UNIVERSIDADE DE LISBOA
INSTITUTO SUPERIOR TÉCNICO

A Modeling Approach to Estimate the Impact of Climate and Societal Scenarios on Water Resources Quantity and Quality

Carina da Conceição Mendes de Almeida

Supervisor: Doctor Ramiro Joaquim de Jesus Neves
Co-Supervisor: Doctor Rodrigo de Almada Cardoso Proença de Oliveira

Thesis approved in public session to obtain the PhD Degree in
Environmental Engineering

Jury final classification: **Pass with Distinction**

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Abstract

The uncertainty in the future in terms of climate and societal behaviour is expected to increase. Mathematical models can be an efficient management tools to prevent and to study the impacts of climate and societal scenarios in water resources. Therefore, the central aim of this thesis is to assess the impacts of future climate and societal scenarios on water quantity and quality under an integrated modelling approach. The MOHID modelling system, the Soil Water Assessment Tool (SWAT) and the CE-QUAL-W2 model were adopted for this purpose.

First, it was investigated the effect of different watershed pressures scenarios including climate change in the hydrological regime and water bodies of the Sorraia River basin (Portugal). The SWAT model was used to simulate water flow and nutrient dynamics in the watershed while considering inputs from two climate models (GFDL-ESM2M and IPSL-CMA-LR) and three societal storylines. The results were indicative of a possible future outcome and may provide guidelines for defining preventive measures to minimize the effect of climate change and growth of environmental pressures in the Sorraia River basin. Afterwards, an integrated modelling approach was followed to investigate water use vulnerability in the Montargil reservoir (in Portugal) under different climate change projections. The SWAT and the MOHID Water models were used to evaluate the impacts of two climate scenarios (GFDL-ESM2M and IPSL-CM5A-LR) on water availability in Montargil's basin and reservoir during two decadal timelines (2030 and 2060). The impacts found indicate the importance of the managing systems in an integrative mode to prevent water resources reduction in the region. Subsequently, an integrated modelling approach was implemented to better understand the trophic status of the Montargil reservoir under climate change scenarios. The SWAT and CE-QUAL-W2 models were applied to the basin and reservoir, respectively, for simulating water and nutrient dynamics while considering the climatic scenario IPSL-CM5A-LR and two decadal timelines. The results showed that even considering measures that involve decreases in 30 to 35% of water use, the eutrophic state is not expected to improve. This raises issues related with fish survival and ecosystems stability, as also the objectives outlined by EU Water Framework Directive.

Besides the primordial investigation carried out, during this thesis, some parallel work was developed. The SWAT model results were integrated with empirical modelling within a common framework, allowing relationships among different ecosystem states to be hierarchized, interpreted and predicted at multiple spatial and temporal scales. The simulations of hydrological and nutrient enrichment stressors and empirical modelling allowed to relate stressors with biotic indicators. Similarly, the SWAT model results were

used in empirical models in order to model the effect of multiple stressors on several biological indicators of the Sorraia river water quality and, subsequently, to model the ecological status.

The outcomes of these test simulations confirm the potential of mathematical models to be considered as a valuable tool for engineering studies and water resources management, especially considering future changes scenarios.

Keywords: Mathematical Models; River Basin Management; Water Resources; Future Scenarios; Climate Change.

Resumo

No futuro é esperado que a incerteza no que diz respeito ao clima e comportamento social aumente. Os modelos matemáticos podem ser ferramentas eficientes de gestão para prevenir e estudar os impactes dos cenários climáticos e sociais nos recursos hídricos. Assim, o objetivo central desta tese é estudar os impactes de futuros cenários climáticos e sociais sobre a quantidade e a qualidade da água seguindo uma abordagem de modelação integrada. O sistema de modelação MOHID, o modelo SWAT (Soil and Water Assessment Tool) e o modelo CE-QUAL-W2 foram os modelos matemáticos adotados para esse fim.

Primeiramente, investigou-se o efeito de diferentes cenários de pressões em bacias hidrográficas, incluindo mudanças climáticas no regime hidrológico e albufeira da bacia do rio Sorraia (Portugal). O modelo SWAT foi usado para simular o caudal e a dinâmica de nutrientes na bacia, considerando os dados de dois modelos climáticos (GFDL-ESM2M e IPSL-CMA-LR) e três linhas sociais. Os resultados foram indicativos de um possível resultado futuro e podem fornecer diretrizes para a definição de medidas preventivas para minimizar o efeito da mudança climática e o crescimento das pressões ambientais na bacia do rio Sorraia. Posteriormente, seguiu-se uma abordagem de modelação integrada para investigar a vulnerabilidade do uso da água na albufeira de Montargil (no Sorraia, em Portugal) sob diferentes projeções de mudanças climáticas. Os modelos SWAT e MOHID Water foram utilizados para avaliar os impactes de dois cenários climáticos (GFDL-ESM2M e IPSL-CM5A-LR) na disponibilidade de água na bacia e no reservatório de Montargil durante duas décadas (2024-2035 e 2054-2065). Os impactes encontrados indicam a importância dos sistemas de gestão de forma integrada para evitar a redução dos recursos hídricos na região. Posteriormente, foi implementada uma abordagem de modelação integrada para melhor entender o estado trófico da albufeira de Montargil sob cenários de mudanças climáticas. Os modelos SWAT e CE-QUAL-W2 foram aplicados na bacia e na albufeira, respectivamente, para simular a dinâmica de água e nutrientes, considerando o cenário climático IPSL-CM5A-LR e duas décadas temporais. Os resultados mostraram que, mesmo considerando medidas que envolvem reduções em 30 a 35% do uso de água, o estado trófico da albufeira mantém-se no nível eutrófico. Isto levanta questões relacionadas

com a sobrevivência dos peixes e a estabilidade dos ecossistemas, como também os objetivos delineados pela Diretiva-Quadro Água da UE.

Além da investigação primordial realizada, durante esta tese, foram desenvolvidos alguns trabalhos paralelos. Os resultados do modelo SWAT foram integrados com a modelação empírica dentro de uma única estrutura, permitindo hierarquizar, interpretar e prever relações entre diferentes estados do ecossistema em múltiplas escalas espaciais e temporais. As simulações de *stressors* hidrológicos e de enriquecimento de nutrientes e modelação empírica permitiram relacionar *stressors* com indicadores bióticos. Da mesma forma, os resultados obtidos com o modelo SWAT foram utilizados em modelos empíricos para modelar o efeito de múltiplos *stressors* em vários indicadores biológicos da qualidade da água do rio Sorraia e, subsequentemente, para modelar o estado ecológico.

Os resultados destas simulações de teste confirmam o potencial dos modelos matemáticos para serem considerados como uma ferramenta valiosa para estudos de engenharia e gestão dos recursos hídricos, principalmente em cenários de alterações futuras.

Palavras-chave: Modelos Matemáticos; Gestão de Bacias Hidrográficas; Recursos Hídricos; Cenários Futuros; Alterações Climáticas.

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Gostaria em primeiro lugar de agradecer ao Prof. Ramiro Neves, pela oportunidade de realizar este trabalho, mas acima de tudo pela liberdade que me deu para pesquisar e aprender o que mais me motiva, pelo apoio e por todas as conversas cheias de conhecimento que tentei absorver. O meu grande obrigada. Ao Prof. Rodrigo Proença de Oliveira, por todas as ideias e opiniões, revisão e críticas construtivas que fez ao longo deste trabalho.

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Chapter 1 Introduction

1.1 Research Goals

Due to rapid population growth, the demand for natural resources and food has been growing. This increase has led to an expansion and intensification of agricultural activity in the last decades and resulted in a growing concern over the quality and quantity of water in rivers, aquifers and reservoirs. The urge to respond to environmental pressures, such as the ones driven by agriculture, is increasing through a more dynamic environmental activism and political impositions, stated in directives and other legal instruments.

In 2000, the European Water Framework Directive (WFD - European Commission, 2000) was published and become the core instrument of the European Union's water policy. The Water Framework Directive (WFD) established as a priority the protection and restoration of aquatic ecosystems and adopted a Drivers-Pressures-State-Impacts-Responses (DPSIR) framework (Voulvoulis et al., 2017; European Communities, 2003a), which aims to provide a systemic understanding of the relationship between environmental effects, their causes and measures taken (Nõges, 2002). This approach requires the development of River Basin Management Plans (RBMP) to achieve and guarantee the good status of all European water bodies, including ecosystems health, through the management of anthropogenic pressures (European Commission, 2000). Equally important, and included in the RBMPs, is the Programme of Measures (PoMs). The Programme of Measures is essential to comply with the legislation on water protection. After implementation of the initial defined PoMs, additional measures identified as necessary to meet the established environmental objectives may be necessary.

Fifteen years after the publication of the WFD, its objectives remain a challenge as 47% of EU surface waters have not reached the good ecological status in 2015 – a central objective of EU water legislation (EEA, 2012 ; European Commission, 2012a). In Portugal only 52% comply with the "good status" goal, according to the diagnosis of the National Water Plan (APA, 2015). According to Backes and van Rijswick (2015) the first WFD cycle, from 2009 to 2015, the number of surface water bodies in “good” state only increased by 10%.

Although the WFD is the core of Europe’s water policy, it is complemented by several other directives with more specific goals: the Directive 91/271/EEC concerning urban waste water treatment, which aims to protect the environment from the effects of urban waste water discharges and discharges from some industrial sectors; the Nitrate Directive

91/676/EEC which aims to protect water quality by preventing nitrates from agricultural sources and promoting good farming practices; the Marine Strategy Framework Directive 2008/56/EC, which establishes a framework for community action in the field of marine environmental policy; the Habitats Directive 92/43/EEC, which aims to ensure the conservation of a wide range of rare, threatened or endemic animal and plant species; and the Floods Directive 2007/60/EC, which aims to reduce and manage the risks floods, specially concerning to human health, the environment, cultural heritage and economic activity. The Blueprint to Safeguard Europe's Water Resources aims at better implementation of existing legislation, reviewing the state of implementation and the successes and pitfalls of these directives.

A recent report by the European Commission indicated that over 90% of RBMPs mentioned agriculture as a significant pressure in basins by contributing, naming particularly the excess of organic matter, nutrients and pesticides. Farm management practices are an integral part of RBMPs due to the frequent field operations, such as fertilizer management, can address non-point source pollution (Cherry et al., 2008). According to Volk et al. (2008), Patoine et al. (2012) and Green et al. (2014) these farm practices can compromised water quality status . Also, the report "Status of Europe's Waters" published by the European Environment Agency (EEA, 2012) lists the most important stressors such as the nutrient enrichment and eutrophication, sediment and pesticide pollution, water abstraction, flash floods, bed and bank modification, and removal of riparian vegetation. Pressures are predicted to intensify in the future given the increase of water demand for agriculture and energy. Moreover, in a scenario of climate change, there is an uncertainty about the real future of water resources availability.

Recently the United Nations resolution entitled "Transforming our world: the 2030 Sustainable Development Agenda" (UN News Centre, 2015), targets 17 objectives, including the availability and sustainable water management for all, and urgent action to combat climate change and its impacts.

Climate change might impact hydrologic processes of watersheds and their reservoirs (IPCC, 2013). In the Mediterranean region this change will possible have a severe effect (IPCC, 2013). According to the Framework Convention on Climate Change (UNFCCC, 2013), climate change is directly or indirectly related with anthropogenic activities and climate variability is related to natural causes. According to the IPCC (2013), Mediterranean region will be mainly affected by extreme events regarding temperature and precipitation in two extreme seasons: a cold season with extreme precipitation events, and a hot season with high temperatures combined with water scarcity. In most prediction studies, climate change may impact nitrogen and phosphorus loads to a greater extent than land use changes (Mehdi et al., 2015).

Since agricultural land can have such a variety of effects on water quality, investigating potential land use and management changes in a basin is necessary to achieve the WFD objectives which will be evaluated during the planning cycles ending in 2021 and 2027. In light of the foregoing, and considering the complexity of watersheds processes, a more sustainable and holistic approach to water management should be consider.

The development of scientific knowledge and computer tools evolved and are now able to respond to the complexity of physical and chemical processes implicit in nature, in particular in the water bodies. Therefore, mathematical models are now acceptable as capable tools to support the design of effective policies.

To determine the degree of impacts of future climate change combined with land use practices, hydrological models are required to explore these influences on surface water quality. Simulation studies have shown that when the vegetation cover is strongly altered, significant impacts to important hydrological processes such as surface runoff, infiltration or evaporation can occur that may be exacerbated by future climate simulations (Pervez and Henebry, 2015; Seo et al., 2018; Wang et al., 2009; Zhang and Werner, 2009). The importance of using predictive models to simulate conditions of water bodies is implicitly defined in the Portuguese Decree-Law no. 77/2006, of March 30, Annex III. Modelling water quality has many advantages, since models allow to analyse present and future state, integrating changes and environmental factors.

The uncertainty in the future in terms of climate and societal behaviour is expected to increase. Although there are already many studies which use mathematical models for predicting water quantity and quality, a more in-depth view is needed for each case study, analysing the processes at the watershed and reservoir scale. This approach should always be carried out in an integrated way, thus continuously allowing scenarios variation and different analytical methodologies in order to effortlessly support water managers and its needs. As so, mathematical models should be an efficient management tools to prevent and to study the impacts in water resources. Therefore, the objectives of the thesis are:

1. To access the impacts of future climate and societal scenarios on water quantity and quality under a basin scale modelling approach;

2. To access the future water demand vulnerability in a reservoir scale under an integrated modelling approach;

3. To access the future trophic status of a reservoir under climate change under an integrated modelling approach.

1.2 Context

The candidate started to work as a researcher at MARETEC in 2009, in mathematical models at different scales: plot, reservoir and watershed. In 2016, the candidate began to work simultaneously in the AQUALOGUS Company, where she continue to develop competences in the scope of mathematical modelling, climate change and water resources management engineer.

From 2009 to 2019 she implement different models (MOHID Land and Water, SWAT, SWMM, and CE-QUAL-W2) in different areas (Portugal, Brazil, Mozambique, Zimbabwe, Greece, Netherlands, etc.), during several national and international research projects, as well as the Sado and Guadiana River Basin Management Plans (2011) and different consultancy projects. The Sorraia river basin was the most studied case by the candidate: an irrigation service was developed with the MARETEC group, with application of plot models with high resolution, where an exhaustive field and modelling work was developed (projects Aquapath-Soil, MyFarm, Figaro, Sensyf, and Irrigasys); study of future scenarios in the basin (MARS project), and the development of detailed reservoir models to be managed operationally (OMeGA project, ongoing with AQUALOGUS and MARETEC), are some examples of work carry out in the Sorraia Basin.

Because of the importance of the Sorraia Valley in Portugal, in particular due to agriculture significance, and being representative of the Mediterranean region in terms of climate, the candidate decided to deepen her knowledge in the climatic and development scenarios, due to the relevance today and in the future, using models as a tool. She hopes, with this thesis, to contribute to water management improvement, showing the importance of this tools in a predictive perspective.

Some of the work published as author and co-author during the PhD period:

Navarro E., Segurado P., Branco P., **Almeida C.**, Andersen H., Predicting the ecological status of rivers and streams under different climatic and socioeconomic scenarios using Bayesian Belief Networks. Limnologica 2019 (submitted).

Almeida, C.; Ferreira T.; Branco, P.; Segurado, P.; Ramos, T.B.; Neves, R.; Proença de Oliveira, R. Evolution of the Trophic Status in a Mediterranean Reservoir under Climate Change: An Integrated Modelling Approach. Hydrology Research 2019 (submitted).

Almeida C., Ramos T., Sobrinho J., Neves R., Proença de Oliveira R. (2019). An Integrated Modelling Approach to Study Future Water Demand Vulnerability in the Montargil Reservoir Basin, Portugal. Sustainability. 11. 206. 10.3390/su11010206.

Mateus M., Vieira R., **Almeida C.**, Silva M., Reis F. (2018). ScoRE—A Simple Approach to Select a Water Quality Model. Water. 10. 1811. 10.3390/w10121811.

Almeida C., Ramos T, Segurado P., Branco P., Neves R., Proença de Oliveira R. (2018). Water Quantity and Quality under Future Climate and Societal Scenarios: A Basin-Wide Approach Applied to the Sorraia River, Portugal. Water. 10. 1186. 10.3390/w10091186.

Santos, C., **Almeida C**., Ramos T., Rocha F., Proença de Oliveira R., Neves R. (2018). Using a Hierarchical Approach to Calibrate SWAT and Predict the Semi-Arid Hydrologic Regime of Northeastern Brazil. Water. 10.3390/w10091137.

Deus S, Neves R., Jauch, E, **Almeida C.,** Faial K., Medeiro A., Mendes R., Faial K., Leite J., Deus, R.. (2018). Streamflow forecasts due precipitation water in a tropical large watershed at Brazil for flood early warning, based on SWAT model. 4. 10.5935/2447-0228.20180027.

Segurado P., **Almeida C.,** Neves R., Ferreira T., Branco P., (2017) Understanding multiple stressors in a Mediterranean basin: combined effects of land use, water scarcity and nutrient enrichment, Science of the Total Environment, 624, 1221–1233. https://doi.org/10.1016/j.scitotenv.2017.12.201;

Ramos T.B., Simionesei L., Jauch E., **Almeida C.,** Neves R., (2017) Modelling soil water and maize growth dynamics influenced by shallow groundwater conditions in the Sorraia Valley region, Portugal, Agricultural Water Management, 185, 27–42. https://doi.org/https://doi.org/10.1016/j.agwat.2017.02.007;

Simionesei L. Ramos T., Brito D., Jauch E. Leitão P., **Almeida C**., Neves R.,(2016) Numerical simulation of soil water dynamics under stationary sprinkler irrigation with MOHID-LAND. Journal of Irrigation and Drainage 2016 https://doi.org/10.1002/ird.1944;

Silva M., Aguiar A., Neves R., Vasco A., **Almeida C.,** Faccioli G., (2015) Sensitivity analysis and calibration of hydrological modeling of the watershed Northeast Brazil Journal of Environmental Protection 06(08):837-850 10.4236/jep.2015.68076 2015;

Mateus M., **Almeida C**., Brito D., Neves R.; From Eutrophic to Mesotrophic: Modelling Watershed Management Scenarios to Change the Trophic Status of a Reservoir. Int. J. Environ. Res. Public Health 2014, 11(3), 3015-3031;

Almeida C, Branco P, Segurado P, Ferreira T, Neves R, Water Quantity And Quality Under Future Climate And Development Scenarios: A Basin-wide Approach." 14th International Water Association (IWA) Specialist Conference on Watershed and River Basin Management, South Africa. October 2017 (winner of the Best Presenter Award)

Almeida C., Sobrinho J., Jauch E., Neves R., Integrated modeling approach to study the impact of reservoirs in the watershed: the case study of the Sorraia River basin. EWRA 2015 - 9th World Congress of the European Water Resources Association, Turquia, Istambul, 10 - 13 Junho 2015.

1.3 Thesis Structure

The structure of this thesis is based on the objectives described above.

Chapter 2 – State of the art, focused on the mathematical modelling methodology.

Chapter 3 presents the application of the SWAT hydrological model to investigate water quantity and quality under future and societal scenarios in the Sorraia river basin.

Chapter 4 integrates the results from the SWAT model applied in previous chapter in the MOHID WATER reservoir model to study future water demand vulnerability in the Montargil Reservoir.

Chapter 5 integrates the results from the SWAT model applied in the Chapter 3 in the CE-QUAL-W2 reservoir model to study the trophic status under climate change in the Montargil Reservoir.

Chapter 6 provides a general conclusion related to the accomplishment of the objectives of this thesis, as well as recommendations for future work.

The last part of this thesis (**APPENDIXES**) includes three papers with some relevant work done throughout this period. This work shows the importance of integrating modelling in different approaches.

