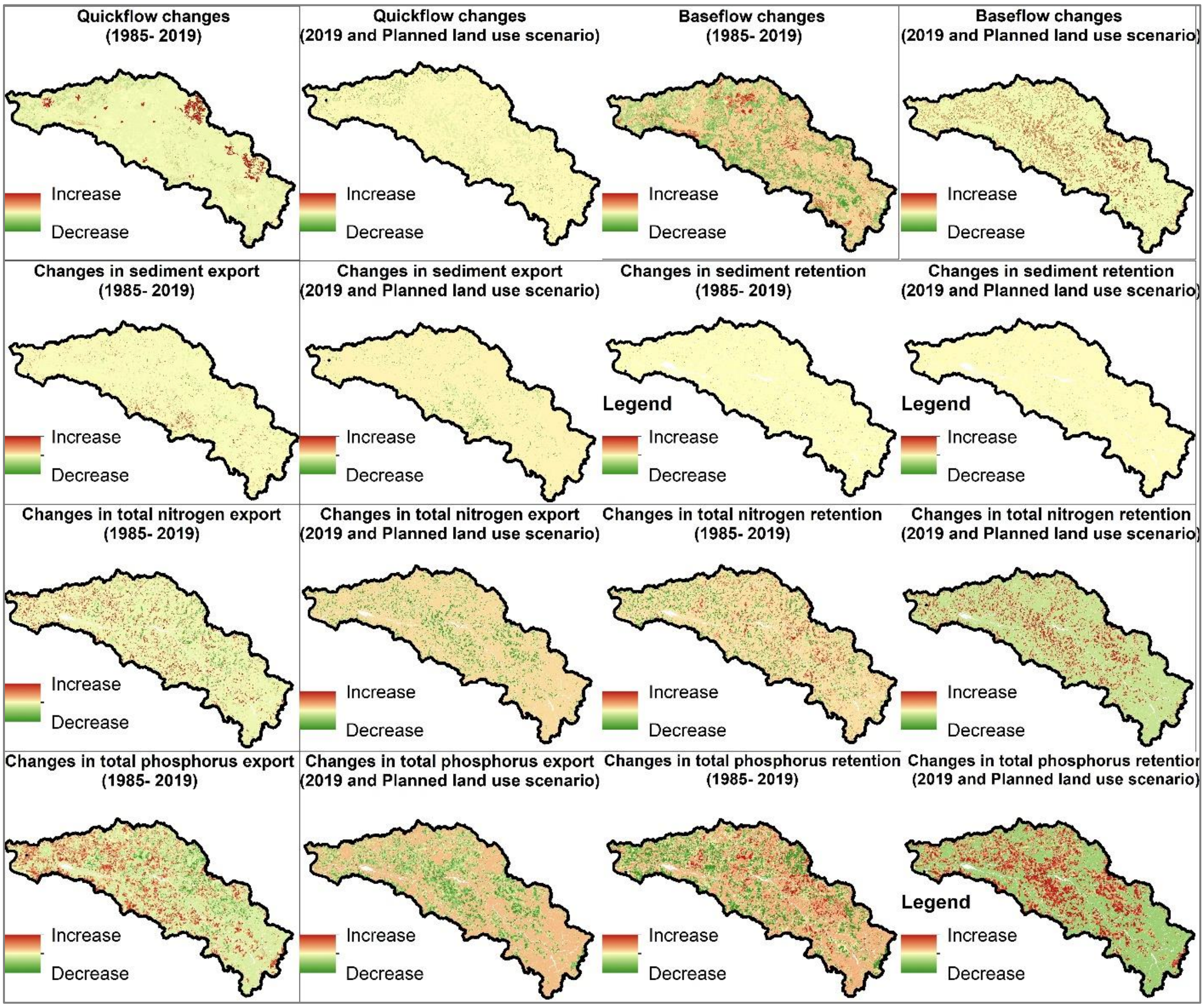

Figure S 4.1. Changes in water ecosystem services indicators between the period of 1985 and 2019, and 2019 and planned land use scenario.

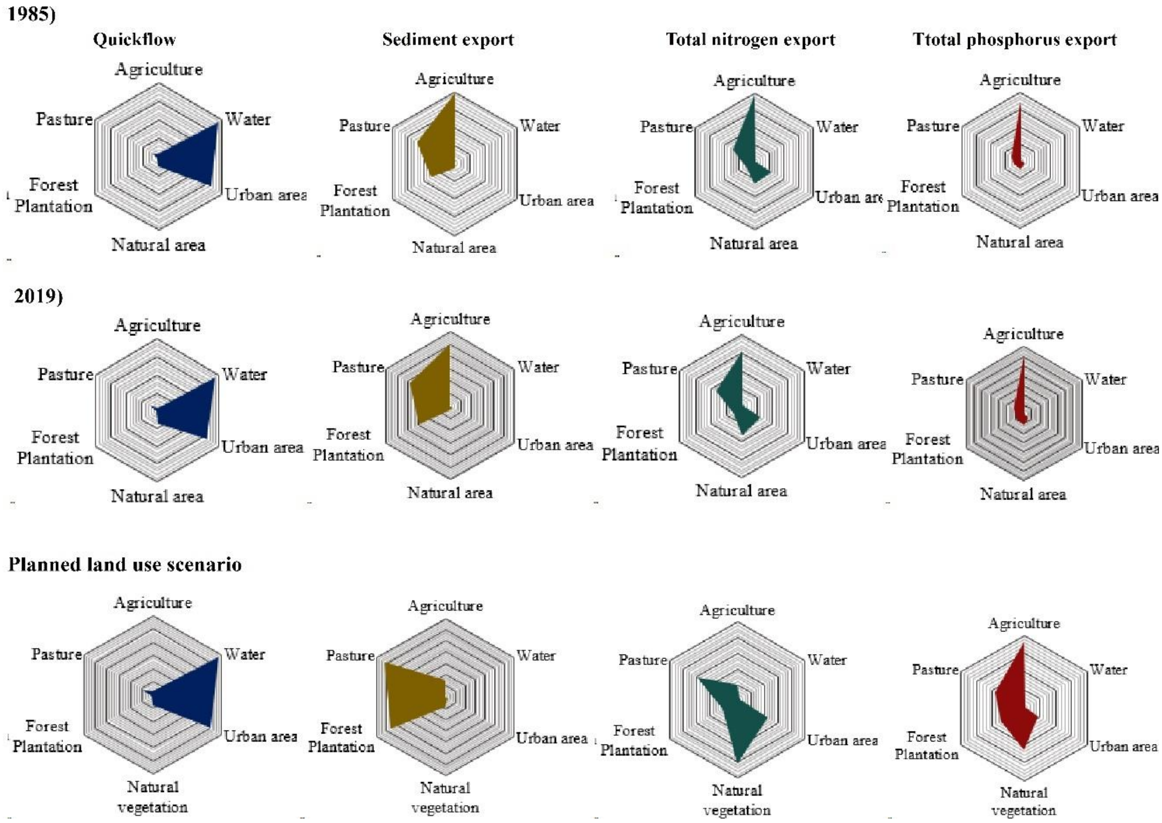

Figure S 4.2. Effects of land use and land cover types on surface runoff and exports of sediments and nutrients in Jacaré-Guaçu River Basin.

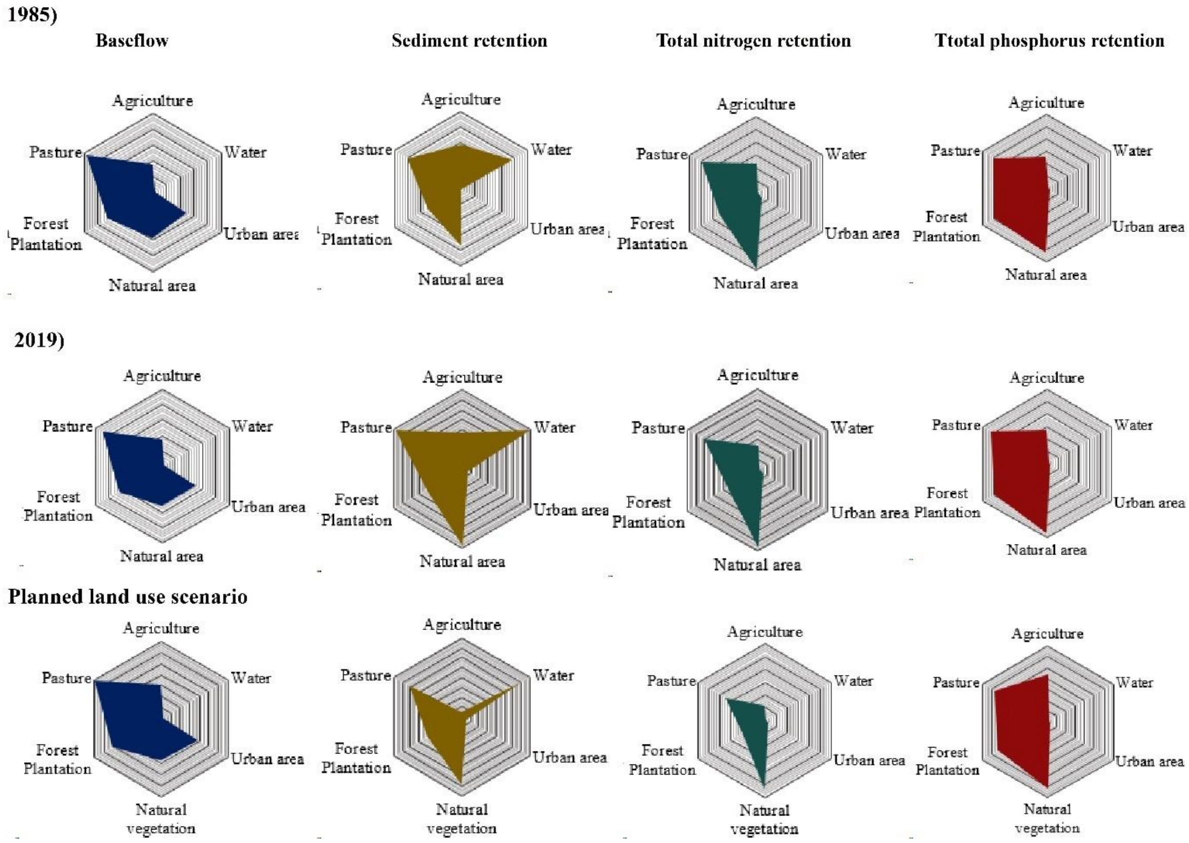

Figure S 4.3. Effects of land use and land cover types on water ecosystem services in Jacaré-Guaçu River Basin.