Chapter 2 State of the Art

2.1 Mathematical Modelling

Mathematical modelling is a world-wide tool with the purpose of assisting the study of processes in nature, tracing scenarios and supporting management decisions. These include studying water balance of a water body, analysing or predicting flood events, analysing risks of erosion and its origin, studying water quality issues or assisting the operation of reservoirs, among others. Models are commonly categorised as physical-based or empirical-statistical depending on the basis of the extent to which they represent the physics of the processes involved. Physical-based models incorporate equations that express hydrologic dynamics and transport. Empirical-statistical models derive functional relationships between hydrologic variables. Each method has advantages and disadvantages and usually the choice of method depends on the data available and the purpose of the simulation. Mathematical models can be classified as deterministic or stochastic (non-deterministic). A significant difference between these two model types consists of the quantitative results of the simulated variables. Deterministic models result in discrete values for it state variables. In water quality models, for example, this result is generally expressed in the parameters concentrations. Stochastic models, on the other hand, present ranges of values, specifying the probability (in %) of the state variables results to be within the ranges adopted. With the increasing of computer capacity that has been verified over the last decades, deterministic models (process oriented and distributed in space and time) have been used more regularity. Models can be spatial represented as lumped, distributed or pseudo or semi-distributed. In lumped models the dependent variables are a function of time, and in distributed models dependent variables are functions of time and one or more spatial variables. A semi-distributed model is a variation of the lumped method and is sometimes referred to as a pseudo-distributed approach.

In 1822-1922, Mulvaney's developed the rational formula, as considered as the first mathematical hydrological model. In the 50's - 60´s the Stanford Watershed Model (SWM) elaborated by Crawford and Linsley in 1966 was developed focussing on water, named rainfall-runoff modelling (Donigian A and Imhoff, 2006).

Since then, a wide range of hydrological models has been developed. Models use to simulate basins hydrology and water quality have been used on a large scale and are crucial in a modern water management: the SWAT – Soil and Water Assessment Tool (Neitsch et al., 2009) from USDA Agricultural Research Service (USDA-ARS) and Texas A&M AgriLife Research, part of The Texas A&M University System, a two-dimensional model derived from the SWRBB (Arnold et al. 1990), CREAMS, GLEAMS, EPIC and QUAL2E models, and focused on land management at river or basin scale and; the HSPF - Hydrologic Simulation Program Fortran (Donigian et al., 1984) from U.S. EPA that simulates the watershed hydrology and water quality for both conventional and toxic organic pollutants; the MIKE SHE model (Refsgaard and Storm, 2005) from Dutch Hydraulic Institute, as one of the references in a generation of physically based, integrated, distributed watershed models; and the MOHID Land model developed by MARETEC at IST- UTL as an integrated model grouping 4 mediums (atmosphere, porous media, soil surface and river network) and with water movement through the mediums based on mass and momentum balances (Trancoso et al., 2009). The MIKE SHE and MOHID Land models are extremely detailed and the main difference between them is the spatial method to solve equations where finite differences is used in the MIKE SHE model and finite volumes in the MOHID Land.

On the other hand, models have been developed to study the hydrodynamics and water quality processes in larger water bodies such as reservoirs, including: the WASP - Water Quality Analysis Simulation Program (Wool et al., 2003) from U.S. EPA with the capability to simulate water and water quality constituents transport; the SisBaHIA (Sistema Base de Hidrodinâmica Ambiental), developed by COPPETEC - COPPE/UFRJ (Rio de Janeiro, Brazil) to simulate coastal and in-land water bodies (Rosman, 2001), which is composed of a 3D hydrodynamic model coupled to a water quality model; the QUAL2Kw, which is the recent development of models in the QUAL 2 series (Pelletier et al., 2006), released by the U.S. EPA, is a 1D steady-state model for rivers, tributaries and well-mixed lakes; the CE-QUAL-W2 model (Cole and Wells, 2015) from US Army Corps of Engineers that is a laterally averaged 2D hydrodynamic and water quality, and the 3D numerical MOHID Water (Neves, 1985; (Braunschweig et al., 2003; Deus et al., 2013) from MARETEC (Marine and Environmental Technology Research Center) at Instituto Superior Técnico (IST) which belongs to Technical University of Lisbon (UTL).

To formulate hypotheses about the basin dynamics, and to simulate several scenarios in complex watersheds with reservoirs, many works have been done, using the integrated modelling approach, such as Xu et al. (2007) that studied the calibration and validation of inked models HSPF and CE-QUAL-W2 in a Virginia, USA watershed, or Debele et al. (2008) that used SWAT and CE-QUAL-W2 to study the upland watershed and downstream waterbody hydrodynamic and water quality. In Portugal, Portuguese Water Institute (INAG – Instituto Nacional da Água) carried out an integrated modelling study of the trophic levels of 30 reservoirs under the scope of the Waste Water Treatment Plant directive (INAG, 2009). Specifically in the Southern Portugal, where more eutrophication and water management issues occurred, Brito et al. (2018) integrated the SWAT and CE-QUAL-W2 models, to study the water quality in the Enxoé eutrophic, or Fontes (2010) where Alqueva Reservoir was modelled to access the water quality and consequently the trophic state.

2.2 Conceptual Modelling - Watershed

A watershed is defined by natural topographic boundaries and usually involve complex ecosystems or highly urbanized and anthropogenic areas. Watershed processes can be fragmented into functions and characteristics, including: soil processes and erosion, nutrient cycling, pollution transport, riparian habitat and stream buffers, stream morphology and channel characteristics, hydrology, and water quality.

A watershed is a three-dimensional (3D) entity, where it is assumed the river network as 1D domain defined from the digital elevation model, the surface land as 2D horizontal dimension and the soil as a 3D domain including the surface land (Figure 2.1). The three-dimensional models can therefore describe the complex processes with accuracy.

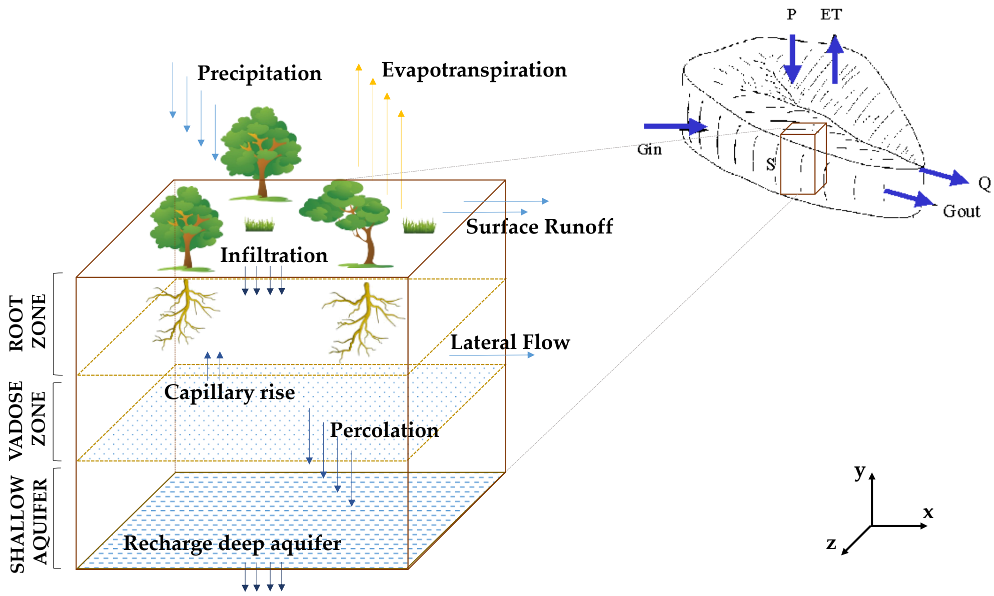

Figure 2.1 Schematic view of the three-dimensional structure in a watershed.

MOHID Land is an example of a 3D model which can described the watershed processes with high detailed. MOHID Land is a physically-based and spatially distributed model, continuous and with a variable time step for the water and property cycles occurred in watersheds. The model is based on finite-volumes organized into a structured grid, rectangular in the horizontal plane, and Cartesian type in the vertical plane. Fluxes are computed over the faces of the finite volumes and state variables are computed at the centre to assure conservation of transported properties.

MOHID Land is an integrated model with four compartments or mediums (atmosphere, porous media, soil surface, and river network). Water moves through the mediums based on mass and momentum conservation equations. The atmosphere is not explicitly simulated but provides data necessary for imposing surface boundary conditions to the model (precipitation, solar radiation, wind, etc.) that may be space and time variant.

Due to the complexity and computational demand of the 3D models the use of these models may have limitations:

- Simulations of large basins with high resolution;
- The need of testing different management strategies, where can be performed without excessive investment of time or money;
- To study long-term impacts.

Therefore, in this thesis, to assess the future impacts on a river basin, under different climatic and social scenarios, involving long-term analysis, the SWAT model was chosen. A comparative analysis was developed for several existing models showed in Appendix III (Mateus et al., 2018). In the future, and with the computer evolution, mathematical model will tend to be 3D. It is described below the model functionalities used in this thesis.

The Soil and Water Assessment Tool (SWAT)

The SWAT is a 2D model widely used to simulate watershed processes (Neitsch et al., 2009). SWAT is a semi-distributed watershed model focused on land management at a basin scale, and most of the formulas are empirical. The model splits the watershed into sub-basins, and each sub-basin is divided by areas with the same land use, soil and topographic characteristics, which form a Hydrologic Response Unit (HRU); a basic computational unit assumed to be homogeneous. The soil domain may be divided into vertical layers. The relative straightforward formulation used in SWAT allows the model to run more demanding simulations within a reasonable time. The hydrology of the model is based on the daily water balance equation, as follows:

$$SW_t = SW_0 + \sum_{i=1}^{n} (R_{day} - Q_{surf} - E_a - W_{seep} - Q_{gw}) \qquad \text{Equation 2.1}$$

Where:
SW_t is the final soil water content (mm),
SW_0 is the soil water content at the initial time step (mm),
R_{day} is the daily precipitation (mm),
Q_{surf} is the surface runoff (mm),
E_a is the actual evapotranspiration (mm),
W_{seep} is the percolated water (mm),
Q_{gw} is the return flow (mm),
all referring to day i, which varies from 1 to the number of simulated days (n).

The surface runoff is computed from daily precipitation using the empirical formula of the Soil Conservation Service Curve Number (SCS-CN) method (Mishra and Singh, 2003).

$$Q_{surf} = \frac{(R_{day} - I_a)^2}{(R_{day} - I_a + S)} \qquad \text{Equation 2.2}$$

Where:

I_a is the initial abstractions which includes surface storage, interception, and infiltration prior to runoff (mm),

S is the retention parameter which varies with the soil type, land use, land management, slope, and soil water content.

When the water leaves the deepest soil layer by percolation, it can recharge the shallow and deep aquifers according to a fraction established by the user. These fraction is crucial during the calibration process. The recharge formulation is based on an exponential function proposed by Sangrey et al. (1984), and depends on the soil water retention capacity, the antecedent conditions and a parameter called GW_DELAY. The equation simulates the time delay since the water exits the soil profile until it recharges the aquifers.

$$W_{rchrg,i}=\left[1-\exp\left(\frac{-1}{GW_{DELAY}}\right)\times W_{seep}+\exp\left(\frac{-1}{GW_{DELAY}}\right)\right]\times W_{rchrg,i-1} \qquad \text{Equation 2.3}$$

Where:

$W_{rchrg,i}$ is the amount of recharge entering the aquifers on day i (mm),

GW_DELAY is the delay time of the overlying geologic formations (d),

W_{seep} is the percolation from the deepest layer, that is the total amount of water exiting the bottom of the soil profile on day i (mm),

$W_{rchrg,i-1}$ is the amount of recharge entering the aquifers on day i-1 (mm).

Shallow aquifer can contribute to the rivers baseflow. In SWAT model the constant baseflow recession, expressed by the ALPHA_BF parameter. The ALPHA_BF parameter is established by the user, and crucial during the calibration process. This parameter is a direct index of groundwater flow response to changes in recharge (Smedema and Rycroft, 1983):

$$Q_{gw,i}=Q_{gw,i-1}\times\exp(-ALPHA_{BF}\times\Delta t)+Q_{rchrg,sh}\times(1-\exp(-ALPHA\_BF\times\Delta t)) \qquad \text{Equation 2.4}$$

Where:

$Q_{gw,i}$ is the groundwater flow into the main channel on day i (mm),

$Q_{gw,i-1}$ is the groundwater flow into the main channel on day i-1 (mm),

ALPHA_BF is the baseflow recession constant (-),

Δt is the time step (d),

$W_{rchrg,sh}$ is the amount of recharge entering the shallow aquifer on day i (mm).

In SWAT model the potential evapotranspiration can be calculated with the method of Hargreaves (Hargreaves et al., 1985), Priestley-Taylor method (Priestley and Taylor 1972) or by the Penman Monteith (Monteith, 1965). The latter method, considered in this thesis, is referred as an international standard method, being widely used:

$$ET_0=\frac{0.408\,\Delta(R_n-G)+\gamma\frac{900}{T+273}u_2(e_s-e_a)}{\Delta+\gamma(1+0.34u_2)}$$ Equation 2.5

Where:
ET_o reference evapotranspiration [mm day^{-1}],
R_n net radiation at the crop surface [MJ m^{-2} day^{-1}],
G soil heat flux density [MJ m^{-2} day^{-1}],
T mean daily air temperature at 2 m height [°C],
u_2 wind speed at 2 m height [m s^{-1}],
e_s saturation vapour pressure [kPa],
e_a actual vapour pressure [kPa],
e_s - e_a saturation vapour pressure deficit [kPa],
Δ slope vapour pressure curve [kPa $°C^{-1}$],
γ psychrometric constant [kPa $°C^{-1}$].

The actual evapotranspiration is calculated as the sum of three components: evaporation from plant canopy, plant transpiration and soil evaporation. For the calculation of transpiration the leaf area index (LAI) is necessary. This parameter is estimated for each HRU using a standard plant growth. SWAT calculates the potential plant growth for each day of simulation as a function of the energy that plant intercepts and the efficiency of its conversion into biomass. The energy is estimated as a function of solar radiation and leaf area index. The maximum biomass growth is dependent on the quantity of photosynthetically active radiation intercepted by leaves and the efficiency of radiation use. Actual growth and actual LAI are dependent on the stress factors such as water, temperature and nutrients. Whenever the base temperature is higher than the base temperature of the plant, growth is accumulated. The difference between daily temperature and the base temperature of the plant accumulated daily basis is called the "heat unit". Optimal LAI is related with crop stage which in turn depends on the crop heat units. These heat units are defined in the SWAT database for each crop. Therefore LAI is simulated as a function of heat units:

$$fr_{PHU}=\frac{\sum_{i=1}^{d}HUi}{PHU}$$ Equation 2.6

Where:
fr_{PHU} is the fraction of potential heat units accumulated for the plant on day d in the growing season,
HU is the heat units accumulated on day i (heat units),
PHU is the total potential heat units for the plant (heat units).

LAI is defined as the area of green leaf per unit area of land (Watson, 1947). Once the maximum LAI is reached, it remains constant until leaf senescence begins to exceed leaf growth. Once leaf senescence becomes the dominant growth process, the LAI is calculated as (Neitsch et al., 2009):

$$\mathrm{LAI} = 16\,\mathrm{LAI}_{\mathrm{mx}}\,(1 - \mathrm{fr}_{\mathrm{PHU}})^2 \qquad \text{Equation 2.7}$$

Where:

LAI is the leaf area index for a given day,

LAI_{mx} is the maximum leaf area index,

fr_{PHU} is the fraction of potential heat units accumulated for the plant on a given day in the growing season.

Therefore the total leaf area index for a given day is calculated in SWAT as:

$$\mathrm{LAI}_i = \mathrm{LAI}_{i-1} + \Delta\mathrm{LAI}_i \qquad \text{Equation 2.8}$$

Where:

ΔLAI_i is the leaf area added on day i,

LAI_i and LAI_{i-1} the leaf area indices for day i and i-1 respectively.

Water which is not evapotranspirated nor infiltrated in the soil due to field capacity condition, is superficially drained. Surface runoff is a major component of the water cycle and it is the primary agent along with precipitation, in soil erosion by water. Soil erosion in SWAT is computed from rainfall and surface runoff with the Modified Universal Soil Loss Equation (MUSLE) (Williams, 1975), which is a modified version of the Universal Soil Loss Equation (USLE) developed by Wischmeier and Smith (1978). In MUSLE, the rainfall energy factor is replaced with a runoff factor, as follows:

$$\mathrm{sed} = 11{,}8 \times \left(Q_{surf} \cdot q_{peak} \cdot area_{hru}\right)^{0{,}56} \times K_{USLE} \times C_{USLE} \times P_{USLE} \times LS_{USLE} \times CFRF \qquad \text{Equation 2.9}$$

Where:

sed is the sediment yield on a given day (ton),

q_{peak} is the peak runoff rate ($m^3\ s^{-1}$),

$area_{HRU}$ is the area of the HRU (ha),

K_{USLE} is the USLE soil erodibility factor,

C_{USLE} is the USLE cover and management factor,

P_{USLE} is the USLE support practice factor,

LS_{USLE} is the USLE topographic factor,

CFRG is the coarse fragment factor.

The erosion process is very relevant for the entrainment of nutrients to the aquatic system, as well as for soil impoverishment. The nutrient component includes inputs from agriculture, transport with runoff and groundwater, consumption by plants, and mineralization processes occurring in the soil (Neitsch et al., 2009). The SWAT model can further simulate the nitrogen (N) and phosphorus (P) cycles.

The N present in the soil is represented by five different pools, considering mineral and organic forms. The mineral N is divided into two pools: ammonia (NH_4^+) and nitrate (NO_3^-). The organic N is divided into three pools: active, stable (associated to the humic substances) and fresh pool (associated to the crop residue). N transport occurs mainly in the nitrate and organic N forms. Nitrate may be transported with surface runoff, lateral flow or percolation, using the following generic formula (Neitsch et al., 2009):

$$NO3 = \beta_{NO_3} conc_{NO3,mobile} \ Q_x \qquad \text{Equation 2.10}$$

Where:

NO3 is the nitrate removed by each of the physical transport mechanisms here considered (i.e., surface runoff, lateral flow, percolation) (kg ha^{-1}),

β_{NO3} is concentration of nitrate in the mobile water for the top 10 mm of soil (kg ha^{-1}) (only considered for surface runoff and subsurface lateral flow in the top layer),

Q_x is the physical transport mechanism considered (surface, lateral flow, or percolation).

The Nitrate component entering the shallow aquifer through percolation (leaching) from the soil profile may remain in the aquifer, be moved with groundwater flow into the main channel, be transported out of the shallow aquifer with water moving into the soil zone in response to water deficiencies, or be moved with recharge to the deep aquifer.

On the other hand, organic N is mainly transported with sediment to the stream, similarly to P transport. Daily organic N runoff losses estimation are based on the sediment yield, the N enrichment ratio, and the concentration of N in the topsoil layer, which is dependent of the amount of organic N in the fresh, stable, and active pools (Neitsch et al., 2009).

In SWAT, molecular nitrogen is added naturally by biological and atmospheric nitrogen fixation. Anthropogenic activities and agricultural practices such as the use of fertilizers also act as sources of N in the environment. After fixation, N is converted to NH_4^+ in the soil and then consumed by plants in the form of NO_3^-. Mineralisation is considered by the fresh organic pool associated with crop residues and the active pool associated with soil humus.

The remained fraction of crop residues after harvest is included into the first soil layer. N is removed from the soil through volatilisation, denitrification, erosion, and leaching (NO_3^- form). The total amount of NH_4^+ lost by volatilisation or nitrification is calculated considering the NH_4^+ amount and environmental factors. The SWAT code calculates the denitrification process according to the soil carbon and nitrate source, a rate coefficient, and different environmental factors such as temperature and soil water content. The denitrification process occurs in anaerobic conditions.

$$N_{denit}=NO3\times\left(1-\exp\left(-CDN\times\gamma_{temp}\times Corg\right)\right)$$ Equation 2.11

Where:
N_{denit} is the amount of nitrogen lost by denitrification (kg N ha^{-1}),
NO3 is the amount of nitrate in the layer (kg N ha^{-1}),
CDN is the rate coefficient for denitrification (d^{-1}),
γtemp is the nutrient cycling temperature factor (-),
Corg is the amount of organic carbon in the layer (%).