Table S 4.3. Simulated runoff, sediment export, nutrient export, baseflow, sediment retention and nutrient retention values for the planned land use and land cover scenario.

Land use and land cover	**Baseflow**	**Quick flow**	**Sediment export**	**Sediment retention**	**Total nitrogen export**	**Total nitrogen retention**	**Total phosphorus Export**	**Total phosphorus**
	(mm/yr)		**(t/yr)**		**(kg/yr)**		**(kg/yr)**	
Agriculture	153	56	3,134	484,073	54,206	245,097	19,133	91,789
Water	13	1,153	1	53,174	78	283	4	38
Urban area	192	1,004	59	50,686	11,722	7,602	476	592
Natural vegetation	187	144	1,367	4,546,069	139,390	741,536	7,976	84,266
Forest Plantation	253	28	1,515	497,008	7,352	51,530	984	13,870
Pasture	345	172	7,436	3,256,356	80,741	392,365	4,946	62,289
JGRB	211	151	13,512	8,887,365	293,489	1,438,413	33,518	252,843

Chapter 5

CAN GREEN SCENARIOS IMPROVE WATER ECOSYSTEM SERVICES AND MITIGATE THE EFFECTS OF CLIMATE CHANGE? A CASE STUDY IN A RIVER BASIN IN SOUTHEASTERN BRAZIL

ABSTRACT

Recent studies indicate that ecological restoration can enhance ecosystem services and mitigate the adverse effects of climate crisis. However, there is still limited research on the effectiveness of these projects, particularly when it comes to restoring native vegetation. This study assesses the effects of different climate scenarios (RCP 4.5 2040-2069, RCP 4.5 2070-2099, RCP 8.5 2040-2069, RCP 8.5 2070-2099) and land use and land cover (LULC) scenarios (trend, economic, green) on water ecosystem services (WES) in a river basin in southeastern Brazil. These scenarios were compared with the reference situation in 2019 (baseline). The main objective of this work is to determine whether green scenarios could enhance the WES while mitigating the effects of climate change. Climate and biophysical models from the InVEST package were used to simulate the effects of these scenarios on sediment export and retention (erosion control service), total nitrogen (TN) and total phosphorus (TP) export and retention (water purification service), and quickflow (QF) and baseflow (BF) (water supply). The results indicated that climate change primarily affected the water supply service, especially in the RCP 4.5 scenario (2069-2099), significantly reducing BF and streamflow. LULC changes had more pronounced impacts on water purification and erosion control services. The economic scenario had the greatest impact on nutrient and sediment exports and retentions. Climate scenarios combined with economic and trend LULC scenarios decreased WES provision. However, combining climate scenarios with the green scenario significantly reduced sediment and nutrient exports while mitigating the effects of climate change on water supply. The methodology of this study proved effective in understanding how climate and LULC changes affect WES. The results suggest that increasing green areas can improve WES and mitigate future climate change effects. The applied methodology can be replicated in other watersheds.

Keywords: Native vegetation restoration. Land use planning. Natural climate solutions. Water management. Hydrological modeling.

5.1. Introduction

Population growth and socioeconomic development have heightened the demand for natural resources, putting ecosystems at risk and consequently jeopardizing the services they provide (MEA, 2005), especially those related to water, known as water ecosystem services (WES) (VÖRÖSMARTY et al., 2013; PHAM et al., 2019). The latest Millennium Ecosystem Assessment (MEA, 2005) estimated that approximately 60% of ecosystem services have been degraded or used unsustainably, including WES such as water supply and purification. The ongoing decline of wetlands is an illustrative example of the current scenario of environmental degradation. It is estimated that only 13% of the wetlands that existed in 1700 remained by 2000, and the decline rates continue to be significant (0.8 percent per year from 1970 to 2008) (IPBES, 2019).

WES are benefits that terrestrial and aquatic ecosystems provide to society, essential for human development and well-being (GRIZZETTI et al., 2016). Various factors can affect the availability of these services in the environment, with climate and LULC changes being the primary threats to aquatic ecosystem integrity (BUCAK et al., 2018; COUTURE et al., 2018). Globally, changes in LULC have demonstrated significant impacts on terrestrial and freshwater ecosystems, while climate change exerts a relatively lesser impact, yet indicating a growing risk due to the accelerated pace of change and interactions with other factors (IPBES, 2019). Changes in LULC have already affected 70% of the non-ice-covered land surface (IPCC, 2019). Climate change has the potential to alter global precipitation and temperature patterns, expanding and intensifying the impacts already identified by modifications in LULC (IPCC, 2019).

While numerous studies have highlighted the isolated effects of climate and LULC changes on water resources (YANG et al., 2018; HASAN et al., 2020; NEVES et al., 2020a; MILLER et al., 2021), understanding their synergistic interactions and combined effects remains limited (MOLINA-NAVARRO et al., 2018; SEGURADO et al., 2018; BAI et al., 2019). LULC changes directly influence ecohydrological processes responsible for WES, impacting hydrological, sedimentological, and nutrient dynamics (SUN et al., 2017). Studies have emphasized the impacts of LULC changes on WES, such as alterations in nutrient and sediment loads (BAI et al., 2019; KHAN et al., 2019) and water production in watersheds (SRICHAICHANA et al., 2019). Similarly, climate change can alter local hydrological cycles, causing multiple impacts on WES (HOYER; CHANG, 2014; JORDA-CAPDEVILA et al., 2019; PAN; CHOI, 2019). These effects vary geographically, potentially increasing the occurrence of extreme weather events, wildfires, soil erosion, nutrient leaching, and reducing biodiversity (ØYGARDEN et al., 2014; BELL et al., 2018; TRISOS et al., 2020; ABRAM et al., 2021; EEKHOUT; VENTE, 2022).

Effective management and restoration of aquatic ecosystems require a thorough understanding of the combined effects of climate and LULC changes on ecosystem services. This complex chain of cause and effect needs to be synthesized into simple models capable of guiding decisions (HERING et al., 2015). Despite the importance of understanding these stressors, it remains a significant challenge for researchers (BAI et al., 2019).

Nature-based solutions (NBS) are being recognized as promising approaches to mitigate and adapt to the effects of climate change, enhancing ecosystem resilience and the availability of its services (SUSSAMS et al., 2015; GRISCOM et al., 2017; MANES et al., 2022;). Ecological restoration stands out among these solutions, defined as the process of recovering degraded ecosystems to rebuild their structure and function (MCDONALD et al., 2016). The interest in ecological restoration primarily stems from the potential of forests to sequester carbon from the atmosphere, making these measures interesting and strategic for mitigating global warming (BASTIN et al., 2019). However, many other climatic and ecological benefits can be achieved through ecological restoration, provided these projects are considered in planning and decision-making (ELLISON et al., 2017; RIIS et al., 2020).

Many countries are developing and implementing projects in pursuit of forest restoration goals, such as the Bonn Challenge, the New York Declaration on Forests, and the 20 × 20 Initiative (GATICA-SAAVEDRA et al., 2017). While many studies demonstrate the positive effects of ecological restoration on multiple ecosystem services, their concrete effects on WES and their potential for climate change mitigation and adaptation still lack understanding (VAN MEERVELD et al., 2021; FELD et al., 2011), especially concerning native forest restoration (Jones et al., 2022). Within the scope of WES, which in this study encompasses erosion control, water provision, and purification services, some studies suggest that restoration initiatives can bring significant benefits to erosion control and water purification in watersheds (WEN; THÉAU, 2020; GHIMIRE et al., 2021). However, concerning the water supply service, results are diverse and strongly influenced by local physical characteristics (FILOSO et al., 2017; FERREIRA et al., 2019).

This study sought to understand this issue better, exploring the individual and combined effects of climate and LULC changes on WES in a rural watershed located in southeastern Brazil. The tested hypothesis involves evaluating whether green scenarios, based on native vegetation reintroduction, can expand WES provision and mitigate the effects of climate change. In doing so, this study contributes to the growing understanding of NBS as an effective strategy for preserving ecosystem services and addressing challenges posed by global warming.

5.2. Methodology

5.2.1. Study area

The Jacaré-Guaçu River Basin (JGRB) is one of the sub-basins within Water Resources Management Unit No. 13 in the state of São Paulo, Brazil (UGRHI 13) (Figure 5.1). The Jacaré-Guaçu River is a significant tributary of the Tietê River, the largest watercourse in the state of São Paulo, spanning approximately 155 km in length. With a drainage area of 4,172.12 km², the basin covers 15 municipalities, and its surface and groundwater resources serve as important water sources for the central-eastern region of the state of São Paulo (CBH-TJ, 2016).

The hydrography of the JGRB is formed by the Jacaré-Guaçu River, resulting from the confluence of the Lobo and Feijão streams, originating from the Itaqueri and Cuscuzeiro mountain ranges, along with several other smaller rivers. Additionally, the basin is situated above the Guarani Aquifer System (SAG), one of the world's largest groundwater reservoirs, covering approximately 1,200,000 km² (COSTA et al., 2019). Due to the geological characteristics of the JGRB, the region is an important recharge area for the SAG (LUCAS; WENDLAND, 2016), covering around 1,640 km² of the basin. In addition to the SAG, formed by the Botucatu and Piramboia formations, the Bauru and Serra Geral formations also occur in the basin (CBH-TJ, 2016).