In the phosphorus cycle, three inorganic P pools (solution, active, and stable) and three organic P pools (active, stable and fresh) are included in the model. The fresh organic pool is associated with crop residue and microbial biomass, while the active and stable organic pools are associated with the soil humus. The sum of the six pools represents total soil P. P is simulated considering the supply and demand during plant growth. Soluble and organic forms can be removed from the soil via mass flow (runoff). The amount of soluble P removed in runoff is predicted using solution P concentration in the top 10 mm of the soil profile, the runoff volume, and a partitioning factor. Sediment transport of P is then simulated with a loading function (Neitsch et al., 2009). SWAT considers the amount of organic and mineral P transported with sediment to the stream with a loading function developed by McElroy et al. (1976) and later modified by Williams and Hann (1978):

$$sedP_{surf}=0{,}001\times conc_{sedP}\frac{sed}{area_{HRU}}\varepsilon_{P.sed}$$ Equation 2.12

Where:
$sedP_{surf}$ is the amount of P transported with sediment to the main channel in surface runoff (kg ha^{-1}),
$\varepsilon_{P:sed}$ is the P enrichment ratio,
$conc_{sedP}$ is the concentration of P attached to sediment in the top 10 mm (g m^{-3}).

The $conc_{sedP}$ is computed from the amount of P in the different pools, as:

$$conc_{sedP}=100\times\frac{\left(minP_{act,surf}+minP_{act,surf}+orgP_{hum,surf}+orgP_{frch,surf}\right)}{\rho_b\,depth_{surf}}$$ Equation 2.13

Where:
$minP_{act,surf}$ is the amount of P in the active mineral pool (kg ha^{-1}),
$minP_{sta,surf}$ is the amount of P in the stable mineral pool (kg ha^{-1}),
$orgP_{hum,surf}$ is the amount of P in humic organic pool (kg ha^{-1}),

$orgP_{frsh,surf}$ is the amount of P in the fresh organic pool (kg ha^{-1}),
ρ_b is the bulk density of the top soil layer (Mg m^{-3}).

2.3 Conceptual Modelling – Reservoir

Artificial reservoirs have been built to meet needs for water consumption (urban, irrigation or industrial), to produce energy or to regulate river levels/flows. Water quality in a reservoir can be imposed by consumption requirements or by legal issues. The water quality is determined by the internal processes and the inflows, and water residence time is determinant. The processes that occur in the reservoir depend, therefore, mainly on the residence time. Similar to watersheds, a reservoir is a three-dimensional body (Figure 2.2) and extremely complex, especially in environments where stratification occurs. As referred above there are 3D models which can describe the complexity of the natural processes with detailed.

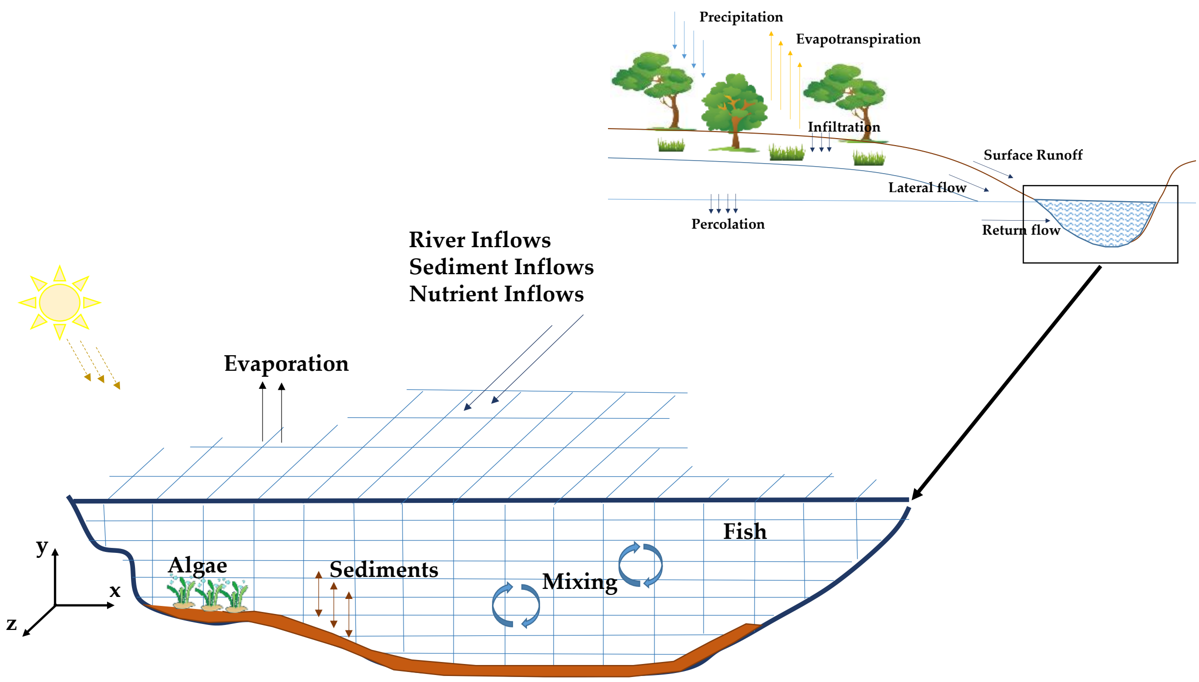

Figure 2.2 Schematic view of the three-dimensional structure in a reservoir.

MOHID Water such as MOHID Land, is a three-dimensional numerical model to simulate surface water bodies such reservoirs. The spatial discretization using the finite volume approach technique (the spatial coordinates are independent, and any geometry can be chosen for every dimension), allow more flexibility in the subdivision of the vertical and horizontal domain, and in implementation of innovative vertical coordinates, adaptable to each particular case. MOHID Water permits to use the model in any dimension (1D, 2D and 3D).

Due to the complexity and computational demand of the 3D models the use of these models may have limitations, such as in the 3D watershed model:

- Simulations of large reservoirs with high resolution;

- The need of testing different management strategies, where can be performed without excessive investment of time or money;

- To study long-term impacts.

Therefore, in this thesis, to assess the future impacts on a reservoir, under different climatic and social scenarios, involving long-term analysis, the MOHID Water in 2D was chosen considering only the water balance in the reservoir, and the CE-QUAL-W2 (2D) to simulate water quality processes, due to the possibility of this model to represent stratification process with accuracy and with a low computational demand, when comparing with MOHID Water 3D. It is described below the MOHID Water and CE-QUAL-W2 models main functionalities used in this thesis.

MOHID Water Modelling System

One of the reservoir model considered in this thesis is the MOHID Water model (from Modelo Hidrodinâmico acronym to hydrodynamic model in Portuguese) Neves 1985 (Braunschweig et al., 2003; Trancoso et al., 2009). MOHID is a 3D water modelling system, developed by MARETEC (Marine and Environmental Technology Research Center) at Instituto Superior Técnico (IST) which belongs to the Universidade de Lisboa in Portugal. MOHID is composed by two main executables: MOHID Water and MOHID Land. This model consists of a set of modules interconnected using an object orientation. Each module is responsible for management of part of information, constituting a total of 40 modules developed over 3 decades of research work. In this thesis the MOHID Water model is considered to simulate reservoir water dynamic.

Since the beginning this model has been applied to a variety of locations subject to different conditions such as: several coastal and estuarine areas, particularly along the Portuguese coast (Martins, 1999). MOHID has also been applied to the several Portuguese fresh water reservoirs such as Monte Novo, Roxo and Alqueva (Braunschweig, 2001), in order to study the flow and water quality (Brito et al., 2018; Deus et al., 2013; Franz et al., 2016; Trancoso et al., 2005). Campuzano F., 2018).

The model solves the three-dimensional incompressible primitive equations. Hydrostatic, Boussinesq and Reynolds approximations are assumed in the equations presented. The momentum balance equations for horizontal velocities are, in differential form and Cartesian coordinates:

$$\frac{\partial u}{\partial t}+\frac{\partial (uu)}{\partial x}+\frac{\partial (uv)}{\partial y}+\frac{\partial (uw)}{\partial z}-fv=-\frac{1}{\rho_0}\frac{\partial p}{\partial x}+\frac{\partial}{\partial x}\left(\mathrm{v_H}\frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mathrm{v_H}\frac{\partial u}{\partial y}\right)+\frac{\partial}{\partial z}\left(\mathrm{v_v}\frac{\partial u}{\partial z}\right) \quad \text{Equation 2.14}$$

$$\frac{\partial \mathrm{v}}{\partial_0}+\frac{\partial (\mathrm{uv})}{\partial x}+\frac{\partial (\mathrm{vv})}{\partial y}+\frac{\partial (\mathrm{vw})}{\partial z}-fu=-\frac{1}{\rho_0}\frac{\partial p}{\partial x}+\frac{\partial}{\partial x}\left(\mathrm{v_H}\frac{\partial v}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mathrm{v_H}\frac{\partial v}{\partial y}\right)+\frac{\partial}{\partial z}\left(\mathrm{v_v}\frac{\partial v}{\partial z}\right) \quad \text{Equation 2.15}$$

Where:

u, *v* and *w* are the components of the velocity vector in the x, y and z directions respectively,

f the Coriolis parameter,

ν_H and ν_v are the turbulent viscosities in the horizontal and vertical directions,
p is the pressure.

Assuming hydrostatic pressure the vertical momentum equation becomes an equation for pressure:

$$\frac{\partial p}{\partial Z}+\rho g=0 \qquad \text{Equation 2.16}$$

And vertical velocity must be computed using the continuity equation (assuming constant density, according to the Boussinesq approach):

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}=0 \qquad \text{Equation 2.17}$$

The Equation 2.17, integrated between bottom and the depth z where w is to be calculated gives:

$$w(z)=-\frac{\partial}{\partial x}\left(\int_{-h}^{z} u\,dz\right)-\frac{\partial}{\partial y}\left(\int_{-h}^{z} v\,dz\right) \qquad \text{Equation 2.18}$$

The free surface equation is obtained integrating the equation of continuity over the whole water column (between the bottom *(z=-h)* and the free surface elevation *(z=η)*:

$$\frac{\partial \eta}{\partial t}+\frac{\partial}{\partial x}\left(\int_{-h}^{\eta} u\,dz\right)+\frac{\partial}{\partial y}\left(\int_{-h}^{\eta} v\,dz\right)=0 \qquad \text{Equation 2.19}$$

Where:
g is the gravity (m s^{-2}),
ρ is density (g m^{-3}).

If the atmospheric pressure p_{atm} is subtracted from p, and density ρ is divided into a constant reference density ρ_0 and a deviation ρ' from that reference density, after integrating between the depth z where pressure is being calculated and the free surface gets:

$$p(z)=p_{atm}+\rho_0 g(\eta-z)+g\int_{z}^{\eta}\rho'\,dz \qquad \text{Equation 2.20}$$

Deriving this equation in the horizontal directions gets the pressure gradient to be used in the horizontal momentum equations:

$$\frac{\partial p}{\partial x_i}=\frac{\partial p_{atm}}{\partial x_i}+\rho_0 g\frac{\partial \eta}{\partial x_i}+g\int_{z}^{\eta}\left(\frac{\partial \rho'}{\partial x_i}\right)dz+\rho_s' g\frac{\partial \eta}{\partial x_i} \qquad \text{Equation 2.21}$$

$$\frac{\partial p}{\partial x_i}=\frac{\partial p_{atm}}{\partial x_i}+\rho_s g\frac{\partial \eta}{\partial x_i}+g\int_z^{\eta}\left(\frac{\partial \rho'}{\partial x_i}\right)dz \qquad \text{Equation 2.22}$$

The pressure gradient is the sum of the gradients of atmospheric pressure, of sea surface elevation and of the density gradient (baroclinic pressure gradient). The two first terms depend only on the free surface properties and exert their effect over the whole water column (because of that they are called barotropic terms). The value of the latter depends on the vertical density distribution and is called baroclinic term.

As referred, the MOHID model consists of a set of modules interconnected using an object-oriented programming. Each module is responsible for the management of part of information. In this thesis the following modules were considered for simulating water variation dynamics: Model, Atmosphere, Geometry, Hydrodynamic, Atmosphere, Interface Water Air, Turbulence and Discharges. A brief description about each module is given below.

The **Model Module** is the topmost module of the MOHID Water Modelling System and it is responsible for constructing, modifying and destructing each model and for controlling information fluxes between the different modules, and time and mapping evolution.

The **Geometry Module** computes the lateral areas and volumes of the finite volumes, based upon the surface elevation and the bathymetric data. This information is updated as needed, and published to the other modules of the MOHID model.

It also uses a finite volume formulation to discretize the equations, applying each equation macroscopically to each control volume, which is determined by the grid and geometry implemented for the study domain. In this approach, the discrete form of the governing equations is applied macroscopically to a cell control volume. A general conservation law for a scalar U, with sources Q in a control volume Ω is then written as:

$$\frac{\partial}{\partial t}\left(\int_{\Omega} Pd\Omega\right)+\oint_S \vec{F}.d\,\vec{S}=\int_{\Omega} Q\,d\Omega \qquad \text{Equation 2.23}$$

Where:
F are the fluxes of the scalar through the surface,
S embedding the volume.

Discretizing this expression in an elementary control volume Ω_j, it is obtain:

$$\frac{\partial(P_j\Omega_j)}{\partial t}+\sum_{faces}\vec{F}.\vec{S}=Q_j\Omega_j \qquad \text{Equation 2.24}$$

In this equation it is assumed that the volume is small so that properties are uniform. Actually, the control volume can have any shape since only fluxes among cell faces are required (Montero, 1999; Martins et al., 2000).

The **Hydrodynamic module** solves the Navier-Stokes equations, considering the hydrostatic, Boussinesq and Reynolds approximations (Martins et al., 2000; Leitão, 2003):

$$\frac{\partial}{\partial t}\int_V \vec{v}_H dV = -\oint_A \vec{v}_H(\vec{v}.\vec{n})dA + \oint_A \upsilon_T\left(\vec{\nabla}(\vec{v}_H).\vec{n}\right)dA - \frac{1}{\varrho}\oint_A p.\vec{n}_H dA + \int_V 2\vec{\Omega}\times\vec{v}_H dV + \vec{F}$$

Equation 2.25

Where:
V represents the control volume (m^3),
$\vec{v}_H = (u, v)$ the horizontal velocity vector,
$\vec{v} = (u, v, w)$ the velocity vector,
$\vec{n}$ the normal vector to the bounding surface (A),
$\vec{n}_H$ the normal vector related to the horizontal plane,
υ_T the turbulent viscosity,
ρ the water density ($g\ m^{-3}$),
$p = g\int_z^\eta \rho dz + p_{atm}$ the water pressure,
g the gravitational acceleration ($m\ s^{-2}$),
p_{atm} the atmospheric pressure, (kPa)
η the water level (m),
$\vec{\Omega}$ the earth rotation vector,
$\vec{F}$ the external forces, which include the wave-induced force (gradient of the radiation stress) computed by the wave model.

The **Atmosphere module** is responsible for meteorological data needed to compute processes occurring at the water-air interface, such as computing wind shear stress, radiation balances, latent and sensible heat fluxes.

The **Water-Air Interface module** is responsible by processes occurring at the water-air interface, such as computing wind shear stress, radiation balances, latent and sensible heat fluxes. This module uses the Atmosphere Module as a database for meteorological data and combines it with information from, for example, Module Hydrodynamic to compute heat and momentum fluxes across the water-air interface.

The **Turbulence module** is a one-dimensional turbulence model, based on GOTM which stands for General Ocean Turbulence Model (http://www.gotm.net/), and consists of a one dimensional water column for most important hydrodynamic and thermodynamic processes related to vertical mixing in natural waters. Module GOTM is a "wrap-up" module containing GOTM routines which were coupled into MOHID in 2001. This routines consist of a set of turbulence models including a k-ε model and Mellor-Yamada second order turbulent closure model (Mellor and Yamada, 1982).

The **Discharges module** handles all the point discharges in MOHID Water Modelling System. These discharges can be simple water discharges but can also have properties such as properties concentration (temperature, salinity, nutrients, contaminants, etc.) and/or momentum.

Boundary conditions

Boundary conditions are required due to spatial derivatives at free surface, solid boundaries, open boundaries and movable boundaries. Some of boundary conditions depend on the properties inside the model and their calculation must be embedded on the numerical algorithm and other boundary conditions depend only on external variables (e.g. discharges, solar radiation) and they can be imposed as explicit fluxes.

Free surface

Advective fluxes of mass and momentum across the surface are assumed to be null. This condition is imposed by assuming that the vertical flux of *W* at the surface is null:

$$Wflux_{surface} = 0$$

Diffusive flux of momentum is imposed explicitly by means of a wind surface stress, τ_w:

$$\frac{\partial \overline{v_H}}{\partial z}\Big|_{surface} = \vec{\tau}_w$$

Wind stress is calculated according to a quadratic friction law:

$$\vec{\tau}_w = C_D \rho_a \vec{W} |\vec{W}|$$

Where

C_D (varying between 0.001 and 0.002) is a drag coefficient that increases with the wind speed,

ρ_a is air density

W is the wind speed at the reference height used to estimate the drag coefficient (10 m above the sea surface).

Bottom boundary

Advective mass and momentum fluxes across the bottom interface are null and diffusive flux of momentum is estimated by means of a bottom stress that is calculated by a non-slip assumption. A quadratic law is assumed to account for turbulent flow. So, the diffusive term at the bottom is written as:

$$v \frac{\partial \vec{v}_H}{\partial Z}\Big|_{bottom} = \frac{\vec{\tau}_b}{\rho} = C_f \ddot{\vec{V}}_H |\ddot{\vec{V}}_H|$$

C_f is the bottom friction coefficient calculated according to the velocity $\vec{V}_H$ used to compute the bottom shear.

Assuming a logarithmic profile

$$|\vec{V}_H| = \frac{U^\tau}{k} ln\left(\frac{z}{Z_0}\right)$$

$$U^\tau = \sqrt{\frac{\tau_b}{\rho}}$$

Where
k is the von Karman constant *(k≅0.41)*
Z_0 is rugosity length, i.e. the height above the bottom where according to the logarithmic law the velocity would be zero.

The law of the wall describes the physical distance above the bottom from which the logarithmic law applies. It is clear that between this height and the wall the logarithmic law can not be applied.

The rugosity length must be determined empirically and tend to decrease with the flow velocity.

From equations above:

$$C_f = \left(\frac{k}{\ln\left(\frac{z}{z_0}\right)}\right)^2$$

The friction coefficient depends on the depth at which the velocity is computed.

Lateral closed boundaries

At these boundaries, the domain is limited by land and velocity is parallel to the boundary. This is imposed in the model nullifying the velocity component perpendicular to the closed boundary. In reality there is a velocity gradient perpendicular to the solid boundary that generates a diffusive flux of momentum. The ratio between this flux and the vertical flux associated to the bottom shear is proportional to the ratio between flow depth and width and consequently it is important only in deep and narrow channels and its accurate calculation requires the use of fine horizontal grid. When that is not the case it is more convenient to assume a free slip condition, i.e. to neglect horizontal diffusion. The typical boundary condition to be used are:

$$\frac{\partial \vec{V}_H}{\partial \eta} = 0$$

$$\vec{V}.\vec{n} = 0$$

In the finite volume formalism, these conditions are implemented specifying zero normal water fluxes and zero momentum diffusive fluxes at the cell faces in contact with land.

CE-QUAL-W2- Hydrodynamic and Water Quality Model

The CE-QUAL-W2 is a bi-dimensional model developed by a collaboration between the U.S. Army Corps of Engineers and the Water Quality Research Group at Portland State University (Cole and Wells, 2015). Since Version 3.5, the model is maintained by the Water Quality Research Group at Portland State. The current version (version 4.1) used in this thesis, simulates the systems hydrodynamics and water quality both vertically and longitudinally in both stratified and not stratified systems. The model assumes lateral homogeneity and supports vertical and horizontal gradients of all calculated properties (Cole and Wells, 2015).

The model was developed to allow simulation of water bodies where resolution of water quality gradients over time in longitudinal as well as vertical axes are required (Cole and Wells, 2015). The geometry of the computational grid is determined by representative bathymetry; longitudinal segments (identified as lengths), vertical spacing of layers (identified as heights), and average reservoir cross-sections (identified as widths). The model allow to include flow boundary conditions, branches, multiple withdrawals, and other features.

This model is based on the finite difference solution of laterally averaged equations of fluid motion. The governing equations are obtained by performing a mass and a momentum balance of the fluid phase about a control volume, as presented simplified below (Cole and Wells, 2015):

x-momentum:

$$\frac{\partial UB}{\partial t}+\frac{\partial UUB}{\partial x}+\frac{\partial WUB}{\partial z} = gB\sin\alpha + g\cos\alpha B\frac{\partial \eta}{\partial X} - \frac{\partial \cos\alpha B}{\varrho}\int_{\eta}^{z}\frac{\partial \varrho}{\partial X}dZ + \frac{1}{\varrho}\frac{\partial B\tau_{xx}}{\partial X} + \frac{1}{\varrho}\frac{\partial B\tau_{x}}{\partial X} + \frac{1}{\varrho}\frac{\partial B\tau_{xz}}{\partial Z} + qBU_x$$

Equation 2.26

z-momentum:

$$0 = g\cos\alpha - \frac{1}{\varrho}\frac{\partial P}{\partial Z}$$

Equation 2.27

Free surface equation:

$$B_\eta \frac{\partial \eta}{\partial t} = \frac{\partial}{\partial X} \int_\eta^h UBdz \qquad \text{Equation 2.28}$$

Continuity:

$$\frac{\partial UB}{\partial x} + \frac{\partial WB}{\partial z} = qB \qquad \text{Equation 2.29}$$

Equation of state:

$$\rho = f(T_W, \Phi_{TDS}, \Phi_{SS}) \qquad \text{Equation 2.30}$$

Conservation of mass/heat:

$$\frac{\partial B\Phi}{\partial t} + \frac{\partial UB\Phi}{\partial X} + \frac{\partial WB\Phi}{\partial Z} - \frac{\partial \left(BD_x \frac{\partial \Phi}{\partial X}\right)}{\partial X} - \frac{\partial \left(BD_z \frac{\partial \Phi}{\partial Z}\right)}{\partial Z} = q_\Phi B + S_\Phi B \qquad \text{Equation 2.31}$$

Where:
B is the width (m),
U is the longitudinal velocity (m s^{-1}),
W is the vertical velocity (m s^{-1}),
q is the inflow per unit width (m s^{-1}),
α is the channel angle (°),
Φ is the concentration or temperature,
η is the water surface elevation (m),
P is the pressure,
h is the depth (m),
Tw is the water temperature (°C),
ΦTDS is the concentration of TDS (mg/l),
Φss is the concentration of suspended solids (mg/l),
ρ is the density (g m^{-3}).

A lake can exchange heat with the atmosphere, inflows, out flows, and the bed sediments.

In the CE-QUAL-W2 model the surface heat exchange can be formulated as a term-by-term process using the explicit adjacent cell transport computation as long as the integration time-step is shorter than or equal to the frequency of the meteorological data, and are depending on water surface temperatures. Term-by-term surface heat exchange is computed as:

$$Hn = Hs + Ha + He + Hc - (Hsr\ Har\ Hbr) \qquad \text{Equation 2.32}$$

Where:
Hn is the net rate of heat exchange across the water surface (W m^{-2}),
Hs is the incident short wave solar radiation (W m^{-2}),
Ha is the incident long wave radiation (W m^{-2}),
Hsr is the reflected short wave solar radiation (W m^{-2}),
Har is the reflected long wave radiation (W m^{-2}),
Hbr is the back radiation from the water surface (W m^{-2}),
He is the evaporative heat loss (W m^{-2}),
Hc is the heat conduction (W m^{-2}).

This model computes biogeochemical processes such as nitrogen, phosphorus, carbon and oxygen cycles, as well as the dynamics of algae and organic matter. In the organic matter (OM), the dissolved non-refractory OM (LDOM), the dissolved refractory OM (RDOM), the particulate non-refractory OM (LPOM) and the particulate refractory OM (RPOM) are considered in the model. The concentrations properties are calculate based on a philosophy of source/sink associated to each cell of the model in order to conserve mass. In order to calculate the evolution of algal species concentration, their maximum growth, respiration, excretion and mortality rates are considered, as well as limiting factors, such as light intensity, nutrients concentration and water temperature. In order to solve the 2D advection-diffusion equation, the source/sink term, must be specified:

$$S_g = K_0 \theta_g^{(T-20)} - K_1 \theta_g^{(T-20)} \Phi_g - \omega_g \frac{\partial \Phi_g}{\partial Z} - \alpha I_0 (1-\beta) e^{-\lambda z} . \Phi_g + \frac{A_{sur}}{V_{sur}} K_L (\Phi_s - \Phi_g) \qquad \text{Equation 2.33}$$

Where:
θ_g is the temperature rate multiplier (-),
T is the water temperature (°C)
α is the photo degradation parameter (m^2 J^{-1}),
I_o is the radiation at surface (W m^{-2}),
λ is the light extinction coefficient (m^{-1}),
β is the fraction of short wave solar absorbed on the surface,
ωg is the settling velocity (m s^{-1}),
K0 is the zero order decay coefficient (g m^{-3} s^{-1} at 20°C),
K1 is the first order decay coefficient (s^{-1} at 20°C),
ϕg is the generic constituent concentration (g m^{-3}),
ϕs is the generic constituent concentration gas saturation in the atmosphere (g m^{-3}),
Asur is the surface area (m^2),
Vsur is the surface volume (m^3),
KL is the surface gas transfer coefficient (m s^{-1}).

Typically, the algal community is represented as a single assemblage or is broken down into diatoms, greens, and cyanobacteria. The rate equation for each algal group is:

$$S_a=K_{ag}\Phi_a-K_{ar}\Phi_a-K_{ae}\Phi_a-K_{am}\Phi_a-\omega_a\frac{\partial\Phi_a}{\partial z}-\sum\left(Z_\mu\Phi_{zoo}\frac{\sigma_{alg}\Phi_a}{\sum\sigma_{alg}\Phi_a+\sigma_{pom}\Phi_{lpom}+\sum\sigma_{zoo}\Phi_{zoo}}\right)$$

Equation 2.34

Where:
z is the cell height
$Z\mu$ is the net growth rate of a zooplankton species,
σ is the zooplankton grazing preference factors,
Kag is the algal growth rate (sec^{-1}),
Kar is the algal dark respiration rate (sec^{-1}),
Kae is the algal excretion rate (sec^{-1}),
Kam is the algal mortality rate (sec^{-1}),
ω_a is the algal settling rate (m sec^{-1}),
ϕ_a is the algal concentration (g m^{-3}).

Algal growth rate is computed by modifying a maximum growth rate affected by temperature, light, and nutrient availability:

$$K_{ag}=\gamma_{ar}\gamma_{af}\lambda_{min}K_{ag\ max}$$

Equation 2.35

Where:
γ_{ar} is the temperature rate multiplier for rising limb of curve
γ_{af} is the temperature rate multiplier for falling limb of curve
λ_{min} is the multiplier for limiting growth factor (minimum of light, phosphorus, silica, and nitrogen)
K_{ag} is the algal growth rate (sec^{-1}),
$K_{ag\ max}$ is the maximum algal growth rate (sec^{-1}).

Phosphorus is an important element in aquatic ecosystems since it serves as one of the primary nutrients for phytoplankton growth (Figure 2.3). In many fresh waters, phosphorus is considered to be the nutrient limiting maximum production of phytoplankton biomass (Schindler, 1971; Schindler et aI., 1973; Vollenweider, 1968, 1976). Phosphorus is assumed to be completely available as ortho-phosphate (PO,) for uptake by phytoplankton. Macrophytes are specified as either taking P from the sediments or from the water column.

Nitrite is an intermediate product in nitrification between ammonium and nitrate. Nitrate is used as a source of nitrogen for algae and epiphyton during photosynthesis. Preferential uptake of ammonium over nitrate by algae and periphyton is now included. Nitrogen may be the limiting nutrient for algae in systems with high phosphorus loadings or in estuaries. Some species of blue-green algae are capable of fixing atmospheric nitrogen for use in photosynthesis. This process can be included by setting the nitrogen half-saturation concentration for algal growth to zero (Figure 2.4).

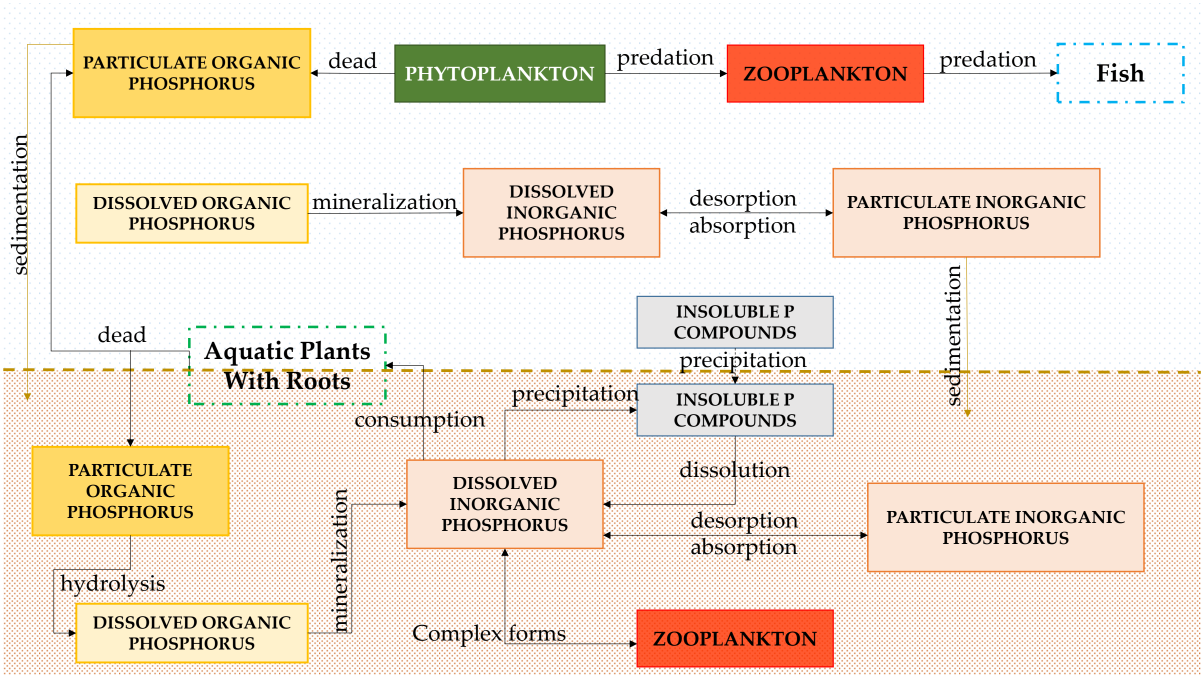

Figure 2.3 Scheme of the main phosphorus processes in the CE-QUAL-W2 model.

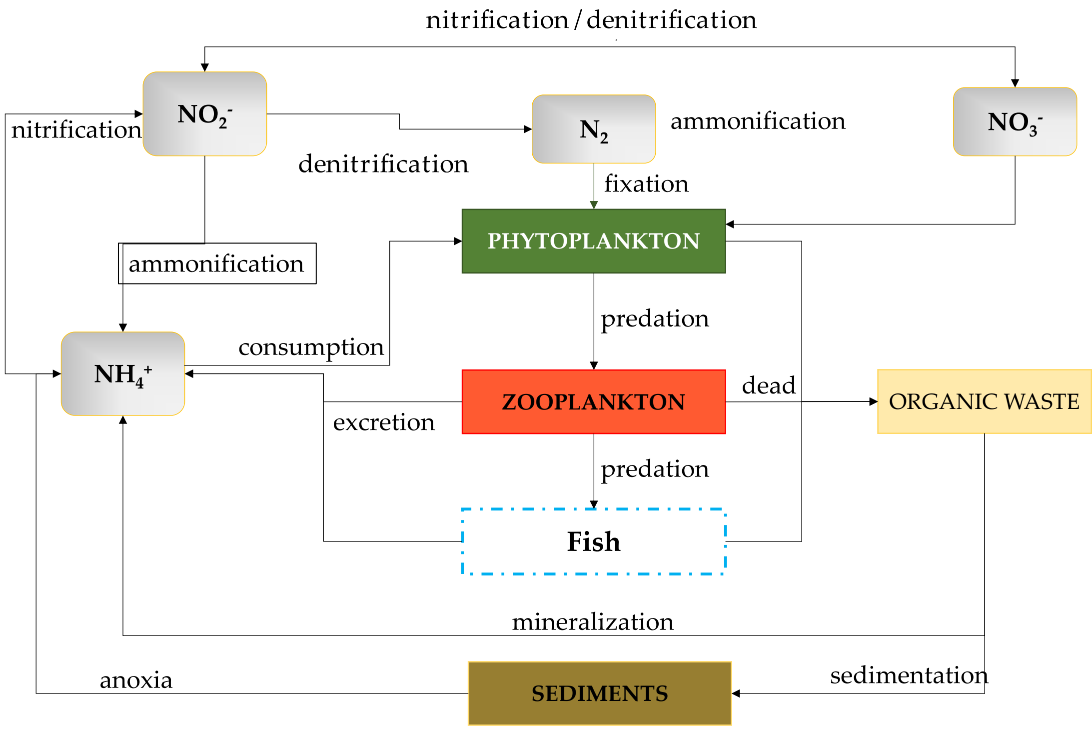

Figure 2.4 Scheme of the main nitrogen processes in the CE-QUAL-W2 model.

Oxygen is one of the most important elements in aquatic ecosystems. It is essential for higher forms of life, controls many chemical reactions through oxidation, and is a surrogate variable indicating the general health of aquatic systems. The model includes both aerobic and anaerobic processes. Simulations can be used to identify possibilities for both metalimnetic and hypolimnetic oxygen depletion and its impact on various water control management alternatives. If a single variable were to be measured in aquatic systems that would provide maximum information about the system state, it would be dissolved oxygen. The DO concentration was calculated as fractions of the saturated DO concentration (DO_{sat}), itself a function of water temperature.

$$DO_{sat}=\exp\left(-139{,}3441+\left(\frac{1{,}5757\times10^{5}}{T}\right)-\left(\frac{6{,}642\times10^{7}}{T^{2}}\right)+\left(\frac{1{,}2438\times10^{10}}{T^{3}}\right)-\left(\frac{8{,}622\times10^{11}}{T^{4}}\right)\right)$$

Equation 2.36

Where:

DO_{sat} is the saturated DO concentration (mg l^{-1}),

T is the water temperature (K).

DO concentration in inflow water to the reservoir is assumed as 80% saturation.

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Chapter 3 Water Quantity and Quality under climate and societal scenarios: a basin-wide approach

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Abstract

Water resources are impacted by several stressors that compromise their availability; including population growth and climate change. These stressors are expected to progressively intensify in most regions of the world, with direct impact on watersheds and river systems. This study investigates the effect of different watershed pressures scenarios including climate change in the hydrological regime and water bodies of the Sorraia River basin (Portugal). This catchment includes one of the largest irrigated area in the country, being thus strongly influenced by anthropogenic activities, associated to hydrological (irrigation, flow regulation, damming) and nutrient stressors. The Soil Water Assessment Tool (SWAT) was used to simulate water flow and nutrient dynamics in the watershed while considering inputs from two climate models (GFDL-ESM2M and IPSL-CMA-LR) and three societal storylines. Results showed that the foreseen rainfall reductions will have a significant impact on river flow and nutrients concentrations when compared to baseline conditions. River flow will expectably decrease 75%, while N and P concentrations in the river water will expectably increase by up to 500 and 200%, respectively. These differences are more evident for storylines that consider increasing pressures such as population and agriculture growth, poor management practices and diminishing technology evolution. Results are thus indicative of a possible future outcome and may provide guidelines for defining preventive measures to minimize the effect of climate change and growth of environmental pressures in the Sorraia River basin.

Keywords: modelling; climate change; basin management scenarios; Sorraia River basin.

3.1 Introduction

Agriculture is one of the main factors responsible for variation in the landscape of a region (Burgi et al. 2004). Unsustainable agricultural practices and excessive urban expansion have drastically affected the hydro morphological characteristics of river systems in the wake of climate change. The ever-increasing world population and globalisation of food products is one of the major reasons for the expansion of agroecosystems. High demands from the global food market have turned small and large-scale farmers towards excessive mechanized farming, the overuse of fertilizers and pesticides, as well as the unsustainable water abstraction for irrigation purposes. Diffused pollution from these sources has also degraded the water quantity and quality, thereby compromising vital ecosystem services and disrupting the local and regional hydrological balance (Hazell and Wood, 2008; Hering et al., 2015a, 2010; Segurado et al., 2018). A study conducted in Portugal observed that of the total water used in agriculture, about 80% is for irrigation consumption (EEA, 2012).

In the future, pressures such as diffuse pollution or water abstraction are predicted to further increase (Alexandratos and Bruinsma, 2012; FAO, 2011; Ruttan and Alexandratos, 2006; Sun et al., 2015), with climate change scenarios bringing great uncertainty to the water resources' availability. According to the Intergovernmental Panel on Climate Change (IPCC)'s Fifth Assessment Report (IPCC and IPCC5 WGII, 2014), the Mediterranean climate, which is comprised of two contrasting seasons, i.e., the wet season with mild temperatures and the dry season with high temperatures, will show extreme variations due to climate change. This region will be highly affected by extreme events like droughts, floods and heat waves. These extreme events will greatly reduce the water availability, hydropower potential and crop productivity of the region. Additionally, health risks and the frequency of other stochastic events will also significantly increase.

The study area, i.e., the Sorraia River basin, also lies under the influence of the Mediterranean climate. This basin is greatly modified by anthropogenic activities such as the construction of dams and weirs to respond to residential, agricultural and industrial demands (Cordovil et al., 2018). It has been predicted that climate change phenomena will further degrade the hydrological balance of the basin, leading to many socio-economic problems at both local and regional scales, further enhancing the water scarcity in the region. Hence, it is of utmost importance to accurately assess the impact of climate change on water resources to develop effective mitigation policies and a framework for management strategies. Better management strategies at the river basin level will not only maximize the benefits of irrigation and other anthropogenic modifications of the ecosystem but also minimize its impacts on water quantity and quality. Thus, the assessment of the impacts of climate change is essential to counter the effects of environmental stressors and improve the ecosystem equilibrium (Gasith and Resh, 1999; Hosseinzadehtalaei et al., 2017; Ning et al., 2015; O'Neill et al., 2017).

Hydrological models can forecast the outcomes of different management practices, thus providing guidance for water managers in defining cost-effective measures for future application (Brito et al., 2015; Hering et al., 2015b; Mateus et al., 2014; Simionesei et al., 2018; Williams et al., 2013). Although there are many unforeseeable events, the use of models in river systems is accepted as a standard practice with relevant information derived from them (Brito et al., 2018; Mateus et al., 2014; Segurado et al., 2018). A study carried out by Brito et al. (Brito et al., 2018) aimed at understanding the relationship between the eutrophication process of the downstream reservoir and soil erosion and nutrient losses related to flood events in a river basin (southern Portugal). Additionally, Mateus et al. (Mateus et al., 2014) conducted an integrated study using basin and reservoir models to depict the influence of river basins on the eutrophication of downstream water bodies, obtaining results that allowed to test different management practices that affect the reservoir trophic status. Watershed modelling is also an important part of the Portuguese River Basin Management Plans at the national level (APA, 2012). However, no such records exist that consider the effect of climate change on water and nutrient dynamics in the Sorraia River catchment area through hydrological modelling. This constitutes a significant gap in terms of knowledge.

The aim of this study is to assess the impacts of climate change and management practices on the water quantity and quality of the Sorraia River using the hydrological model Soil Water Assessment Tool (SWAT) (Neitsch et al., 2011). The main objective is to predict the effects of multiple biotic and abiotic stressors at the basin scale (Hering et al., 2015b). These stressors result from unsustainable anthropogenic activities and negatively affect the indicators of ecological quality and service. In addition, the study also has the following specific objectives:

(i) to simulate the baseline conditions in terms of hydrology and nutrients (N and P) in the Sorraia River basin using the SWAT model (Neitsch et al., 2011);

(ii) to simulate three distinct storylines which combine alternative trends in the evolution of the society and practices with climate change scenarios;

(iii) to compare scenario results for accuracy and efficiency.