The region's climate is characterized by dry winters and wet summers, falling under the CWA and CWB climate zones, according to the updated Köppen-Geiger classification

(PEEL et al., 2007). Average temperatures range from 17.4 °C in June to 23.7 °C in February, with an annual average precipitation of approximately 1400 mm (ANJINHO et al., 2022).

The relief of the JGRB is predominantly flat, composed of gently undulating hills (about 80%). Steeper areas are concentrated mainly near the sources of the Jacaré-Guaçu River and the watercourses in the central part of the basin. The altitude varies from 372 m to 1024 m. Soils consist mainly of Latosols, Red-Yellow Argisols, and Quartzarenic Neosols (ROSSI; KANASHIRO, 2017).

The natural vegetation of the basin comprises remnants of the Brazilian Cerrado (savannah) and Atlantic Forest, two significant Brazilian biomes (CBH-TJ, 2016). The sugarcane sector is the region's primary economic activity, with sugarcane being the main driver of LULC change (Trevisan et al., 2021). Currently, agriculture occupies 51% of the basin, followed by pasture areas (22%), natural vegetation (17%), planted forests (5%), urban areas (4%), and water bodies (1%) (Chapter 4).

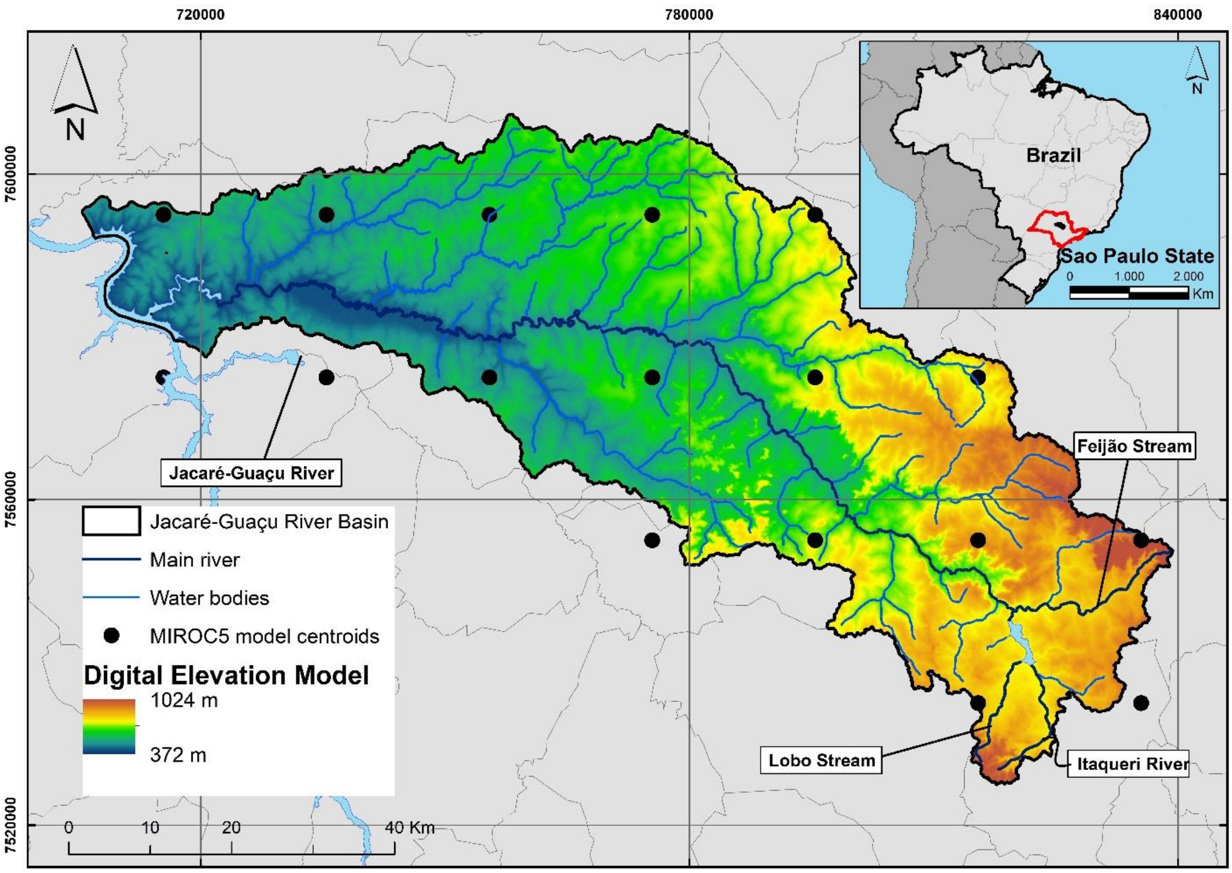

Figure. 5.1. Location of Jacare-Guaçu River Basin, digital elevation model, water body, and centroids referring to the MIROC5 model.

5.2.2. Data acquisition and methods description

Data from various government agencies were used to assess the effects of climate and LULC changes on WES. The dataset includes ALOS-PALSAR images (12.5 meters spatial resolution) from the Alaska Satellite Facility (ASF, 2021), 2019 LULC data from the Brazilian Annual Land Cover and Use Mapping Project (MAPBIOMAS, 2021), meteorological information from the Water Resources and Environmental Studies Center (CRHEA) at the School of Engineering in São Carlos, University of São Paulo, precipitation data from the National Water and Basic Sanitation Agency (ANA) (ANA, 2021), and high-resolution precipitation data from the Climate Hazards Group Infrared Precipitation with Stations (0.05°), obtained through Google Earth Engine (FUNK et al., 2015). Additionally, soil data for the state of São Paulo at a scale of 1:100,000 were utilized (ROSSI; KANASHIRO, 2017). Precipitation, average air temperature, and reference evapotranspiration (ET_0) data from the ETA MIROC5 model (TAVARES et al., 2023), regionalized for South America, were also incorporated to evaluate the effects of climate changes on WES.

Biophysical models from the InVEST 3.12.0 package (NATURAL CAPITAL PROJECT, 2022) were employed to simulate the impacts of climate and LULC changes on WES. Details regarding the relationship between input data and the InVEST biophysical models are available in Table 5.1. Three LULC change scenarios (trend, economic, and green) and four climate change scenarios (RCP 4.5 2040–2069, RCP 4.5 2070–2099, RCP 8.5 2040–2069, and RCP 8.5 2070–2099) were projected, in addition to the baseline scenario previously assessed by Anjinho et al. (Chapter 4), which references 2019 LULC data and meteorological data equivalent to the long-term average (1985-2019). The following subsections describe the methods employed in projecting scenarios of climate and LULC changes, analyzing trends in climate data, formulating combined scenarios of climate and land use changes, and the biophysical models used to quantify WES.

Table 5.1. Input data used in InVEST biophysical models.

Data	Input	Type	Model	Source
Digital Elevation Model	Digital Elevation Model	Raster	SWY, SDR e NDR	ASF (2021)
Land use and Land cover	Land use and Land cover	Raster	SWY, SDR e NDR	MAPBIOMAS (2021)

Precipitation	Average monthly precipitation	Raster	SWY	ANA (2021), Funk et al. (2015), and Tavares et al. (2023)
	Erosivity Index	Raster	SDR	
	Nutrient Runoff Proxy	Raster	NDR	
Meteorological	Monthly average reference evapotranspiration	Raster	SWY	CRHEA and Tavares et al. (2023)
Pedological	Soil Erodibility	Raster	SDR	Rossi and Kanashiro (2017)
	Soil Hydrologic Group	Raster	SWY	
Biophysical tables	Biophysical tables	CSV	SWY, SDR e NDR	Anjinho et al. (2022)

Seasonal Water Yield model (SWY), Nutrient Delivery Ratio model (NDR), and Sediment Delivery Ratio model (SDR).

5.2.3. Projection of land use and land cover change scenarios

The effects of LULC changes on WES were determined by altering the current (2019) LULC pattern of JGRB. Scenarios were projected based on MAPBIOMAS data, resulting in three scenarios used as input for the water ecosystem services models, in addition to the baseline scenario (2019). These scenarios include: i) baseline, representing the 2019 LULC pattern; ii) trend; iii) economic; and iv) green.

The trend scenario was projected assuming the economy would maintain the same growth level and compliance with environmental guidelines. This scenario was determined based on the analysis of LULC dynamics between 1985 and 2019, conducted by Anjinho et al. (Chapter 4). The goal was to analyze the trend of each LULC class and identify classes that showed significant increases during the analyzed period. In this scenario, 15% (609 km^2) of the JGRB area was modified, with projections indicating a 25% increase (474 km^2) in sugarcane areas, 40% (85 km^2) in forestry, and 30% (50 km^2) in urban areas. This change primarily occurred through the replacement of pasture areas (-50%, equivalent to 465 km^2) and natural vegetation (-20%, equivalent to 144 km^2). This trend aligns with another study conducted in the region (Santos, 2018).

The economic scenario focused on the economic development of JGRB, driven by a significant expansion of agricultural areas. This expansion was fueled by increasing sugarcane cultivation for ethanol production, one of the main economic products of the state of São Paulo, following the trend of this crop's expansion in the state (RUDORFF et al., 2010). The trend scenario served as the basis for projecting the economic scenario, where all pasture and other agricultural areas were replaced by sugarcane cultivation.

The green scenario aimed at the sustainable use of natural resources, where current environmental laws regulate economic development. This scenario was based on the LULC planning proposed by Anjinho et al. (Chapter 4), which combined biophysical models and multicriteria analysis to zone the JGRB area and suggest a planned LULC scenario that promotes an increase in WES supply. Furthermore, for the green scenario, this study considers the legal provisions of the Brazilian Forest Code (BRAZIL, 2012), assuming that all legally protected areas, Legal Reserves (LRs), and Permanent Preservation Areas (PPAs) were implemented correctly in JGRB. In other words, it simulates the restoration of 100% of PPAs and LRs.