The storylines and management scenarios considered in this study should serve as guidelines for defining mitigation measures in the catchment.

3.2 Materials and Methods

3.2.1. Study Area

This study was carried out in the Sorraia River (southern Portugal), the tributary of the Tagus River with the largest basin area, with ~7730 km2 (Lat: 38.59° to 39.50°; Long: −8.99° to −7.24°), and with a longitudinal length of ~155 km (Figure 1). The climate in the region is dry sub-humid, with dry and hot summers, and mild and wet winters. Records from 14 meteorological stations (SNIRH, 2017) for a 20-year period (1996 to 2015) showed that the annual precipitation in the region varied from 200 to 900 mm, with the average of ~500 mm. The average monthly precipitation was ~50 mm, fluctuating up to 25 mm from April to September and 70 mm between October and March. The average annual surface air temperature was ~15 °C, varying from ~9 to ~22 °C. The reference evapotranspiration estimated according to Allen et al. (G. Allen et al., 1998) reached ~900 mm. The dominant soil types found in the region are Cambisols, Luvisols, and Regosols (IUSS Working Group WRB, 2014). Fluvisols are also found at higher concentrations in the downstream irrigated areas.

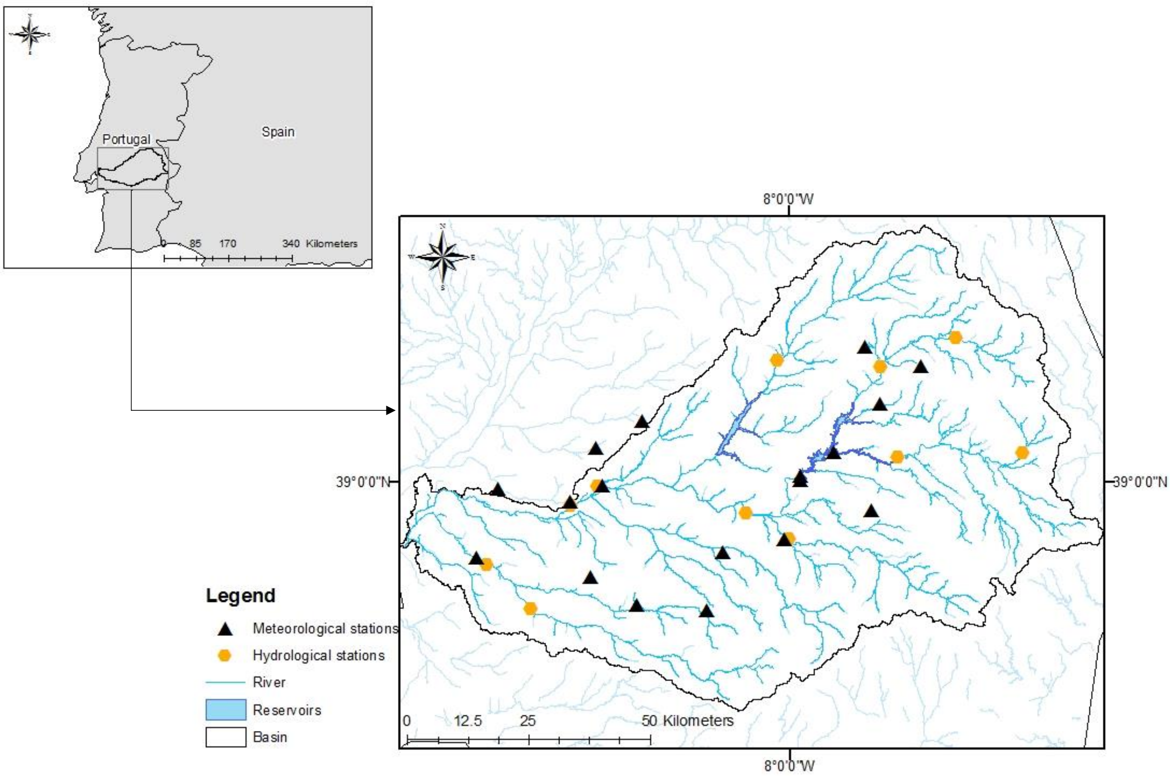

Figure 3.1 The Sorraia River Basin.

Two major reservoirs, Montargil and Maranhão, were built in the watershed during the second half of the twentieth century as a part of the Sorraia Valley Irrigation Implementation Plan. Currently, the Sorraia Valley is one of the largest irrigation areas in

Portugal, totalizing 16,000 ha, in which corn (*Zea mays* L.), rice (*Oryza sativa* L.) and tomato (*Solanum lycopersicum* L.) predominate. The land use in the remaining area of the watershed is characterized by holm oak forest, rainfed cereals and pasture.

In terms of human population, the Sorraia watershed has a total of 153,100 inhabitants, with a density of 20 inhabitants km^{-2} (INE, 2011). The population is mainly concentrated in three core cities: Ponte de Sôr (16,700 inhabitants), Samora Correia (17,123), and Coruche (19,950). According to the River Basin Management Plan (RBMP) (APA, 2016), hydro-morphological changes, diffuse pollution, municipal discharges, flow regulation, and water abstraction are the main pressures in the basin.

3.2.2. Hydrological Modelling

The Soil and Water Assessment Tool (SWAT) Model

The SWAT model (Neitsch et al., 2011) is widely used to simulate watershed processes (Du et al., 2013; Koch Stefan A4 - Bauwe, Andreas A4 - Lennartz, Bernd, 2013; Mateus et al., 2014; Santhi et al., 2006; Williams et al., 2013; Zhang et al., 2011). SWAT is a semi-distributed watershed model focused on land management at a basin scale. The model splits the watershed into sub-basins that are assumed to be homogeneous in their Hydrologic Response Units (HRU), i.e., in terms of land use, soil and topographic characteristics. The relative straightforward formulation used in SWAT allows the model to run more demanding simulations within a reasonable time. The hydrology of the model is based on the daily water balance equation, as follows:

$$\mathrm{SW_t} = \mathrm{SW_0} + \sum_{i=1}^{n}(\mathrm{R_{day}} - \mathrm{Q_{surf}} - \mathrm{E_a} - \mathrm{W_{seep}} - \mathrm{Q_{gw}}) \qquad 1)$$

where SWt is the final soil water content (mm), SW0 is the soil water content at the initial time step (mm), Rday is the daily precipitation (mm), Qsurf is the surface runoff (mm), Ea is the actual evapotranspiration (mm), Wseep is the percolated water (mm), and Qgw is the return flow (mm), all referring to day i, which varies from 1 to the number of simulated days (n). In this study, the potential evapotranspiration rates were estimated using the Penman–Monteith method (G. Allen et al., 1998), with Ea being then dependent on soil water availability. Surface runoff was computed from daily precipitation using a modification of the Soil Conservation Service Curve Number (SCS-CN) method (USDA-SCS, 1972). Groundwater recharge was estimated by combining a storage routing technique and a crack-flow model. The lateral flow was simulated using a kinematic storage method (Neitsch et al., 2011).

The SWAT model can further simulate the nitrogen (N) and phosphorus (P) cycles. The N present in the soil is represented by five different pools, considering mineral and organic forms. The mineral N is divided into two pools: ammonia (NH4+) and nitrate (NO3−). The organic N is divided into three pools: active, stable (associated to the humic substances) and fresh pool (associated to the crop residue). Molecular nitrogen is added naturally by biological and atmospheric nitrogen fixation. Anthropogenic activities and agricultural practices such as the use of fertilizers also act as sources of N in the environment. After fixation, N is converted to NH_4^+ in the soil and then consumed by plants in the form of NO_3^-. Mineralisation is considered by the fresh organic pool associated with crop residues and the active pool associated with soil humus. At harvest, the remaining fraction of crop residues is incorporated into the first soil layer. N is removed from the soil through volatilisation, denitrification, erosion, and leaching (in the NO_3^- form). The total amount of NH_4^+ lost by volatilisation or nitrification is calculated considering the NH_4^+ amount and environmental factors. The SWAT code calculates the denitrification process according to the soil carbon and nitrate source, a rate coefficient, and different environmental factors such as temperature and soil water content. The denitrification process occurs in anaerobic conditions. In the case of the phosphorus cycle, the model includes three inorganic P pools (solution, active, and stable) and three organic P pools (active, stable and fresh). The fresh organic pool is associated with crop residue and microbial biomass, while the active and stable organic pools are associated with the soil humus. The sum of the six pools represents total soil P. P is simulated considering the supply and demand during plant growth. Soluble and organic forms can be removed from the soil via mass flow (runoff). The amount of soluble P removed in runoff is predicted using solution P concentration in the top 10 mm of the soil profile, the runoff volume, and a partitioning factor. Sediment transport of P is then simulated with a loading function (Neitsch et al., 2011).

In this study, the SWAT model was applied to the Sorraia basin using the ArcGIS extension from ESRI (Redlands, CA). The model application relied on available Geographical Information System maps for topography (SRTM), land use maps from Earth Observation (GSE Land M2.1) and soil maps and data from Cardoso (Cardoso , 1965). Daily discharge data provided by the reservoirs' manager (ARBVS—Farmers Association from the Sorraia Valley) were used in the model from 1996 to 2015. Meteorological time series were downloaded for the basin area from the National Water Resources Institute website (SNIRH). The input data considered for the present conditions (hereafter referred to as the baseline) are summarized in Table 3.1. In order to stabilize the model conditions, the period between 1996 and 2000 was considered as the warm-up period, and the baseline simulation was defined for the period 2001–2015.

Table 3.1 The input data used in the Soil Water Assessment Tool (SWAT) model application.

Data Type	Source	Data Description	Resolution
Topography	Shuttle Radar Topography Mission (SRTM) NASA	-	90 m
Soil type	Cardoso (Cardoso, 1965)	Soil physical properties	1:25,000
Land Use	GSE Land M2.1	Land use classification 1996–2015	20 m and 300 m
Meteorology	Serviço Nacional de Informação dos Recursos Hídricos (SNIRH)	Precipitation, temperature, relative humidity and wind speed	Daily time series

Calibration and Validation

The SWAT model was calibrated by manually modifying one parameter at a time, considering the most sensitive parameters that determined the best results for simulating daily/monthly river flows. The hydrograms were analysed, and the parameters that affected flow peaks and baseflow were selected and modified until deviations between the model outputs and measured flow data were minimised (Table 3.2). The previously calibrated parameters were then validated by comparing the results of the simulations with an independent dataset. Model calibration was thus performed for the period between 2001 and 2006, while the validation exercise was carried out from 2006 to 2015.

Table 3.2 The values of the calibrated parameters used in the SWAT model (parameter, description and default according to Neitsch et al., 2011).

Parameter	Description	Default	Calibrated Value
CN2	SCS runoff curve number for moisture condition II.	25 to 92	80 to 92
ALPHA_BF	Baseflow alpha factor (1/days).	0.048	1
GW_Delay	Groundwater delay time (days)	31	3
SOL_AWC	Available water capacity of the soil layer (mm H2O/mm soil).	0.11–0.14	−40%
SOL_ZMX	Maximum rooting depth of soil profile. (mm).	-	500
SOL_Z1	Depth from the soil surface to the bottom of the first layer (mm).	300 to 800	slope 0–3%, to 800 slope 3–8%, to 500 slope 8–9999%, to 300
SOL_Z2	Depth from the soil surface to the bottom of the second layer (mm).	300 to 800	slope 0–3%, to 1000 slope 3–8%, to 800 slope 8–9999%, to 500

Discharge data from two monitoring stations were used for model calibration and validation. Moinho Novo (Lat. 39.228°; Long. −8.029°) and Ponte Vila Formosa (Lat. 39.216°; Long. −7.784°) were selected as they are not significantly influenced by the operation of existing hydraulic structures. To evaluate the nutrients' concentration, the monitoring station at Ponte de Coruche (38.956°; −8.524°) was considered (SNIRH, 2018). However, its location and the monitoring interval of measured values (usually 15 days to 1 month) hindered the representativeness of the monitoring record.

The goodness-of-fit indicators adopted for comparing model outputs with measured flow data were the coefficient of determination (R^2), the root mean square error (RMSE), the Nash-Sutcliffe model efficiency coefficient (NSE (Nash and Sutcliffe, 1970)), and the Model Bias (Bias). An R^2 value close to 1 indicates that the model explains the variance of observations well. RMSE values close to zero indicate small estimation errors and good model predictions. Bias was defined as the average difference between the estimator and the true value. Bias values close to zero indicate no under or over-estimation of the measured results. NSE values close to 1 indicate a perfect match of modelled discharge to the observed data, hence, indicating that the model predictions are good. On the contrary, when NSE is very close to 0 or negative, there is no gain in using the model.

For N and P, comparison was focused on the magnitude of the simulated and observed values due to data limitation, considering only R^2 and Bias indicators.

Storylines

The storylines defined in this study followed the framework developed within the Managing Aquatic Ecosystems and Water Resources Under Multiple Stress Project-MARS (Feld et al., 2016; Hering et al., 2015b). Here, the storylines are defined as a combination of societal and climate scenarios. Three storylines were considered by combining the work of O'Neill et al. (O'Neill et al., 2014) and Riahi et al. (Riahi et al., 2017). These authors defined Shared Socioeconomic Pathways (SSP's) as reference scenarios describing plausible alternative trends in the evolution of society and ecosystems over a century timescale in the absence of climate change or climate policies. Storylines also considered Moss et al. (Moss et al., 2010) who developed Representative Concentration Pathways (RCPs) for greenhouse emissions. RCP 4.5 assume that greenhouse gas emissions will peak around 2040 followed by a decline, while RCP 8.5 considers that emissions will increase throughout the 21st century.

Climate data considered in this study, such as the surface air temperature and precipitation, was extracted from the Inter-Sectoral Impact Model Intercomparison (ISI-MIP) project as it provided the best temporal and spatial resolution for the study area. In the ISI-MIP project, the bias-corrected time-series of surface air temperature and precipitation were downscaled at a 0.5° resolution (Warszawski et al., 2014). Following the IPCC's Fifth Assessment Report, the ISI-MIP project run specific climate models to obtain data (Wu et al., 2017), which included five of the Coupled Model Intercomparison Project Phase 5 (CMIP5) Global circulation models (GFDL-ESM2M, HadGEM2-ES, IPSL-CM5A-LR, MIROC-ESM-CHEM and NorESM1-M).

As established by Nerc et al. (Nerc et al., 2018) and Birk et al. (Birk et al., 2018), the storylines considered in this study are the following (Figure 3.2):

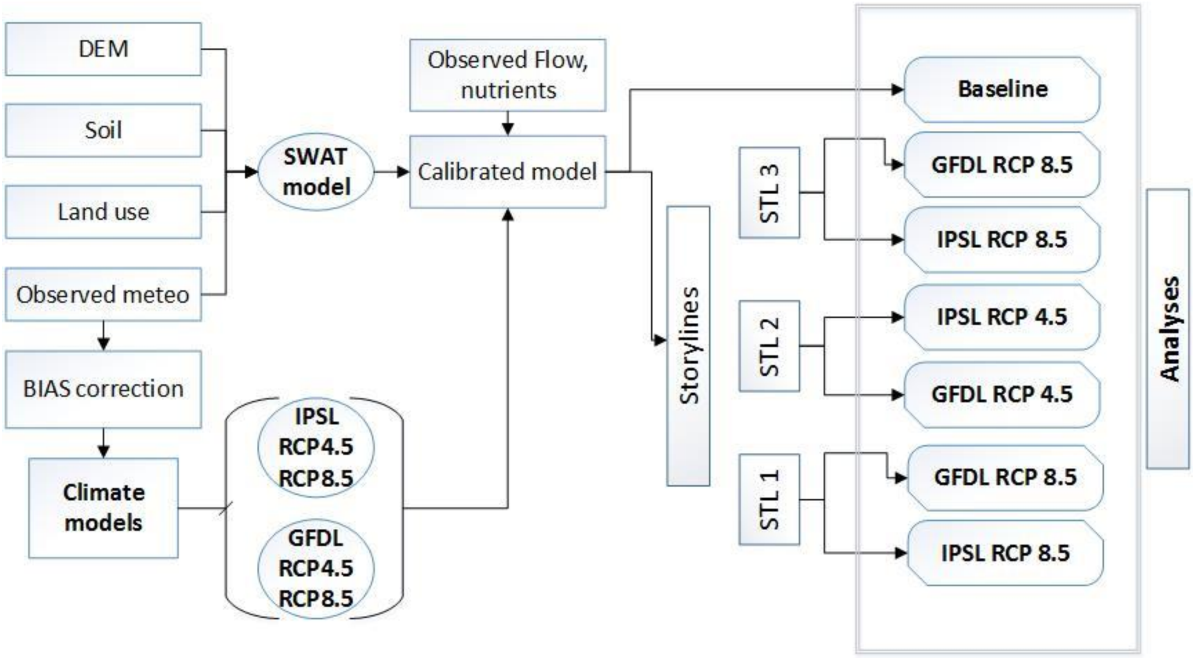

Figure 3.2 The schematic description of the modelling approach and considered scenarios (IPSL, IPSL-CM5A-LR model; GFDL, GFDL-ESM2M model; RCPs, Representative Concentration Pathways, STL, storylines).

Storyline 1 (STL1): Techno World. It represents fast global economic growth, characterised by a rapid technological development but with high energy demands and no real drive to enhance or ignore the health of natural ecosystems. This world is based on a combination of SSP-5 which consider a conventional development and low population (O'Neill et al., 2014) and climate scenario RCP 8.5 (Moss et al., 2010);

Storyline 2 (STL2): Consensus world. It is a world in which the actual policies continue after 2020. The growth of economy keeps to the same pace as now, but with awareness for environment preservation. This world is based on a combination of SSP-2 which is considered as the intermediate stage (O'Neill et al., 2014) and the climate scenario RCP 4.5 (Moss et al., 2010);

Storyline 3 (STL3): Survival of the fittest. It represents a fragmented world, driven by the individual interest of countries, with fast economic growth in NW Europe but with recessions in other regions; with minimal or no investment and effort in environmental protection, conservation and restoration. This world is based on a combination of SSP-3, which consider a rapid technology for fossils, high demand and high economic growth (O'Neill et al., 2014) and climate scenario RCP 8.5 (Moss et al., 2010).

The two climate models adopted for each climate scenario (Figure 2) were:

GFDL-ESM2M (Dunne et al., 2013, 2012): RCP 4.5 was used in Storyline 2 (hereafter referred as STL2 GFDL), and RCP8.5 was used in Storyline 1 (STL1 GFDL) and Storyline 3 (STL3 GFDL);

IPSL-CM5A-LR (Dufresne et al., 2013): RCP 4.5 was used in Storyline 2 (STL2 IPSL), and RCP8.5 was used in Storyline 1 (STL1 IPSL) and Storyline 3 (STL3 IPSL).

GFDL and IPSL were adopted in this study as they give results close to the ISI-MIP median for the Western Europe region (Grizzetti et al., 2014). These two models differ in terms of the atmospheric prognostic state and of the spatial resolution of their atmospheric grid (2.5° lon. by 2.0° lat. for GFDL, and 2.5° lon. by 3.75° lat. for IPSL). Further conceptual differences between the GFDL and IPSL models, and the downscaling of variables at the basin-scale acquired from the outputs of these two models are given in Warszawski et al. (Warszawski et al., 2014) and references therein. Bias-corrected time-series of air temperature and precipitation downscaled at a 0.5° resolution (Hempel et al., 2013) were considered. Additional bias correction for the Sorraia basin was applied on precipitation (Figure 3.3) and surface air temperature (Figure 3.4) values following Shrestha (Shrestha, 2015) and Shrestha et al. (Shrestha et al., 2017) and considering the measured data from 2006–2015. This is a statistical downscaling method known as Linear scanning bias correction based on the average difference between monthly observed and historical time series for the same period.

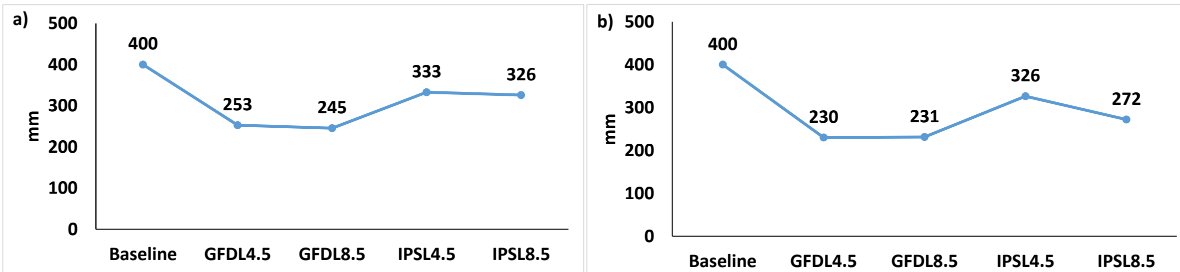

Figure 3.3 The annual average precipitation (mm) for the baseline conditions and climate scenarios: (a) timeline 2030; (b) timeline 2060. For clarification on the modelled scenarios.

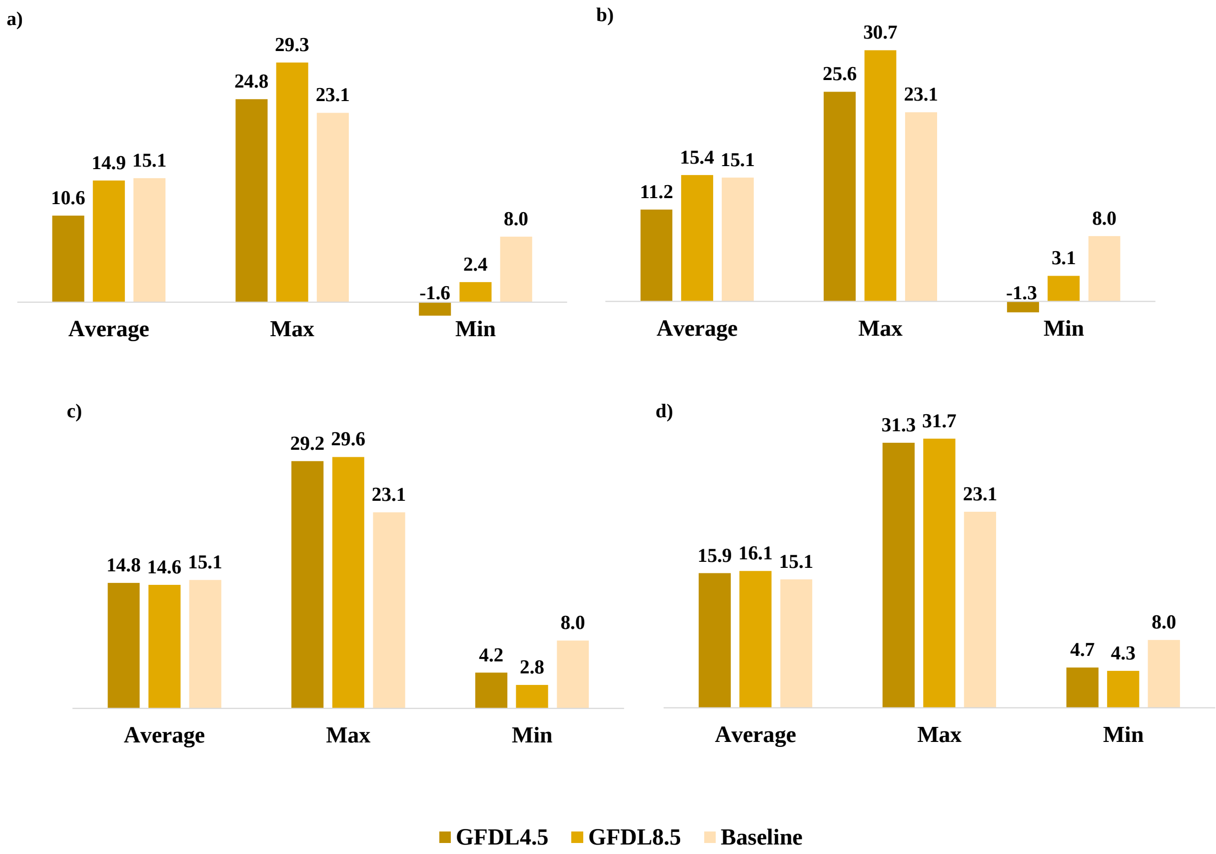

Figure 3.4 The average, maximum, and minimum daily temperature (°C) for the present conditions (baseline) and climate scenarios: (a) and (c) timeline 2030; (b) and (d) timeline 2060. For clarification on the modelled scenarios.

Two distinct temporal intervals were set up to run the simulations: 2030 (defined as a 10-year average from 2025 to 2034) and 2060 (defined as a 10-year average from 2055 to 2064). Thus, the term “climate change” refers here only to decadal changes. The period 1996–2015 was selected as a reference for the baseline simulation (present condition).

The downscaling of the socio-economic factors and foreseen management practices change in the Sorraia catchment was performed with the help of local water board stakeholders (Associação de Regantes e Beneficiários do Vale do Sorraia). Therefore, each storyline was naturally translated into quantitative data assuming that the Mediterranean climate imposes additional stress on the agriculture (Grizzetti et al., 2014). This additional stress was defined in terms of management practice changes, namely on the amount of fertilizer and irrigation applied to crops (Table 3). That assumption considered that in a changing environment, with temperatures increasing, higher irrigation needs are required to fulfil crop requirements. Additionally, higher temperatures lead to higher mineralisation rates and, thus, higher use of fertilizers. It also considered that higher usage of fertilizers and irrigation lead to larger diffuse pollutions from agricultural fields and greater environmental risk. Model inputs were thus related to the level of agriculture intensification and the environmental protection awareness considered in each Storyline. Fertilizers were applied to prevent nutrient stress by plants. The percentage variation (increase or decrease) defined in Table 3.3 for each storyline and timeline was applied on the baseline values and used as an input in the model.

Table 3.3 The input values used for simulating the storylines in the Soil Water Assessment Tool (SWAT).

Storyline	Timeline	Management Practices	Variation (%)	Baseline	Amount
STL1	2030	Fertilization (kg/ha)	10+	492	541
	2060		15+		566
	2030	Irrigation (mm)	10−	430	387
	2060		15−		366
STL2	2030	Fertilization (kg/ha)	10−	492	443
	2060		15−		418
	2030	Irrigation (mm)	20−	430	344
	2060		25−		323
STL3	2030	Fertilization (kg/ha)	30+	492	640
	2060		35+		664
	2030	Irrigation (mm)	30+	430	559
	2060		35+		581

3.3 Results and Discussion

3.3.1. Model Calibration/Validation

Model calibration was carried out considering the period between 2001 and 2006, and validation was performed considering the period between 2006 and 2015. The statistical indicators obtained after comparing the daily and monthly simulated and measured flow values at the selected monitored stations are presented in Table 3.4. At Moinho Novo, the R^2 value of 0.71 for monthly data shows that a considerable proportion of variability of the observed data was explained by the model (Table 3.4 and Figure 3.5). The RMSE value of 6 m3/month indicates a small error of model estimates, while the NSE value of 0.71 indicates that the residual variance results were much smaller than the measured data variance (Table 4 and Figure 5). The comparison of daily values produced, as expected, worse results, with errors being mostly minimized during the monthly analysis due to data aggregation. For the validation period, the indicators were found to be similar, indicating a reasonable calibration of model parameters when considering all the uncertainties related to measurements.

Table 3.4 The daily and monthly flow statistics at Moinho Novo and Ponte Vila Formosa.

Statistics	Moinho Novo				Ponte Vila Formosa			
	Calibration		Validation		Calibration		Validation	
	Daily	Monthly	Daily	Monthly	Daily	Monthly	Daily	Monthly
Obs. Average	6.05	6.71	7.57	7.07	3.17	3.31	5.68	5.61
Mod. Average	6.95	7.04	6.50	5.81	6.09	6.27	5.22	5.19
Bias	0.90	0.33	−1.07	−1.27	2.93	2.97	−0.46	−0.42
RMSE	13.1	6.00	16.6	7.51	12.61	6.04	15.21	5.93
R^2	0.41	0.71	0.41	0.68	0.31	0.58	0.24	0.54
Model Efficiency	0.22	0.71	0.39	0.67	−3.05	−1.26	0.11	0.40

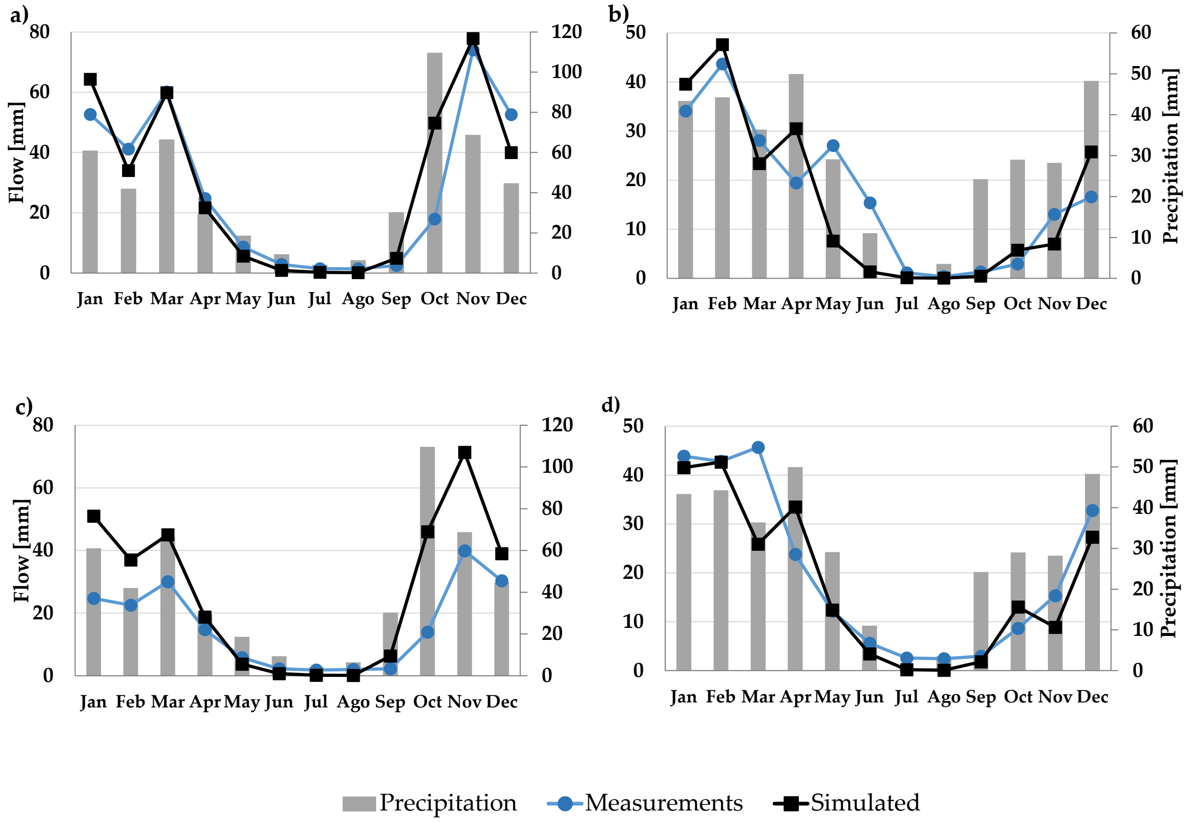

Figure 3.5 The monthly average flow (mm) in Moinho Novo: (a) calibration period; (b) validation period; and Ponte Vila Formosa location; (c) calibration period; (d) validation period.

3.3.2. Scenario Analysis

Water Quantity

After calibration and validation, the SWAT model was used to evaluate the developed storylines. Climate models showed a decrease in precipitation from 400 mm year^{-1} to an average of 264 mm year^{-1} on both timelines (Figure 3.6). As a result, the simulated scenarios showed a substantial reduction of monthly flows for the 2030 and 2060 timelines (Figure 3.7). Flow reduction evidenced a non-linear relationship between precipitation and monthly river flow averages. This resulted from the uncertainty associated with climate models, particularly in the forecast of extremes events (Figure 3.6). The monthly average flow for the baseline simulation was 42 m^3 s^{-1} (Table 3.5), while the IPSL model showed a decrease by half of this value in the timeline 2030 (to about 19 m³ s⁻¹), and a further decrease in the timeline 2060 (to 10 m³ s⁻¹). More severe results were obtained with the GFDL model for the same scenarios, predicting a decrease in the precipitation average to half of the present value, which resulted in monthly flow averages of 4.5 m³ s⁻¹ and 2.5 m³ s⁻¹ for the timelines 2030 and 2060, respectively (Table 3.5). Moreover, the increasing temperature trend predicted by both climate models combined with decreasing precipitation further led to more hazardous agricultural practices for the environment, with irrigation and fertilizer requirements increasing as considered in STL1 and STL3. Even for the scenario with more sustainable agricultural practices (STL 2), the changes in the climate variables had the same severe effect on river flow (Figure 3.6). For both climate scenarios, the decrease in irrigation in STL2 resulted in small differences in the monthly flow average when compared with the previous results (Table 3.5).

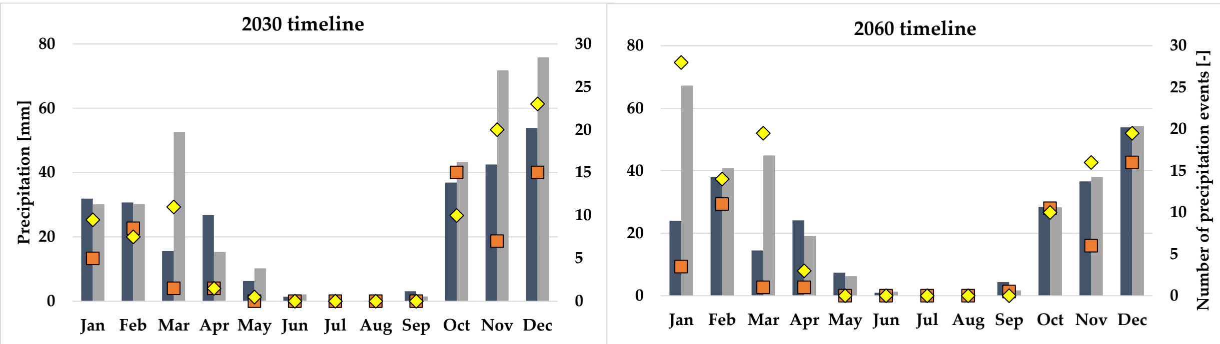

Figure 3.6 The monthly average precipitation (mm) for each climate model (bars), and the number of daily precipitation events > 10 mm (−) for all period (symbols), for each timeline.

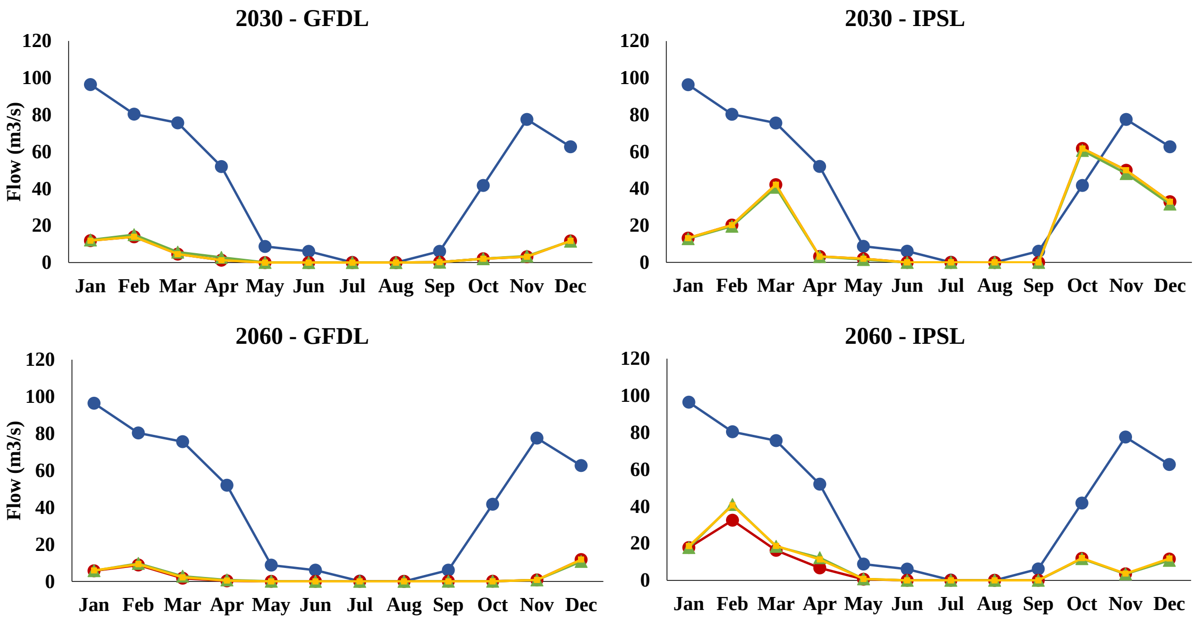

Figure 3.7 The monthly average of modelled river flow (m3 s−1) for each storyline and baseline. For clarification on the modelled scenarios.

Table 3.5 The monthly averages for river flow ($m^3\ s^{-1}$), total N ($mg\ N\ L^{-1}$), and total P ($mg\ P\ L^{-1}$) in each scenario.

Monthly Average	Baseline	STL1	STL2	STL3	STL1	STL2	STL3	STL1	STL2	STL3	STL1	STL2	STL3
		2030 GFDL			2030 IPSL			2060 GFDL			2060 IPSL		
River flow ($m^3\ s^{-1}$)	42.3	4.1	4.5	4.1	18.8	18.2	18.8	2.5	2.6	2.5	8.4	9.7	9.8
Total N ($mg\ N\ L^{-1}$)	0.7	3.3	2.2	3.9	1.1	0.9	1.2	5.5	2.6	6.2	1.4	1.2	1.5
Total P ($mg\ P\ L^{-1}$)	0.2	0.1	0.1	0.1	0.3	0.3	0.4	0.2	0.2	0.2	0.2	0.2	0.2

The simulated storylines focused on distinct management practices in the watershed. Changes were associated with climate change models IPSL and GFDL developed for this purpose. All simulated scenarios showed a significant decrease in water quantity, clearly visible in the reduction of river flow (Figure 3.7). This outcome was a direct consequence of the significant decrease in precipitation generally estimated by all climate models, especially for Mediterranean countries, due to the increased anticyclonic circulation that yields increasingly stable conditions, and to a northward shift of the Atlantic storm track (Erol and Randhir, 2012; Giorgi and Lionello, 2008; IPCC and IPCC5 WGII, 2014). Similarly, Bucak et al. (Bucak et al., 2017) predicted flow variations between +18 and −59% for the Beyşehir watershed (Turkey), depending on the climate scenario considered. Pascual et al. (Pascual et al., 2015) reported the largest reductions (34%) in mean streamflows (for 2076–2100) to be expected in the headwaters of two humid catchments in Catalonia (Spain), while lesser variations (25% of mean value for 2076–2100) were to be expected in a drier area. Additionally, in all three catchments, the most notable projected decreases in streamflow were observed in autumn (50%) and summer (30%). The largest reductions in the Sorraia river flow were associated with agriculture activities, namely irrigation, which, combined with climatic change, augmented the problem. Therefore, while water availability in several Mediterranean basins is mostly conditioned by precipitation, the results of this study in the Sorraia River basin show that other processes related to agricultural practices also contribute to water scarcity, such as evapotranspiration and irrigation.

Water Quality

In the Sorraia basin, irrigated crops are traditionally sown during mid-April/May and harvested in mid-September/October (Cameira et al., 2007; Ramos et al., 2017). This leads to an increase of Total N concentration in the Sorraia River during those periods as noticed in all storylines, especially in STL3 (Table 3.5 and Figure 3.8), which results from the water reduction in the basin and increased use of fertilizers (STL1 and STL3). Total N concentrations were perceptibly higher when using the GFDL climate model due to the lower precipitation amount predicted. An increase of the total N concentration in the river during the crop growth periods was also predicted due to nutrient runoff and leaching. The most marked increase was observed immediately after the harvest season (Figure 3.8), coinciding with the mineralisation of crop residues and the beginning of the rainy seasons. The increase of soil water content further promoted nitrate leaching, as well as losses by the lateral flow. Therefore, precipitation reduction played a fundamental role in the future projections of catchment dynamics.