PPAs refer to areas of vegetation that play a vital role in preserving water resources, landscape, geological stability, and biodiversity. They also help facilitate the gene flow of fauna and flora, protecting the soil, and ensuring the well-being of human populations. These areas were identified using a Geographic Information System (GIS) based on specific legal criteria (BRAZIL, 2012). The criteria included a radius of 50 meters around springs, a 50-meter strip along the Jacaré Guaçu River, a 30-meter strip for other watercourses in JGRB, and a radius of 100 meters around artificial reservoirs. Additionally, areas with a slope greater than 45° were considered APPs. No hilltop APPs were found in the study area, following the guidelines of the Brazilian Forest Code.

LRs are designated areas within rural properties that aim to ensure the sustainable use of natural resources, help in the restoration of ecological processes, and promote biodiversity conservation (BRAZIL, 2012). The percentage of the rural property area allocated for maintaining or restoring native vegetation varies depending on the location in Brazil. In this study, data related to LRs from the Brazilian Rural Environmental Cadaster National System (SICAR) were integrated into the green scenario. This data includes both the existing LRs and the proposed ones for rural properties.

5.2.4. Projection of climate change scenarios

The Model for Interdisciplinary Research on Climate, version 5 (MIROC5), was employed to develop the climate scenarios in this study. MIROC5 is a climate model developed by Japanese institutions and widely used in studies assessing the impacts related to climate change (BARBOSA et al., 2022; OLIVEIRA SERRÃO et al., 2023; RIQUETTI et al., 2023). Grounded in mathematical equations, it aims to simulate the natural processes associated with climate change, featuring a spatial resolution of approximately 150 km horizontally and 40 levels vertically (CHOU et al., 2014).

Through the ETA model, regionalized data from the MIROC5 model were utilized to obtain more detailed climate predictions (TAVARES et al., 2023). The ETA model was originally developed by the University of Belgrade and the Hydrometeorological Institute of the former Yugoslavia. In Brazil, its operation began in 1996 and has since been employed by the National Institute for Space Research of Brazil (INPE) to produce climate forecasts for South America at different temporal scales (CHOU et al., 2014). Climate projections of daily precipitation, average air temperature, and ET_0 data, with a spatial resolution of 20 km and bias correction, provided by INPE, were utilized (TAVARES et al., 2023). The ETA model's regionalized projections span the period from 1976 to 2099.

Climate scenarios in this study were projected based on the sixth report of the Intergovernmental Panel on Climate Change (IPCC) (IPCC, 2023). Starting from the fifth IPCC report, climate scenario projections shifted from an emissions-based approach to radiative forcing, known as Representative Concentration Pathways (RCP). In this approach, climate scenarios are defined as total radiative forcing, measured in $W.m^{-2}$, representing the amount of solar radiation retained on the planet. To assess the effects of climate change on WES, RCP scenarios of radiative forcing 4.5 $W.m^{-2}$ and 8.5 $W.m^{-2}$ (RCP 4.5 and RCP 8.5) were selected. The analysis period covered the range from 2040 to 2099, generating four distinct scenarios: i) RCP 4.5 (2040-2069), ii) RCP 4.5 (2070-2099), iii) RCP 8.5 (2040-2069), and iv) RCP 8.5 (2070-2099). RCP 4.5 represents intermediate levels, where emissions are relatively controlled over time. This scenario predicts an increase in the average land temperature of up to 3°C (IPCC, 2023). RCP 8.5 indicates pessimistic conditions, where significant actions to reduce greenhouse gas emissions are not taken. In this scenario, the global average temperature may exceed 4°C, depending on the adopted Shared Socio-economic Pathways (SSP) (IPCC, 2023).

5.2.5. Analysis of meteorological data trends

This study aimed to enhance the understanding of the impacts of climate change on WES through a trend analysis. The study evaluated the direction and magnitude of changes in climatic variables using observed historical data from 1985 to 2019 and projections from 2020 to 2099. The annual average precipitation from rainfall measurement points was calculated using Thiessen polygons, while data from CRHEA were used to analyze the trend in annual average air temperature and ET_0. The non-parametric Mann-Kendall test was applied to identify trends in climatic variables, specifically recommended for this purpose (NEVES et al., 2020b). The test allowed the verification of the presence or absence of trends in the data series by testing two hypotheses: H_0, suggesting the absence of trends in the data, and H_1, indicating the presence of trends.

5.2.6. Combined scenarios of climate and land use changes

Twelve scenarios were created that integrate projections of climate and LULC changes, aiming to assess their effects on WES (Table 5.2). Scenarios S1 to S4 represent climate variations combined with the economic development scenario. On the other hand, scenarios S5 to S8 combine different climatic conditions with the trend-based land use scenario, while scenarios S9 to S12 result from the combination of climate projections and the green land use scenario.

Table 5.2. Scenarios combining climate and land use changes.

Scenarios	**Economic development**	**Trend**	**Green**
RCP 4.5 (2040 - 2069)	SC1	SC5	SC9
RCP 4.5 (2070 - 2099)	SC2	SC6	SC10
RCP 8.5 (2040 - 2069)	SC3	SC7	SC11
RCP 8.5 (2070 - 2099)	SC4	SC8	SC12

5.2.7. Simulation of the effects of climate and land use changes on water ecosystem services

The scenarios of climate and LULC changes were used as input in the biophysical models SWY, NDR, and SDR to assess their effects on eight indicators of WES. The indicators QF and BF are linked to the water supply service, assuming that BF has a direct relationship with water supply, and QF has an indirect relationship. The indicators sediment export, TN export, and TP export are associated with erosion control and water purification services, respectively. The higher the export of sediments and nutrients, the lower the provision of these services. On the other hand, the indicators sediment retention, TN retention, and TP retention are directly related to these services.

The previously calibrated models by Anjinho et al. (2022) were employed to assess the effects of each projected scenario, as well as their combined effects. The InVEST package models used to evaluate WES are based on well-known hydrological simplifications and do not incorporate all the characteristics of hydrological, sediment, and nutrient cycles (VIGERSTO; AUKEMA, 2011). Below, a simplified presentation of the models used in this study is provided. All inputs requiring rainfall and meteorological data (Table 5.1) were generated based on observed historical data (1985 to 2019) from the study by Anjinho et al. (2022). The authors utilized 31 rainfall measurement points (21 monitoring stations and 10 CHIRPS points) and 1 meteorological monitoring station. For scenarios involving future climate data, data from 16 points generated from the MIROC5 model grid (20 km) were used (Figure 5.1). Further information on data, parameters, and calibration and validation methods can be found in Anjinho et al. (2022).

The SWY model was employed to quantify the effects of climate and LULC scenarios on the QF and BF indicators. QF characterizes surface runoff in the watershed, while BF represents the flow of groundwater-feeding rivers during the dry season and, in this study, is considered an indicator for the water supply service. The streamflow of the watershed is determined by the sum of QF and BF. QF is calculated based on an adaptation of the SCS method (NATURAL CAPITAL PROJECT, 2022), while BF represents the portion of local groundwater recharge that properly reaches watercourses. Local recharge for each pixel (L_i) is determined from a simplified water balance between precipitation (P_i), surface runoff (QF_i), and evapotranspiration (AET_i) (Equation 5.1). SWY model outputs are generated on a monthly scale for QF and an annual scale for BF, in mm. pixel^{-1}. Unlike the study by Anjinho et al. (2022), which used the method of Camargo et al. (1990) to calculate ET_0, this study employed the Penman-Monteith method, adapted by FAO (PM-FAO56) (ALLEN et al., 1998), for compatibility with future ET_0 data provided by Tavares et al. (2023).

$$L_i = P_i - QF_i - AET_i \tag{5.1}$$

The sediment export and retention indicators were calculated using the SDR model (NATURAL CAPITAL PROJECT, 2022). This model was developed based on the studies of Borselli et al. (2008) and essentially involves the steps of quantifying annual soil loss, sediment export, and sediment retention. The quantification of annual soil loss per pixel (ton. ha^{-1}. $year^{-1}$) is estimated using the Revised Universal Soil Loss Equation (RUSLE). The annual sediment export per pixel (E_i), which refers to the proportion of soil loss that reaches the watercourse, is calculated by multiplying annual soil loss (RUSLE) by the sediment delivery ratio (SDR) (Equation 5.2). Finally, the sediment retention per pixel (AEX_i), characterizing the erosion control service provided by vegetation, is calculated by the difference between RKLS (referring to RUSLE without the C (soil cover) and P (conservation practices) factors) and RUSLE, multiplied by SDR plus the amount of sediment trapped in upslope pixels (T_i) (Equation 5.3).

$$E_i = RUSLE_i \,.\, SDR_i \tag{5.2}$$

$$AEX_i = (RKLS_i - RUSLE_i) \,.\, SDR_i + T_i \tag{5.3}$$

The NDR model was employed to calculate the export and retention of TN and TP in the study area. It is a simple method that represents the nutrient balance through empirical relationships, without delving into the details of the nutrient cycle. The model assesses nutrient loads according to LULC and retention properties, calculating the proportion of nutrients reaching watercourses, similar to the SDR model (NATURAL CAPITAL PROJECT, 2022). Nutrient loads are determined using the method of average export coefficients associated with different LULC classes. This study used the same export coefficients as Anjinho et al. (2022). Additionally, the model adjusts nutrient loads ($Load_i$) by multiplying them by the potential surface runoff of each pixel (RPI_i), which refers to a proxy generated from the ratio between the pixel's runoff proxy value (RPi) and the average basin runoff value (RP_{av}) (Equation 5.4). Precipitation data was used as a proxy in this study. Nutrient export (N_i) is determined by multiplying the modified nutrient loads of each pixel by their respective nutrient delivery rate (NDR) values (Equation 5.5). This study considered only diffuse nutrient loads. The nutrient retention service was calculated by comparing nutrient exports from a degraded scenario, where all land uses in the watershed were converted to agriculture, with the LULC scenarios analyzed in this study, as recommended by the user manual (NATURAL CAPITAL PROJECT, 2022).

$$RPI_i = RP_i / RP_{av} \tag{5.4}$$

$$N_i = Load_i \cdot NDR_i \tag{5.5}$$

5.3. Results

5.3.1. Land use and land cover scenarios

The spatial distribution and proportion of each LULC class in the projected scenarios are presented in Figure 5.2. In the economic scenario, 73% of the land is used for agriculture, followed by the trend-based scenario with 62%, and the green scenario with 39%. Planted forests occupy 7% of the land in the trend-based and economic scenarios, and 5% in the green scenario. Urban areas occupy 5% in the trend-based and economic scenarios but represent 4% in the green scenario. Pastures cover 11% of JGRB in the trend-based scenario and 19% in the green scenario. In the economic scenario, all pastures were converted to sugarcane. Natural vegetation covers 14% in the trend-based and economic scenarios and 32% in the green scenario.