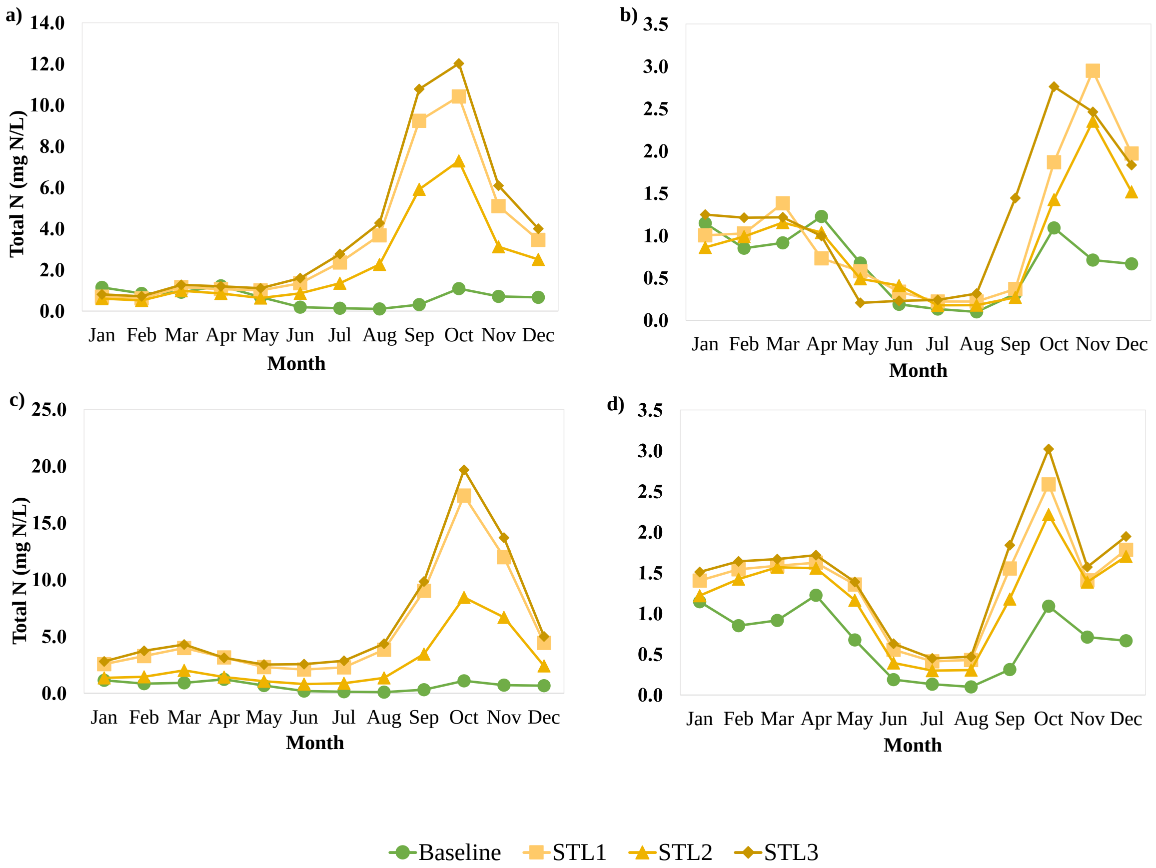

Figure 3.8 The monthly average of modelled Total N concentration (mg N L−1) for each storyline and baseline period: (a) 2030-GFDL; (b) 2060-GFDL; (c) 2030-IPSL; (d) 2060-IPSL. For clarification on the modelled scenarios.

The increase of Total N concentration in all storylines was drastic when compared with the present conditions (0.7 mg N L^{-1}) (Table 3.5). For the GFDL scenarios, despite the agriculture practices outlined in STL2, there was a predicted increase of Total N concentration in the Sorraia River up to 2.2 mg N L^{-1} in the 2030 timeline, and up to 2.6 mg N L^{-1} in the 2060 timeline. For the STL1 and STL3, an average of 3.6 mg N L^{-1} was computed for the timeline 2030, and an average of 5.9 mg N L^{-1} was computed for the timeline 2060. For the IPSL model scenarios, the increase was not so outstanding, especially for STL2, where the monthly averages in the timelines of 2030 and 2060 were predicted to be 0.9 and 1.2 mg N L^{-1}, respectively. For this model, an average of 1.2 mg N L^{-1} was observed for the STL1 and STL3 in the timeline 2030, and an average of 1.4 mg N L^{-1} was noted for the timeline 2060 (Table 3.5).

The projected increase of N concentration in the river resulted from the progressive use of this nutrient as fertilizer in most scenarios, but also as a consequence of natural processes occurring in the soils. This outcome is also visible in the more optimistic scenario (STL2), where the negative impact of water flow reductions on water quality was also high. Nitrate was the most abundant form of N simulated in the river (Figure 3.9), also contributing significantly towards this outcome were nitrate high solubility and leaching susceptibility (Cameron et al., 2013; Lamb et al., 2017), mostly during the periods of higher precipitation, and the type of fertilizers used by farmers (Ramos et al., 2012).

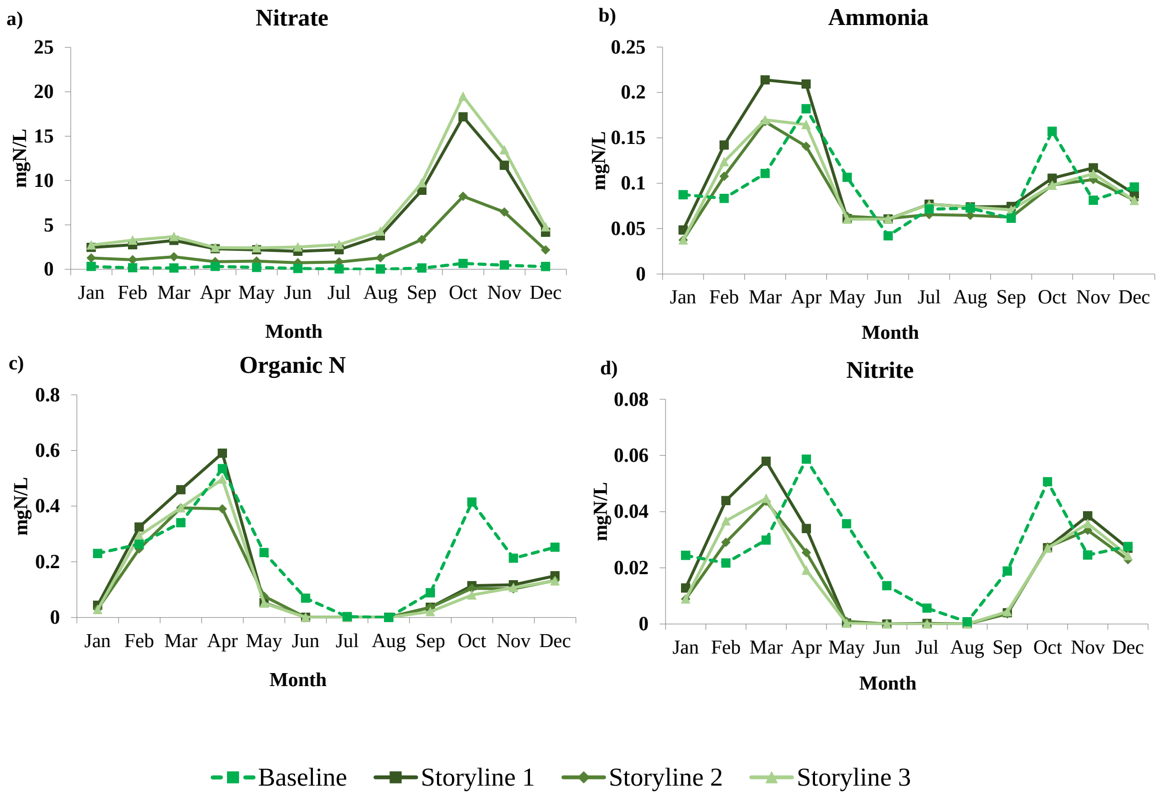

Figure 3.9. The monthly evolution of the N forms (mg N L−1) for each storyline (timeline 2060 and GFDL climate model) and baseline condition: (a) Nitrate; (b) Ammonia; (c) Organic N; and (d) Nitrite.

The most pronounced increase in the nutrients concentration was found to occur during the autumn/winter period, after the harvesting of corn in irrigated areas (September/October). The high temperature and low soil moisture values predicted during this time of the year enhanced the mineralization of crop residues as observed by the increase of simulated organic N in the river (Figure 3.9). Nitrite was the least abundant form of N as its oxidation process occurred very fast. The significant increase in N and P may enhance the eutrophication process, thus contributing towards the degradation of water quality (Brito et al., 2018).

Table 3.5 and Figure 3.10 further describe the monthly behaviour of the Total P concentrations in the baseline simulation and future scenarios while considering the different Storylines and climate models. On average, most of the scenarios led to similar monthly concentrations when compared with the present (0.2 mg P L^{-1}). In the 2030 timeline, a decrease of the Total P concentration in the Sorraia River to 0.1 mg P L^{-1} was predicted for all storylines when using the GFDL model, mainly due to the significant decrease in the precipitation amount which reduced runoff and soil erosion, thus decreasing the transport capacity of P in the basin. In the 2060 timeline, an increase of the Total P concentration to 0.3 mg P L^{-1} in the STL 1 and STL2, and a double-fold increase (0.4 mg P L^{-1}) in the STL3 were predicted, in line with the literature (Serpa et al., 2017). Serpa et al. (Serpa et al., 2017) found a similar decrease of water quality in the Vale do Gaio River (Portugal), located a few kilometres south of the Sorraia River basin, with P concentrations increasing from +29% to +93% depending on the storylines adopted. All climate models and Storylines showed the same concentration averages for the 2060 timeline when comparing with the present monthly average (0.2 mg P L^{-1}). However, the major differences observed between the results from GFDL and IPSL climate models may result from extreme precipitation events as shown above (Figure 3.7).

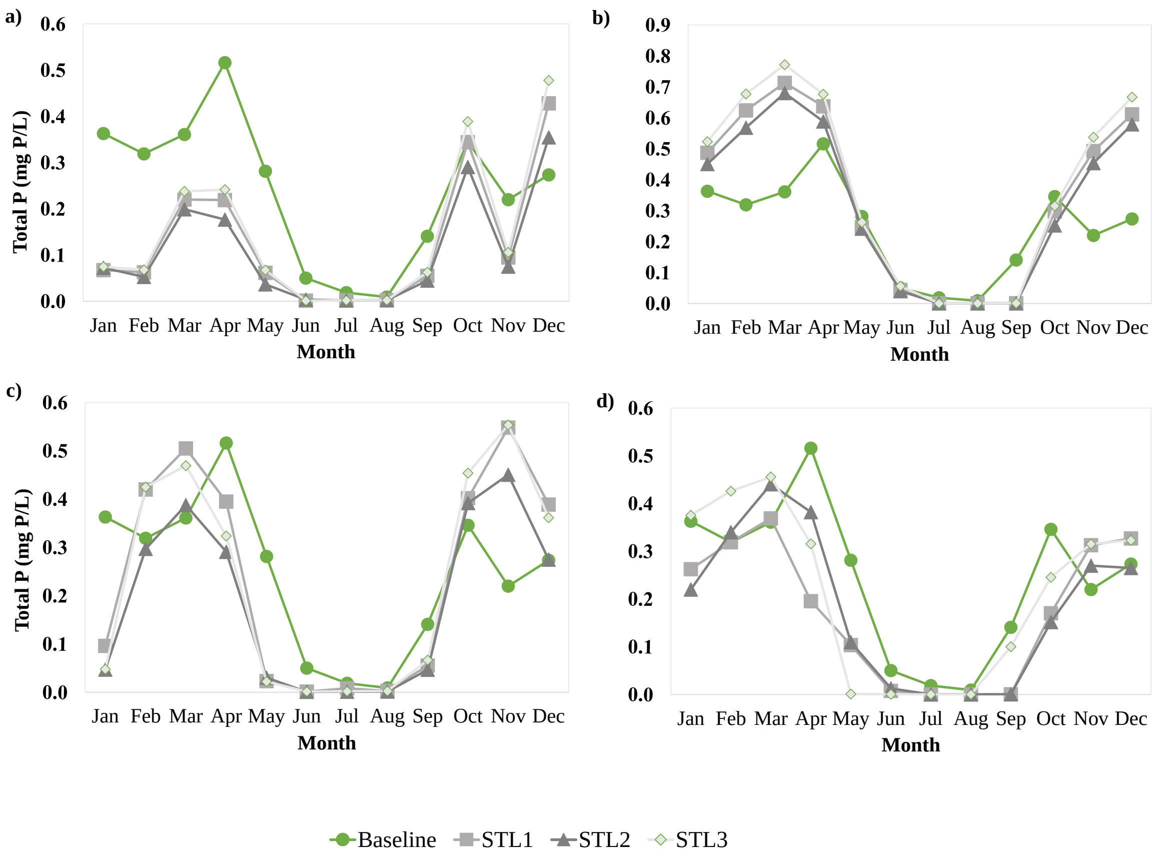

Figure 3.10. The monthly average of the modelled Total P concentration (mg P L−1) for each storyline and baseline: (a) 2030-GFDL; (b) 2060-GFDL; (c) 2030-IPSL; (d) 2060-IPSL.

Interestingly, the mineral P increase resulting from fertilizer use in corn fields was not obvious in terms of water quality results. This outcome can be explained by the fact that P presents low mobility, adsorbing to sediments and depending on rainfall and runoff events to be removed from agricultural fields. As shown in Figures 3.10 and 3.11, P concentrations are expected to exhibit a different behaviour from N in all storylines. However, the fact that P concentrations show a slight increase despite the decrease in precipitation suggests that its continued application will have a significant impact on water quality.

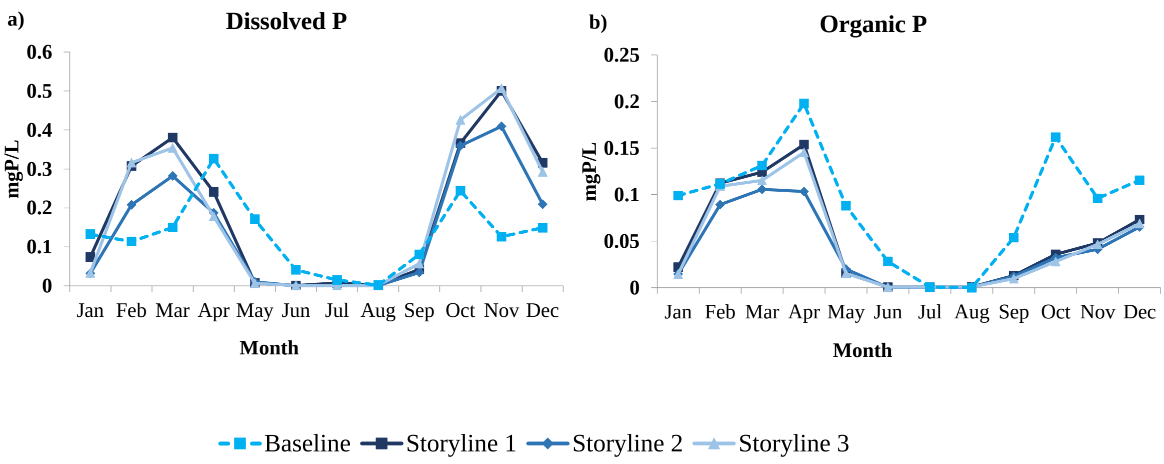

Figure 3.11. The monthly evolution of the P forms (mg P L−1) for each storyline (timeline 2060 and GFDL climate model) and baseline: (a) Dissolved P; and (b) Organic P.

Results have also shown that the decrease of water in the basin had a significant influence on the quality of water in the river. Results for Total N and P concentrations (Figure 3.8 and Figure 3.10) further suggest a significant deterioration of water quality in the Sorraia River, particularly with respect to the Total N.

3.4 Conclusions and Future Research

The modelling approach developed in this work highlighted possible cumulative impacts of future climatic changes in the Sorraia River basin by considering the expected changes in precipitation, temperature, and human activities. A significant decrease in precipitation is expected over the watershed for the near future (between 25% and 50%). It is likely that this decrease will lead to an increase in irrigation and fertilization needs over this basin by 35%. The water quantity is predicted to fall approximately by up to 75%, while water quality shows an unbalanced deterioration, with nutrient concentrations predicted to increase up to 200% for P and up to 500% for N. Such a rise in nutrient concentration is observed to be a consequence of the increased use of fertilizers and decrease in water availability in rivers.

The results show how societal and especially climatic changes can affect river water quantity and quality in the study basin and can be considered as a starting point for defining appropriate management plans to counteract such negative impacts. The SWAT model can be further explored to test the effects of management practices and the degree of stress they introduce on the environment, thereby contributing to a cost-effective adaptive management practice. For instance, the use of winter crops with minimum water requirements, the implementation of no-till practices to improve soil structure and soil infiltration rates, the use of cover crops for reducing soil water evaporation or the establishment of more resilient cropping systems to cope with water scarcity may allow future impacts to be minimised at the basin level.

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Chapter 4 An Integrated Modelling Approach to Study Future Water Demand Vulnerability in the Montargil Reservoir Basin, Portugal

The material on which this chapter is based has been previously published in **Almeida, C.;** *Ramos, T.B.; Sobrinho, J.; Neves, R.; Proença de Oliveira, R. An Integrated Modelling Approach to Study Future Water Demand Vulnerability in the Montargil Reservoir Basin, Portugal. Sustainability 2019, 11, 206.*

Abstract

This paper describes an integrated modelling approach to study water use vulnerability in a typical Mediterranean basin under different climate change projections. The soil water assessment tool (SWAT) and the MOHID (from *modelo hidrodinâmico*) Water model were used to evaluate the impacts of two climate scenarios (GFDL-ESM2M and IPSL-CM5A-LR) on water availability in Montargil's basin and reservoir (Portugal) during two decadal timelines (2030 and 2060). Reservoir performance metrics were estimated considering also two water demand scenarios: an average of the water demand in the last 10 years; and the largest annual demand of the last 10 years. The SWAT model results showed a future decrease of inflows to the reservoir, with its volumetric reliability decreasing from 100% in the historical simulation to about 60–70% in the IPSL-CM5A-LR climate scenario and 40–50% in the GFDL-ESM2M climate scenario. The time reliability also decreased to less than 30%, while the resiliency for the water demand decreased to an average 20–35% for both climate scenarios. These impacts indicate the importance of the managing systems in an integrative mode to prevent water resources reduction in the region.

Keywords: integrating modelling; climate change; water availability; vulnerability; Montargil; basin; reservoir.

4.1 Introduction

In the Mediterranean region, water resources are scarce and exhibit large seasonal and intra-annual variability. Water storage is essential for fulfilling water demand, for producing energy and for controlling flood and drought events. The sustainability and development of many economic activities in the region depends on water storage in reservoirs, with the construction of infrastructures in river valleys also leading to changes in land use that influence the entire water balance and water quality at the basin scale.

Basins are subjected to multiple stressors (Hering et al., 2015; R. Townsend et al., 2008; Segurado et al., 2018), with climate change emerging as a major concern in river water management. In the Mediterranean countries, surface air temperature is expected to increase while the annual amount of precipitation is expected to decrease (IPCC and IPCC5 WGII, 2014; Olesen and Bindi, 2002; Ragab and Prudhomme, 2002; van Vuuren et al., 2011). These changes will result in an increasing frequency of extreme climatic events, including droughts (Giorgi and Lionello, 2008; Iglesias et al., 2007). Examples of these extreme events are already visible in Portugal, where severe drought events occurred during 2005 and 2012 (Botelho and Ganho, 2010). As a result, surface and ground water availability is projected to decrease, especially in the centre and south of Portugal (Nobrega, 2006), stressing the need for developing strategies for adapting water resources management to climate change.