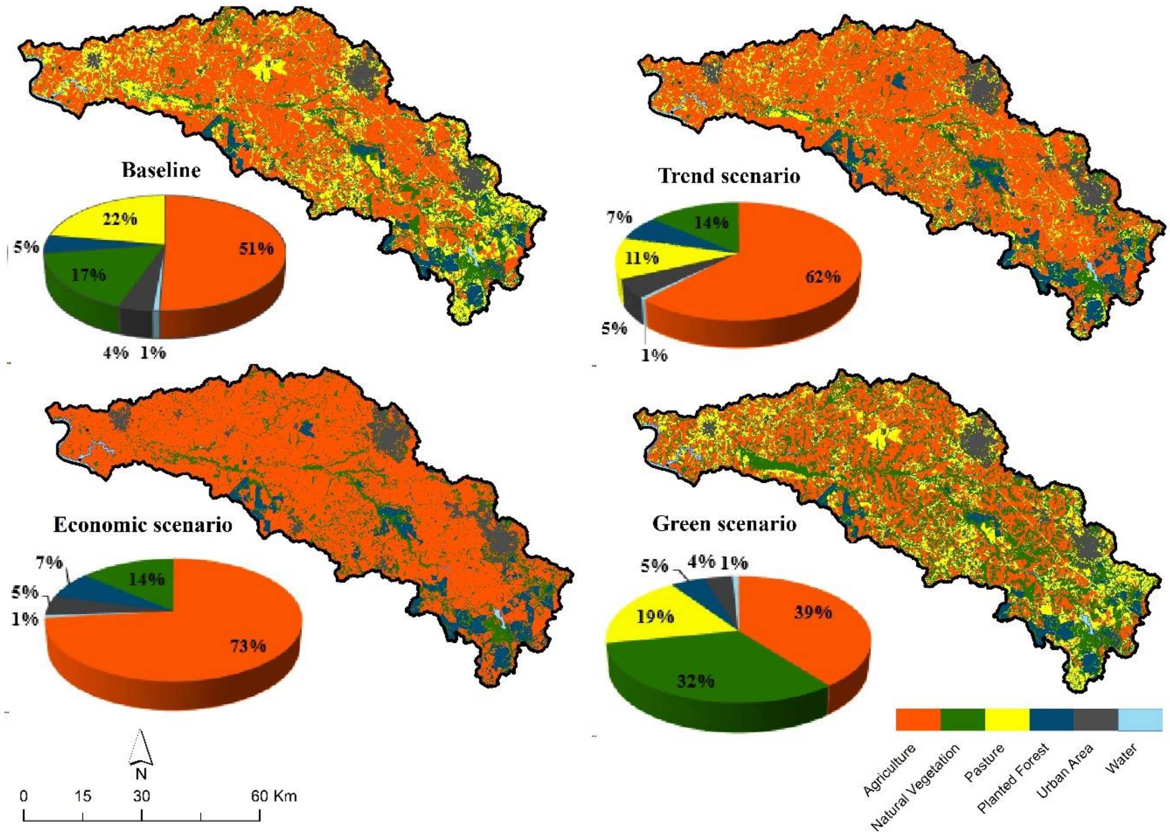

Figure 5.2. Spatial distribution and percentage of the projected land use scenarios for the Jacare-Guaçu River Basin.

5.3.2. Climate change scenarios

The RCPs 4.5 and 8.5 indicated a significant increase (p-value < 0.05) in the trend of average air temperature until the end of the 21st century (Figure 5.3). Starting from 2020, each year recorded average air temperatures above the long-term historical average (1985-2019). For the RCP 4.5 scenarios (2040-2069) and RCP (2070-2099), the increase in average air temperature was 2.3º C (+11%) and 2.9º C (+14%), respectively; and for the RCP 8.5 scenarios (2040-2069) and RCP 8.5 (2070-2099), the respective increases were 3.0º C (14%) and 4.4º C (21%).

Annual cumulative precipitation tends to decrease in both RCPs 4.5 and 8.5 but with a significant trend only for RCP 4.5 (p-value <0.05) (Figure 5.3). In this scenario, below-average precipitation occurred mainly between the years 2023 to 2038 and 2079 to 2099, with some specific years showing slightly above-average values. In RCP 8.5, the reduction was more prominent between 2015 to 2041 and 2086 to 2099. Except for the RCP 4.5 scenario (2040-2069), which showed an increase in average annual precipitation of 49 mm (+4%), all climate scenarios indicated a decrease. Average annual precipitation decreased by

195 mm (-14%) in the RCP 4.5 scenario (2070-2099), 94 mm (-7%) in the RCP 8.5 (2040-2069) scenario, and 19 mm (-1%) in the RCP 8.5 (2070-2099) scenario.

ET_0 showed a significant increasing trend for both RCP 4.5 and 8.5 (Figure 5.3), being more pronounced in RCP 8.5, where, except for a few years, almost all ET_0 values were higher than the long-term historical average. The RCP 4.5 scenarios (2040-2069) and RCP 4.5 (2070-2099) indicated increases of 24 mm (+2%) and 43 mm (4%), respectively, while in the RCP 8.5 scenarios (2040-2069) and RCP 8.5 (2070-2099), the increases were 55 mm (+5%) and 87 mm (7%), respectively.

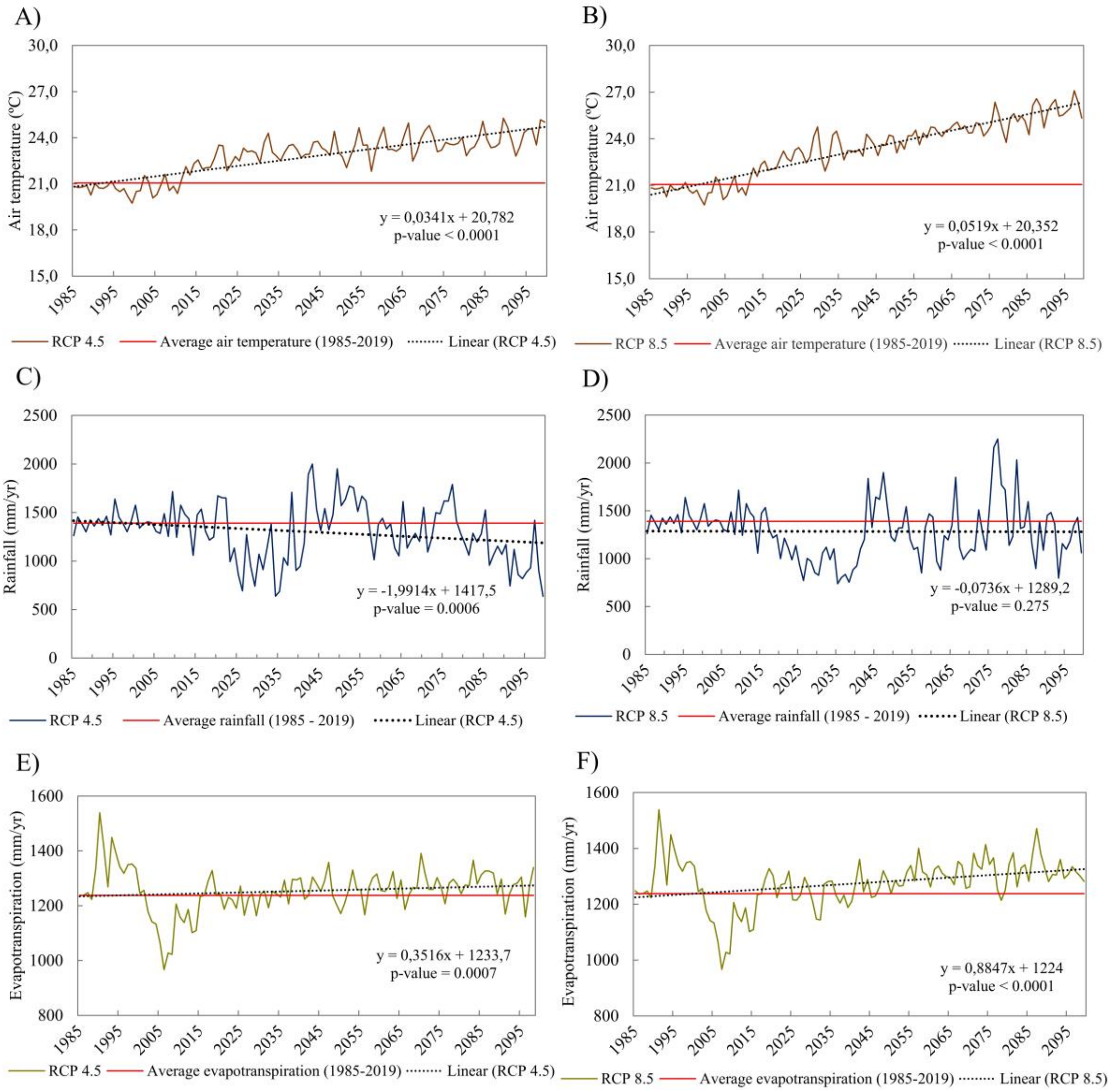

Figure 5.3. Trend of air temperature, precipitation, reference evapotranspiration, and p-values (Mann-Kendall). A) Air temperature trend for RCP 4.5 scenario, B) air temperature trend for RCP 8.5 scenario, C) precipitation trend for RCP 4.5 scenario, D) precipitation trend for RCP 8.5 scenario, E) reference evapotranspiration trend for RCP 4.5 scenario, F) reference evapotranspiration trend for RCP 8.5 scenario.

5.3.3. Effects of land use and land cover changes on ecosystem water services

The projected LULC scenarios showed distinct effects on WES indicators (Figure 5.4). Compared to the baseline, the trend scenario reduced the JGRB streamflow by 6% (Figure 5.5), representing a decrease of 23 mm. year^{-1} (Table 5.3). In the trend scenario, there was a 7% increase in QF and a 13% decrease in BF (Figure 5.5). Sediment export increased by about 106%, while sediment retention services increased by 33% (Figure 5.5). Similarly, TN export increased by 23%, while TN retention decreased by almost 11% (Figure 5.5). Exported TP increased by 24%, and its retention decreased by 10% (Figure 5.5).

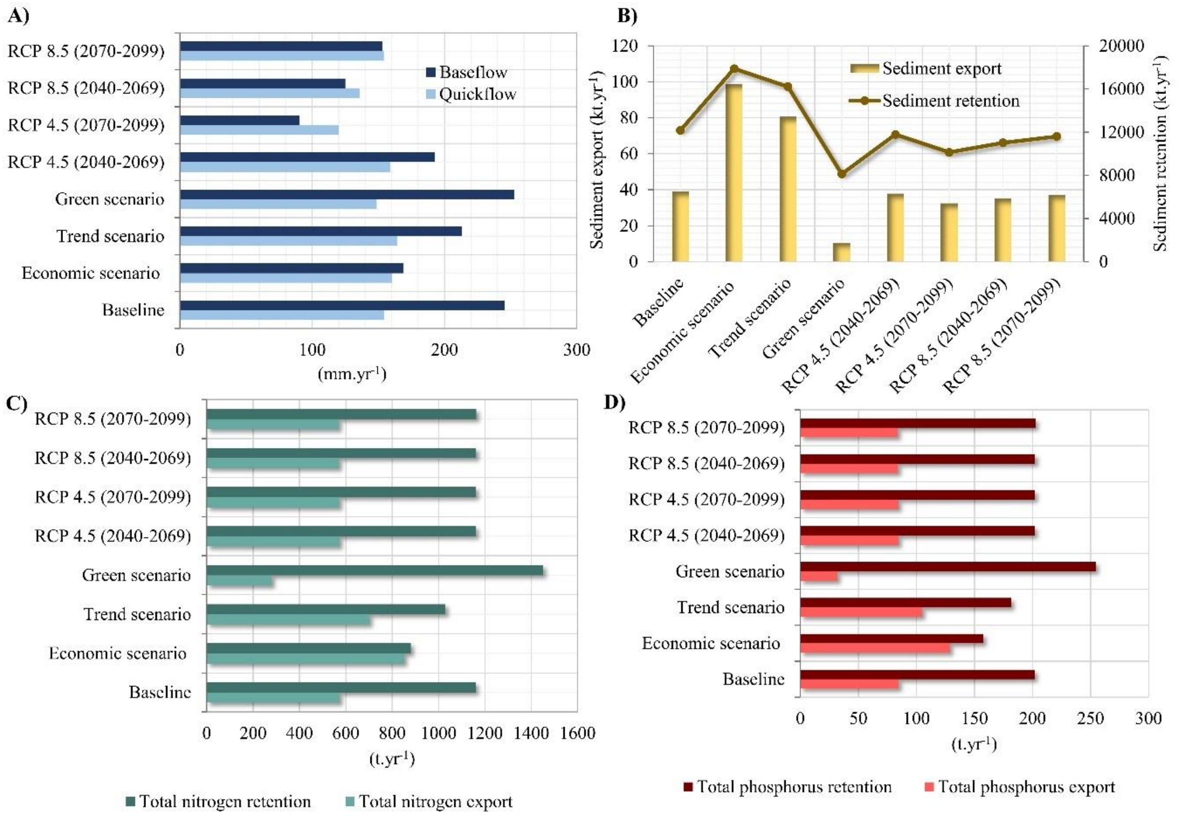

Figure 5.4. Individual response of climate and land use changes on water ecosystem services: A) quickflow and baseflow, B) sediment export and retention, C) total nitrogen export and retention, and D) total phosphorus export and retention.

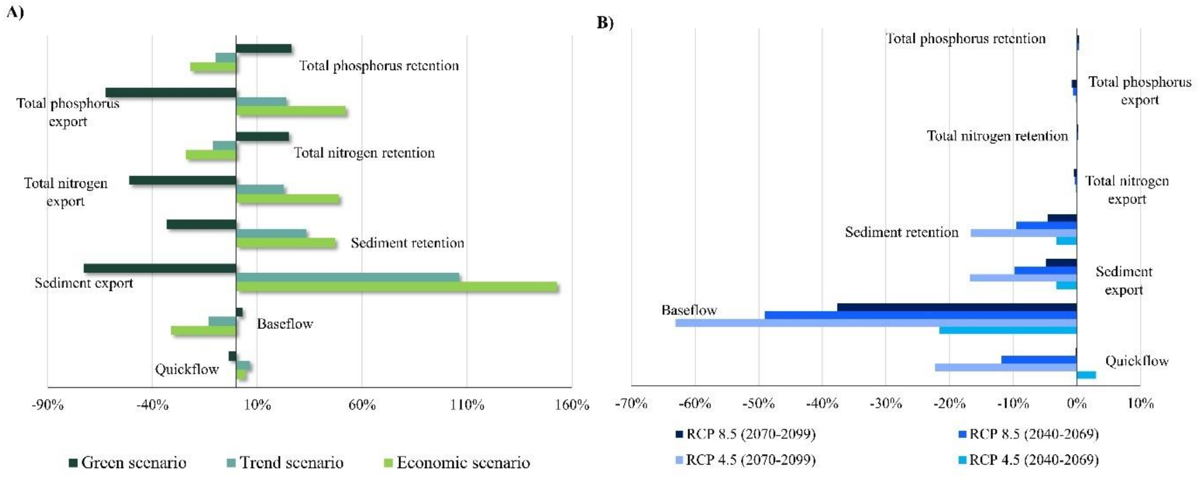

Figure 5.5. Proportion of changes in water ecosystem service indicators for the land use and land cover scenarios (A) and climate change scenarios (B) compared to the baseline.

Table 5.3. Simulated ecosystem service values for each climate and land use and land cover scenario.

	Baseline	**Economic scenario**	**Trend scenario**	**Green scenario**	**RCP 4.5 (2040-2069)**	**RCP 4.5 (2070-2099)**	**RCP 8.5 (2040-2069)**	**RCP 8.5 (2070-2099)**
Quickflow (mm. yr^{-1})	154	161	164	149	159	120	136	154
Baseflow (mm. yr^{-1})	245	169	213	252	193	91	125	153
Streamflow (mm. yr^{-1})	400	330	377	401	351	210	261	307
Sediment export (kt. yr^{-1})	39	99	81	11	38	33	35	37
Sediment retention (kt. yr^{-1})	12,171	17,891	16,220	8,132	11,784	10,144	11,019	11,613
Total nitrogen export (t. yr^{-1})	572	852	702	281	572	571	570	569

Total nitrogen retention ($t. yr^{-1}$)	1,160	880	1,030	1,451	1,160	1,161	1,162	1,163
Total phosphorus export ($t. yr^{-1}$)	85	129	105	32	85	84	84	84
Total phosphorus retention ($t. yr^{-1}$)	202	158	182	254	202	202	202	202

In the economic scenario, there was an 18% reduction (70 $mm. year^{-1}$) in JGRB streamflow compared to the baseline, with a 4% increase in QF and a 31% decrease in BF (Figure 5.5). There was a significant increase in sediment export and retention, with increases of 153% and 47%, respectively (Figure 5.5). TN and TP exports increased by around 50% in the economic scenario, and retentions decreased by approximately 23% (Figure 5.5).

Simulated streamflow for the green scenario remained close to the baseline (~400 $mm. year^{-1}$) (Table 5.3), but small changes in QF (-4%) and BF (+3%) were observed (Figure 5.5). The green scenario reduced sediment export by 73% and sediment retention by 33% (Figure 5.5). TN and TP exports decreased by 51% and 62%, respectively, and retentions for both nutrients increased by approximately 25% (Figure 5.5).

5.3.4. Effects of climate change on water ecosystem services

Climate changes had a more pronounced impact on the SWY model compared to the SDR and NDR models (Figure 5.4). Overall, all climate scenarios led to a reduction in streamflow, BF), and QF in the JGRB, except for the RCP 4.5 (2040-2069) scenario, which increased QF by 3% (Figure 5.5). In this scenario, BF decreased by 22%, and streamflow by 12%. For the RCP 4.5 (2070-2099) scenario, there was a decrease of 22% in QF, 63% in BF, and 47% in streamflow. The RCP 8.5 (2040-2069) scenario showed 12%, 49%, and 35% reductions in QF, BF, and streamflow, respectively. In the RCP 8.5 (2070-2099) scenario, there was no reduction in QF, but reductions of 38% and 23% were found for BF and streamflow, respectively.

The climate scenarios slightly reduced nutrient export and retention compared to the baseline (Figure 5.4), with percentages nearly negligible (~0%) (Figure 5.5). Sediment exports varied between 33 kt. year^{-1} and 38 kt. year^{-1}, and retentions between 10,144 kt. year^{-1} and 11,784 kt. year^{-1}, very close to the values simulated for the baseline (39 kt/year and 12,171 kt/year, respectively) (Table 5.3). The RCP 4.5 (2070-2099) scenario had the greatest impact on sediment dynamics in the JGRB, with a reduction of approximately 16% in sediment export and retention (Figure 5.5). The RCP 8.5 (2040-2069) was the second most influential scenario on sediment dynamics in the basin, followed by RCP 8.5 (2070-2099) and RCP 4.5 (2040-2069) (Figure 5.5).

5.3.5. Combined effects of climate and land use and changes on water ecosystem services

The combined effects of climate and LULC changes are presented in Figure 5.6, and Figure 5.7 shows the proportion of changes in indicators compared to the baseline. All twelve scenarios reduced the streamflow of JGRB but with variations in the magnitude of these effects. In general, scenarios of climate change associated with the economic land-use scenario (SC1, SC2, SC3, and SC4) demonstrated the most substantial reductions compared to the baseline (Table 5.4), followed by climate change scenarios related to the tendential (SC5, SC6, SC7, and SC8) and green (SC9, SC10, SC11, and SC12) land-use scenarios. Among these, scenarios SC2, SC6, and SC10 stood out with the most significant reductions in streamflow. The effects on QF varied, showing increases and decreases compared to the baseline. Scenarios SC1, SC4, SC5, and SC8 increased JGRB's QF, and all green land-use-related climate scenarios reduced the QF. All scenarios reduced JGRB's BF, but green scenarios exhibited the smallest reductions.

Sediment exports and retentions increased in climate scenarios combined with economic and tendential scenarios, and decreased in scenarios combined with green scenarios. Scenarios SC1 and SC4 most affected sediment dynamics in the study area, providing increases of 145% and 142%, respectively, for sediment exports, and 43% and 41%, respectively, for sediment retentions. Green scenarios reduced sediment exports by more than 70% and sediment retentions by more than 30%.

Climate scenarios associated with economic development also significantly affected nutrient exports, resulting in approximately 50% increases in TN and TP exports. Scenarios from SC5 to SC8 increased nutrient exports by around 23%, while green scenarios reduced TN exports by 50% and TP exports by over 60%. Nutrient retentions decreased by more than 20% in climate scenarios associated with the economic land-use scenario, around 10% in scenarios linked to the tendential land-use scenario, and increased by more than 25% in green land-use scenarios.

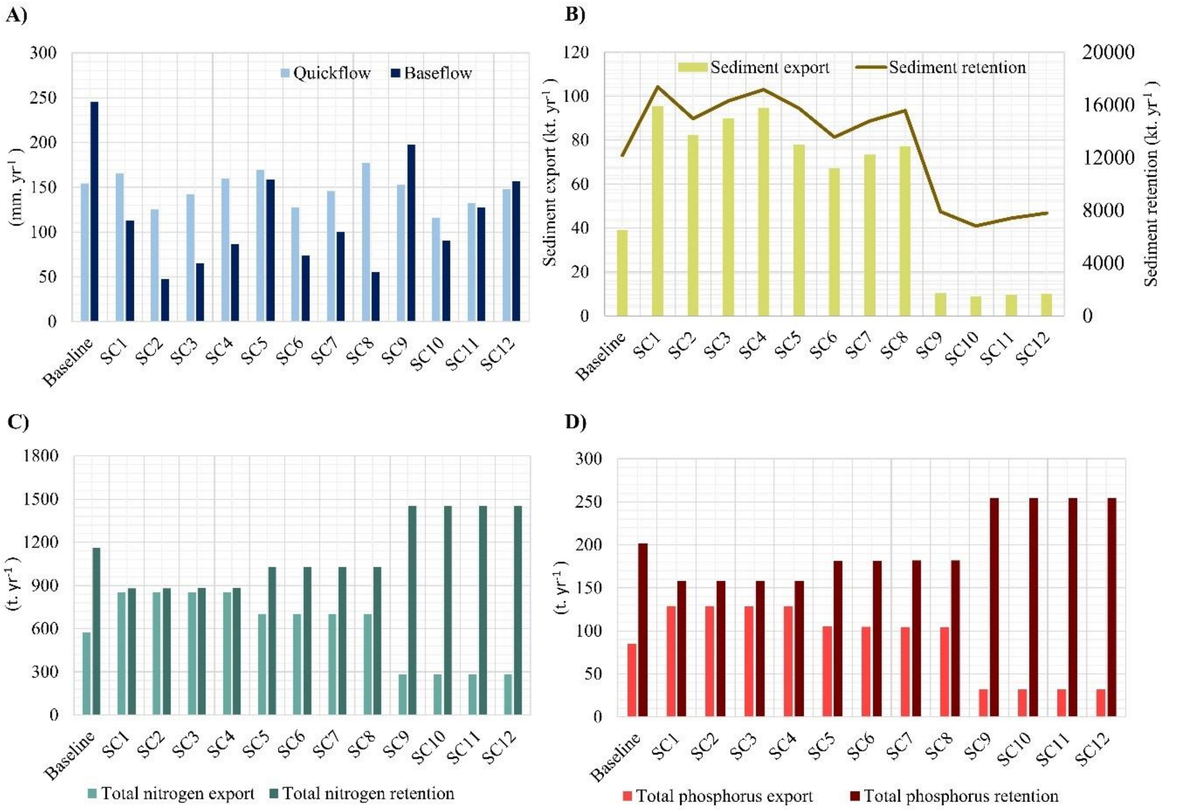

Figure 5.6. Combined effects of climate and land use changes on water ecosystem services indicators: A) quickflow and baseflow, B) Sediment export and retention, C) total nitrogen export and retention, D) total phosphorus export and retention.

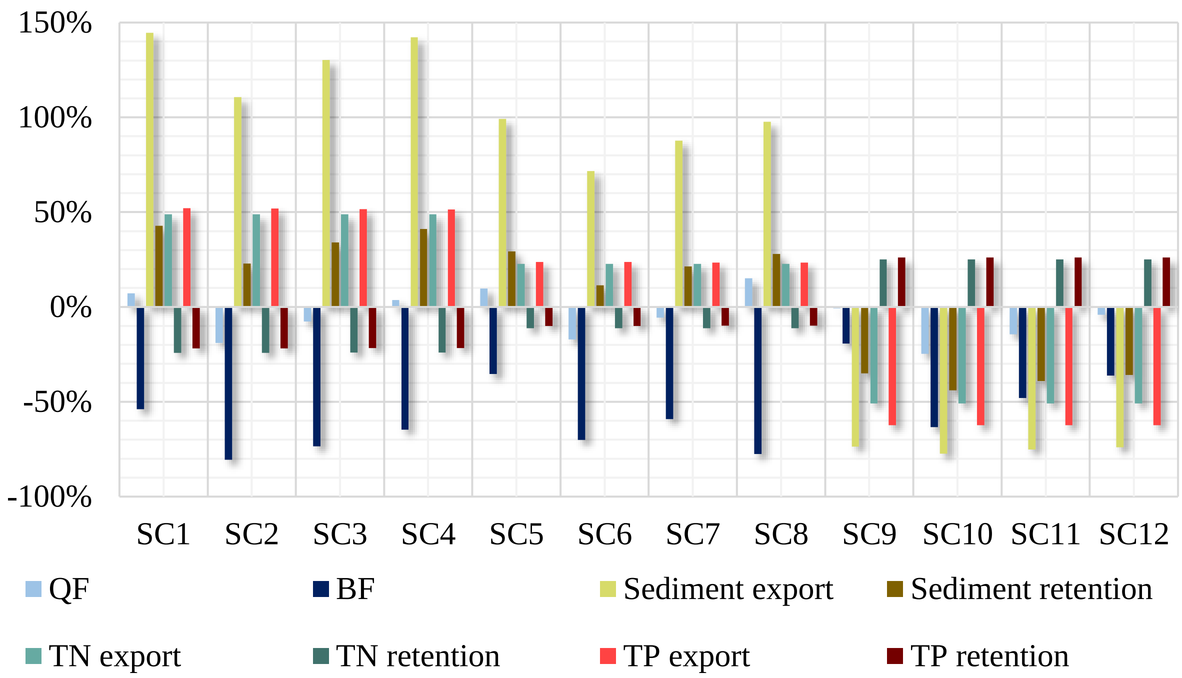

Figure 5.7. Proportion of changes in water ecosystem services indicators for combined scenarios compared to baseline.

Table 5.4. Simulated values of water ecosystem services for combined scenarios of climate change and land use and cover.

Scenarios	Quickflow (mm. yr^{-1})	Baseflow (mm. yr^{-1})	Streamflow (mm. yr^{-1})	Sediment export (kt. yr^{-1})	Sediment retention (kt. yr^{-1})	Total nitrogen export (t. yr^{-1})	Total nitrogen retention (t. yr^{-1})	Total phosphorus export (t. yr^{-1})	Total phosphorus retention (t. yr^{-1})
SC 1	165	113	278	96	17373	852	880	129	158
SC 2	125	48	173	82	14964	852	880	129	158
SC 3	142	65	208	90	16308	851	881	128	158
SC 4	160	87	246	95	17167	851	881	128	158
SC 5	169	159	328	78	15748	702	1030	105	182
SC 6	128	73	201	67	13565	702	1030	105	182
SC 7	146	100	246	73	14781	702	1030	105	182
SC 8	178	55	233	77	15567	702	1030	105	182
SC 9	153	198	351	10	7912	281	1451	32	254
SC 10	116	90	206	9	6817	281	1451	32	254
SC 11	132	128	260	10	7420	281	1451	32	255
SC 12	148	157	305	10	7804	281	1451	32	255

5.4. Discussion

The results of this study suggest that expanding green infrastructure through LULC planning can be a promising strategy to enhance WES provision and mitigate the effects of climate change. They highlight the relevance of these strategies in global warming mitigation, aligning with the recent Intergovernmental Panel on Climate Change (IPCC) report (IPCC, 2023) and other studies (CAPON et al., 2013; SUSSAMS et al., 2015; GRISCOM et al., 2017; SILVA; WHEELER, 2017).

Analyzing meteorological data for JGRB revealed a decreasing trend in annual precipitation, particularly in the RCP 4.5 scenario (p-value < 0.05), accompanied by a significant increase in the annual average air temperature and ET_0 throughout the century. These findings align with previous research in the state of São Paulo (FREITAS et al., 2022; Barbosa et al., 2023) and are consistent with the trend analysis of historical meteorological data for JGRB previously conducted by Neves et al. (2020b).

Similar to other research examining the impacts of climate and LULC changes on watershed hydrology (BAI et al., 2019; GUO et al., 2021; WANG et al., 2022; YIN et al., 2022), this study underscores the pronounced influence of climate change on water supply. These results were already expected, given the heightened sensitivity to precipitation observed in the SWY model when compared to the SDR and NDR models. Overall, the RCP 4.5 and 8.5 scenarios led to a decline in the basin's streamflow due to reduced precipitation and increased evapotranspiration. Of particular concern is the impact of climate change on BF, with reductions ranging from 22% to 63%. Although the study area covers the largest groundwater reservoir in South America (COSTA et al., 2019), the findings of this study raise concerns regarding the region's water availability. This is especially crucial when considering the observed declines over the years, particularly in groundwater availability, which has reached a critical state in UGRHI 13 (CBH-TJ, 2023). This underscores the urgency of addressing future climate change in water resources planning in the region.

Climate changes also affected erosion control services in JGRB but had a nearly negligible effect on water purification. Reduced precipitation decreased annual erosivity, the only climatic variable associated with sediment dynamics calculated by the SDR model (NATURAL CAPITAL PROJECT, 2022). The decline in erosivity led to decreased sediment exports and retentions in JGRB.

Climate changes had minimal impact on nutrient export and retention. This outcome is tied to how precipitation data are utilized in the NDR model. Precipitation in the model serves to modify nutrient load in the pixel to account for its potential surface runoff, based on an index relating local precipitation (pixel) to the average precipitation in the watershed (raster). The precipitation effect is more associated with its configuration in the watershed than its intensity. Therefore, once the spatial pattern of precipitation is preserved, the results obtained will be similar. These findings had been previously noted by Redhead et al. (2018).

The LULC changes exerted a more pronounced effect on erosion control and water purification services, also impacting, to a lesser extent, the water supply service of the JGRB. Similar outcomes were noted by Bai et al. (2019). The expansion of native vegetation in the green scenario moderately increased water supply (BF = 3% and streamflow = 0.4%), yet dramatically reduced sediment and nutrient exports while enhancing nutrient retention. These are direct benefits for erosion control and water purification. These results were expected for nutrient and sediment models, given the inherent potential of natural vegetation to regulate ecohydrological processes related to nutrient and sediment dynamics (TAMBOSI et al., 2015; RIIS et al., 2020). However, concerning water supply, outcomes vary, with some studies indicating increases in streamflow (LARA et al., 2021) and others showing decreases (FILOSO et al., 2017). The primary effect of vegetation on the hydrological cycle lies in partitioning precipitation into evapotranspiration and streamflow (JONEs et al., 2022), and the intensity of these effects varies based on the characteristics of plant species. This variability complicates the identification of a clear pattern in the effects. Other factors such as scale, management practices, geographic location, LULC history, and successional stage are also relevant and influence hydrological processes (ELLISON et al., 2017; JONES et al., 2022).

On the other hand, the increased anthropogenic activities in the trend and economic scenarios, primarily driven by sugarcane cultivation, diminished water supply, water purification, and erosion control services in the JGRB. These outcomes were expected for the basin, given the pronounced effects already evident from past LULC changes (1985 and 2019), as previously analyzed by Anjinho et al. (in press). Other studies conducted in the central-eastern region of the state of São Paulo have also underscored the impact of sugarcane expansion on the water quality of watercourses (TANIWAKI et al., 2017; COUTO-JUNIOR et al., 2019; ANJINHO et al., 2021).

The combination of climate and LULC scenarios resulted in increased sediment and nutrient exports and reduced nutrient retention. The inclusion of green scenarios mitigated these effects, emphasizing the crucial role of vegetation in regulating ecohydrological processes (SUN et al., 2017). All combined scenarios reduced both baseflow and streamflow in the JGRB compared to the baseline, but these effects were less intense in the green scenarios. Using different analytical methods, Ferreira et al. (2019) also observed the positive effects of reforestation on water availability in the southern metropolitan region of São Paulo, Brazil, highlighting its buffering impact against climate change.

Nature-based solutions (NBSs) are fundamental for adapting to climate change and expanding the provision of multiple ecosystem services (MANES et al., 2022). Ecological restoration stands out as a key adaptation strategy (CAPON et al., 2013; SUSSAMS et al., 2015; GRISCOM et al., 2017). In the ongoing study by Anjinho et al. (Chapter 4), the authors have already highlighted the potential of ecological restoration to increase the provision of WES in the JGRB. This study complements the land-use planning proposed by the authors. As per the Brazilian Forest Code (BRAZIL, 2012), the inclusion of legally protected areas enhanced previously calculated WES indicators, showcasing its potential for the study area. Another relevant instrument that could facilitate ecological restoration practices in the JGRB is the National Policy on Payments for Environmental Services (Federal Law No. 14,119/2021), which provides payments to providers of ecosystem services (BRAZIL, 2021). Considering that the JGRB is a rural watershed with more flexible LULC management compared to urban basins, implementing these legal instruments could be instrumental in facilitating ecological restoration projects in the region.

While the methodology employed in this study facilitated understanding the individual and combined effects of climate and LULC scenarios, it is crucial to acknowledge uncertainties and limitations that should be considered in interpreting the results. The InVEST models operate annually, meaning they do not capture seasonal variations in watershed hydrology. This limitation hinders the comprehension of the seasonal effects of climate change on WES. Despite the trend analysis indicating a reduction in annual precipitation and an increase in temperature and ET_0, the intensity and seasonality of these changes vary throughout the year. In the JGRB, for instance, approximately 80% of the annual precipitation occurs between late October and March (ANJINHO et al., 2022), intensifying surface runoff and sediment and nutrient exports during this period (Neves et al., 2021). The difficulty in capturing these seasonal effects also complicates understanding water availability, especially during low precipitation periods when climate and LULC changes may impact BF, something neglected in annual analyses.

In addition to seasonality, it is important to note that this study did not cover other ecosystem services. The effects of climate change may extend beyond the considered WES, impacting services such as climate regulation, habitat availability, pollination, carbon sequestration, among others, aspects not addressed in this research. Therefore, the limitation of these models in capturing seasonal variability and considering a broad range of ecosystem services complicates a comprehensive assessment of the effects of climate change in the studied watershed. For more precise evaluations, it would be necessary to turn to more refined models that account for seasonal variations and the diverse ecosystem services affected by climate change. However, for this study, the models proved to be efficient.

5.5. Conclusion

The methodology adopted in this study allowed for the assessment of the individual and combined effects of climate and LULC changes on WES indicators, enabling the testing of the viability of green scenarios based on increased native vegetation as a management strategy to enhance WES provision and mitigate adverse effects of climate change.

Projected climate changes resulted in a reduction of the water supply service, with a comparatively lesser impact on erosion control services. Nevertheless, sediment export and retention values were lower than those observed in the baseline. Notably, the water purification service remained unaffected by climate changes. This suggests a limitation in the NDR model's ability to assess the impact of climate changes on nutrient export and retention when there is no alteration in the spatial pattern of precipitation within the watershed.

LULC changes exhibited a more pronounced impact on erosion control and water purification services, with the economic scenario identified as the most detrimental to JGRB's WES. On the other hand, the green scenario demonstrated effectiveness in enhancing WES within the study area. In isolated effects, the green scenario led to increased BF, streamflow, and nutrient retention in the watershed while concurrently decreasing QF and exports of sediments, total TN, and TP. When integrated with climate scenarios RCP 4.5 and RCP 8.5, incorporating the green scenario mitigated the individual impacts of climate change, underscoring its potential to mitigate the effects of climate change.

The approach employed in this study offers valuable insights into ecological restoration as an effective strategy for preserving ecosystem services and addressing climate change. While the methodology has demonstrated efficiency and applicability to other regions, evaluating its limitations and interpreting the results with caution is imperative. Nonetheless, the findings highlight the utility of this methodology in guiding sustainable LULC planning to support the WES conservation.

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Chapter 6

FINAL CONSIDERATIONS.

This research aimed to enhance our understanding of how climate and land use changes impact water ecosystem services. The focus was on exploring how green land use scenarios can increase and mitigate the effects of climate change on these services. The analysis of the four articles developed in this research yielded valuable conclusions and guidance for future investigations. The following highlights the main recommendations and findings.

In the third chapter, when analyzing the performance of the InVEST biophysical models, the need for using complete sets of historical data and establishing an integrated and continuous monitoring system for streamflow and water quality was observed. The absence of an integrated monitoring approach in the studied basin compromises the accuracy in estimating nutrient and sediment loads, essential for model calibration and validation.

The annual values simulated by the InVEST biophysical models obscured the seasonal effects of climate and land use changes on basin hydrology, which can lead to misconceptions in water resource planning. Additionally, the proposed environmental zoning criteria were limited to erosion control, water supply, and water purification services, limiting the methodology's applicability. Thus, the adoption of more sophisticated models and a broader range of ecosystem services is suggested to develop comprehensive strategies that improve the provision of multiple ecosystem services. The use of artificial intelligence and the increased availability of satellite imagery can also assist in monthly and seasonal assessments of ecosystem services.

This research focused exclusively on the watershed scale to assess the impacts of climate and land use changes. Integration of InVEST models with hydraulic and water quality models is recommended for a more detailed analysis of water resources in the studied area. Such integration will allow for a deeper understanding of sediment and nutrient transport and dispersion in water bodies and facilitate a more accurate assessment of reservoir impacts on water, sediment, and nutrient flows, as well as water quality parameters.

Additionally, the inclusion of economic valuation and mapping of demand for ecosystem services in the studied watershed is suggested. This approach is essential to emphasize the importance of preserving ecosystem services in the region, providing a more solid foundation for decision-making in monetary and biophysical terms.

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