In southern Portugal, several reservoirs were built in the middle of the 20th century, mainly for irrigation. New irrigated areas were created, with crops having their growing season in the summer season when evapotranspiration needs are higher (Valverde et al., 2015). This production system is highly dependent on water stored in reservoirs during the rainy season and on the existence of hydraulic structures to distribute water.

In the past, infrastructure planning and operations, namely reservoir water management, was based on the analysis of historical records, which were assumed to be stationary. In the context of climate change that may not be the most appropriate strategy. Instead, a growing number of studies have pointed to the importance of integrating mathematical models in the decision-making process (Brito et al., 2018a; Silva-Hidalgo et al., 2009; Skoulikaris, 2008). Mathematical models can provide managers with an integrative analysis of the processes and time variables concerning the basin status (Labadie, 2006; Lettenmaier D.P., Dennis P., Alan F. Hamlet, Tazebe B., 2008), which otherwise would be difficult to assess only with available monitoring results. Models can also provide, directly or indirectly, performance indicators related to water resource use that can be used to evaluate its operating rules, determining the supply guarantee, the vulnerability of water needs, and the system's resilience (Hashimoto et al., 1982; Jinno, 1995).

By considering climate change and related uncertainty, those modelling tools can be used for predicting water availability in the near future. This results in a direct benefit when estimating inflows or planning of best operation practices, particularly in basins where agriculture is heavily dependent of reservoirs supply. Additionally, while most of the uncertainty associated to long-term hydrological predictions refers to the ability of climate model to forecast future precipitation for the river basin, climate models have been consistent in the projected trends allowing to draw reliable future scenarios.

The complexity of the dynamics and properties of each water body such as lakes, rivers or coastal areas, or even artificial systems such as reservoir or urban systems further require the integration of mathematical models for improving water resources management. Thus, extensive integration of mathematical models has been performed during the last decades. For example, Brito et al. (Brito et al., 2015) integrated the basin (soil and water assessment tool (SWAT) model) and reservoir model (CE-QUAL-W2) to study the water quality and to test different management scenarios to reduce nutrient loads in an eutrophic reservoir in southeast Portugal. Brito et al. (Brito et al., 2015) developed an operation management tool for simulating flows from the main watersheds of the Iberia Peninsula, where the basin model MOHID Land (from *modelo hidrodinâmico*) were integrated in the coastal model MOHID Water.

In this study, two climate models were used as input to a basin model, which in turn was integrated into a reservoir model. The main objective was to investigate water resources availability in the Montargil reservoir (southern Portugal) and respective vulnerability under future climate scenarios. The specific objectives were: (1) to assess and model climate change scenarios over the study area; (2) to determine the water balance and flows at the basin scale; and (3) to analyse the vulnerability of the reservoir while considering those future scenarios. This study is particularly original in performing an integrated analysis of water resources availability in the Mediterranean region under the context of climate change. This study further promotes the development of tools to support sustainable water resources management in the study area.

4.2 Materials and Methods

4.2.1. Study Area

This study was carried out in the Montargil Reservoir, located in the Sôr River sub basin, which is part of the Sorraia River (southern Portugal), the tributary of the Tagus River with the largest basin area (~7730 km^2) (Figure 4.1). Montargil, with its drainage area of ~1200 km^2, is one of the largest Portuguese reservoirs on a dry area. This reservoir is part of the Sorraia Valley watering system with two other reservoirs: Magos and Maranhão. The system was created between 1951 and 1959 and benefits a total of 16,351 ha of irrigated agricultural land in six municipalities. The watering system is managed by the Farmers Association of the Sorraia Valley (ARBVS) since 1970. Thus, while each reservoir has an independent drainage area, they are managed together according to water availability.

Over the last years, the Montargil reservoir has been increasingly used for recreational purposes, benefiting from short distances to major urban habitation areas (about 100 km from Lisbon) and warm water temperatures during the bathing season. The reservoir has also been used for electric power generation, fishing, and water sports. The climate in the region shows two typical seasons, one with dry and hot summers, and another with mild and wet winters (Figure 4.2).

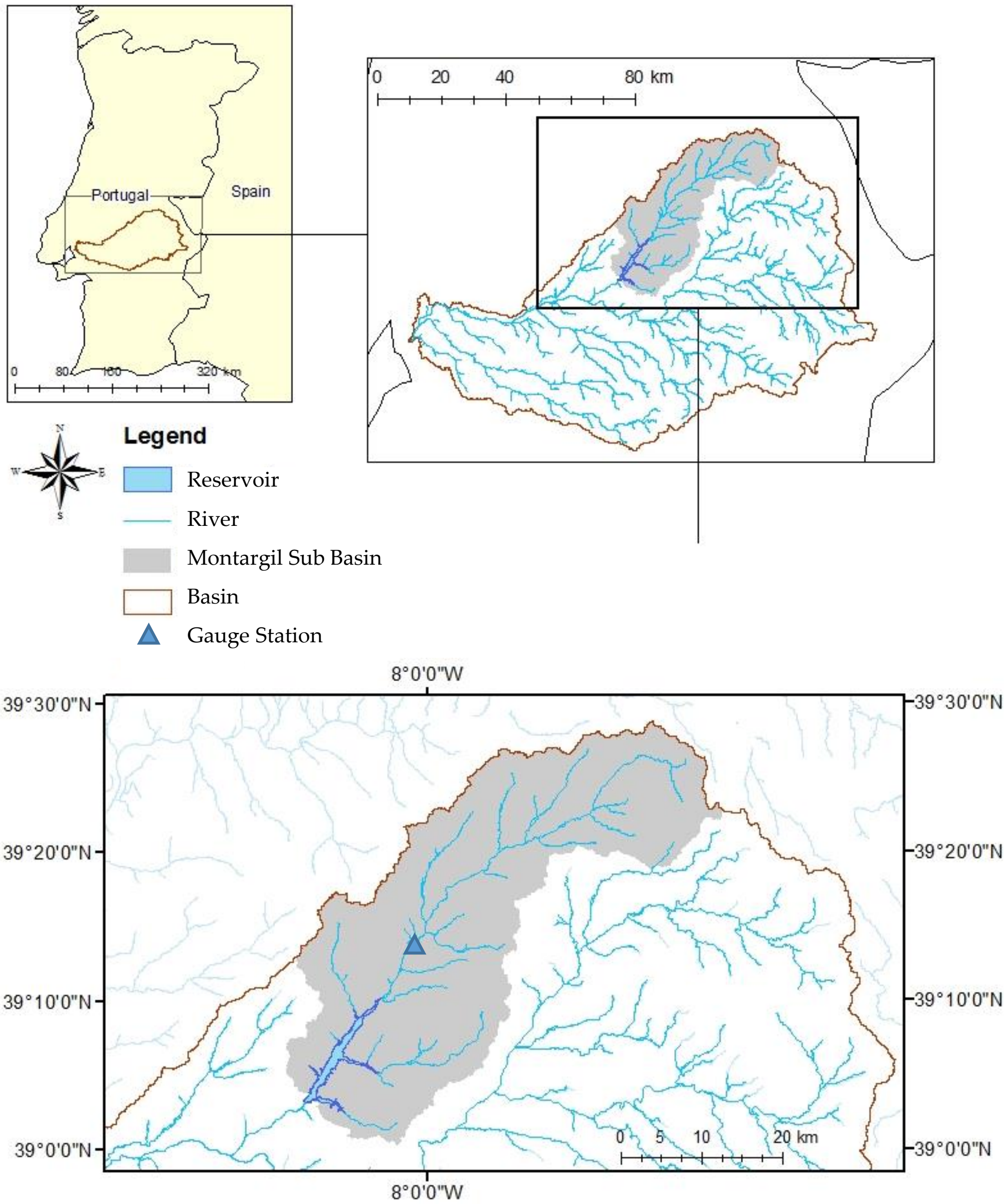

Figure 4.1. Location of the Montargil sub basin and reservoir.

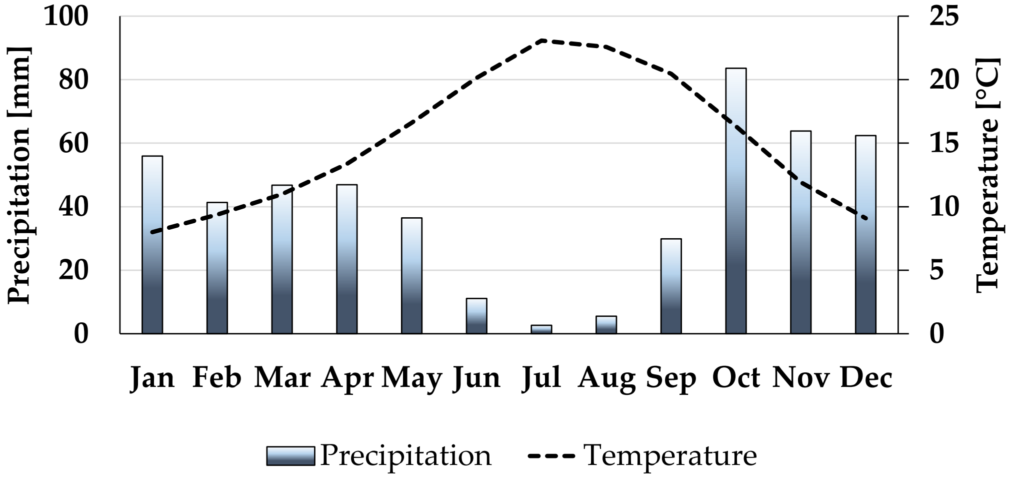

Figure 4.2. Monthly average temperature and precipitation in Montargil basin (average of last 20 years).

The main land uses in the Montargil basin area are forest (63%), range-grass (22%), agriculture (8%), orchard (3%), urban and industrial (1%) and pasture (1%) (Mateus et al., 2009) (Figure 4.3). The elevation ranges from 45 to 358 m a.s.l (Figure 4.3). The dominant soil types are Cambisols, Luvisols and Regosols (IUSS Working Group WRB, 2014).

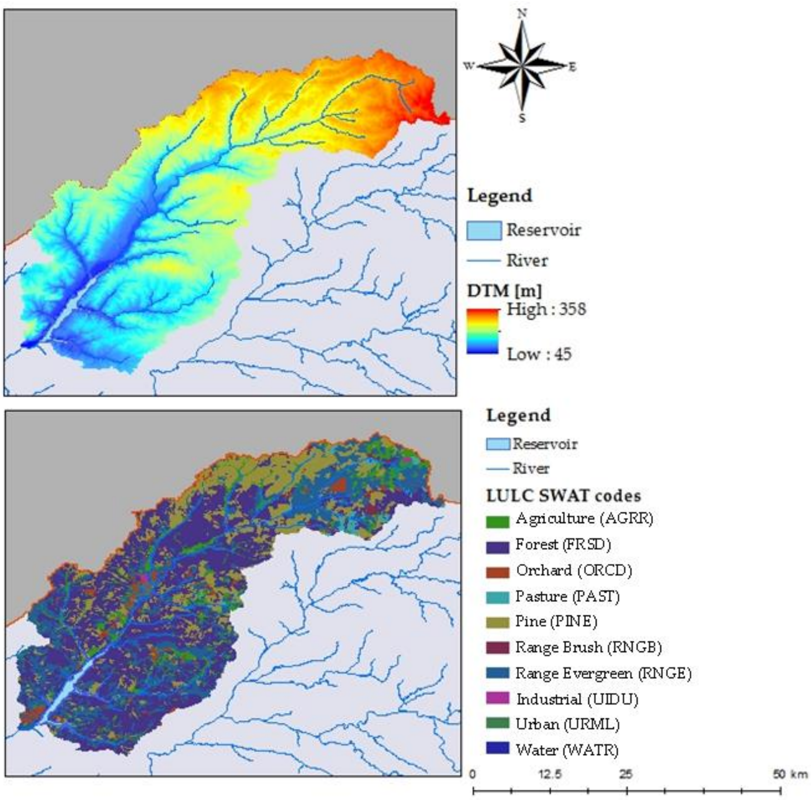

Figure 4.3. Digital terrain model and land use/land cover map in Montargil sub-basin.

The Montargil reservoir provides mainly water for irrigation, and to a less extent for industry purpose. The water level is thus regulated by irrigation water demand and depends on climatic conditions. Accordingly, the reservoir is filled between autumn and spring and the water is used gradually during the summer irrigation season (Figure 4.4). The outflow from the reservoir is controlled by several structures. The maximum reservoir capacity is about 164 hm^3, with a water surface elevation of 80 m and minimum surface height of 30 m. The minimum water surface elevation acceptable for operation is 65 m above water surface elevation, which corresponds to ~143 hm^3.

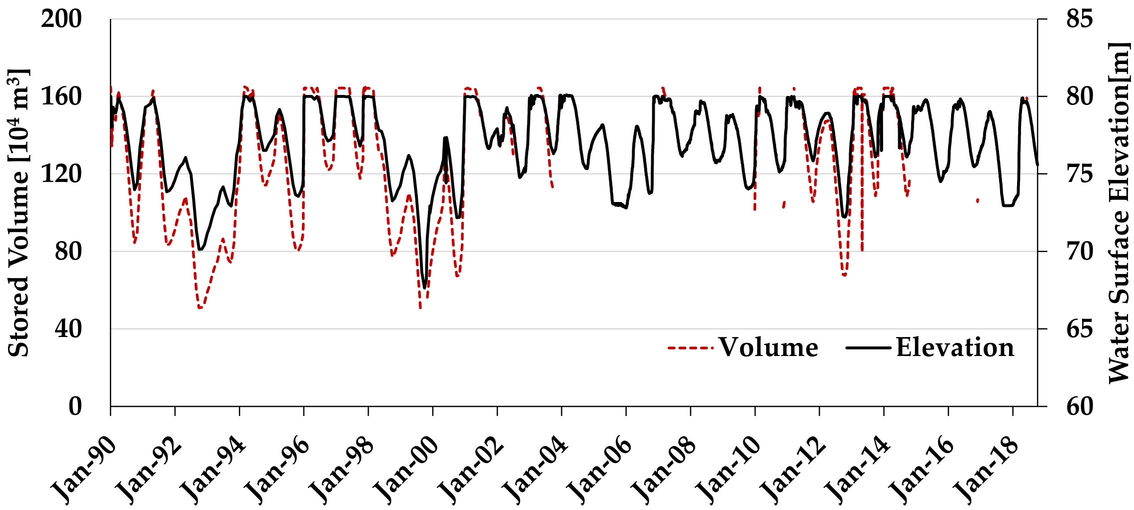

Figure 4.4. Observed reservoir stored volume with missing values found (m3) and water surface elevation (m) during the last 28 years in the Montargil reservoir.

4.2.2. Integrated Modelling Approach

Figure 4.5 describes the framework of the integrated modelling approach considered in this study. The SWAT (Neitsch et al., 2011) was used for modelling flows at the basin scale. The basin modelling considered the digital terrain model (DTM), soil data, land use, and meteorology from historical data as inputs. The model was calibrated and validated by comparing simulated flows with measured data. The baseline simulation was defined for the period between 1996 and 2015. The SWAT model was calibrated manually for the period between 2001 and 2006, while the validation exercise comprised the period from 2006 to 2015. Flow results from SWAT were then integrated as boundary conditions to the reservoir MOHID Water model (Neves, 1985). This model was calibrated and validated for simulating the elevation-volume curve, levels, and volumes during the historical period (Figure 4.5). After model validation, future scenarios were defined using projections from the GFDL-ESM2M and IPSL-CM5A-LR climate models (Dufresne et al., 2013; Dunne et al., 2013) as boundary conditions to SWAT and MOHD Water. The description of each model can be found in the sections below.

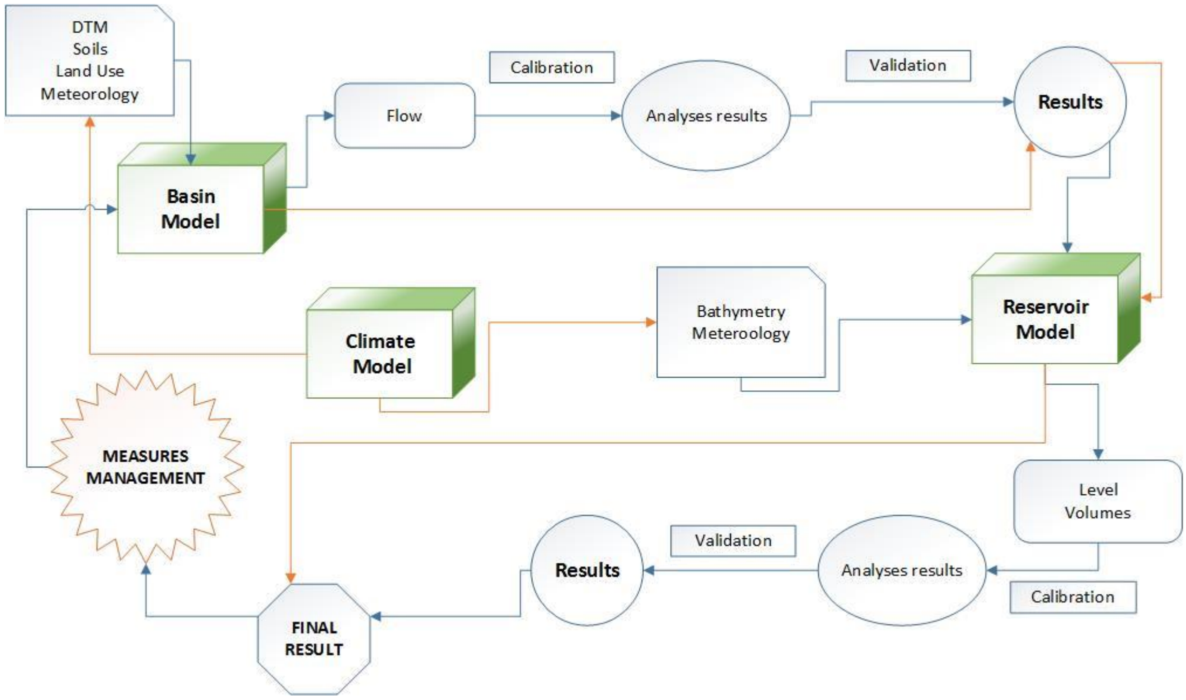

Figure 4.5. Schematic description of the modelling approach considered: basin model, reservoir model and climate models integration; blue connections are related to baseline modelling, and yellow connections are related to scenarios.

4.2.2.1. Basin Model

TheSWAT (Neitsch et al., 2011) is a semi-distributed widely used model for simulating watershed processes and assessing land management practices at the basin scale using a daily time step. The SWAT model was already successfully calibrated/validated for simulating streamflow and nutrient dynamics in the Sorraia basin (Almeida et al., 2018; Segurado et al., 2018), with results providing the necessary basis for conducting this study. The model splits the watershed into sub-basins that are assumed to be homogeneous in their hydrologic response units (HRU), i.e., areas with homogeneous properties in terms of slope, land use, and soil type. The hydrology of the model relies on solving the water balance equation, as follows:

$$SW_t = SW_0 + \sum_{i=1}^{t}(R_{day} - Q_{surf} - E_a - W_{seep} - Q_{gw}) \tag{1}$$

where SW_t is the final soil water content (mm), SW_0 is the soil water content at the initial time step (mm), R_{day} is the precipitation on day i (mm), Q_{surf} is the surface runoff on day i (mm), E_a is the actual evapotranspiration on day i (mm), W_{seep} is the percolated water on day i (mm), and Q_{gw} is the return flow on day i (mm).

Crop evapotranspiration is computed following the Penman Monteith method (G. Allen et al., 1998), and dependent on soil water availability. Infiltration and groundwater flow are computed based on empiric or semi-empiric formulations (as the Soil Conservation

Service (SCS) rainfall-runoff curves or soil-shallow aquifer-river transfer times). Details on individual simulation components can be found in Neitsch et al. (Neitsch et al., 2011).

In this study, the SWAT model was applied to the Montargil sub-basin using the ArcGIS extension from ESRI (Redlands, CA, USA). Available geographic information system (GIS) maps of topography from Shuttle Radar Topography Mission (SRTM) with 90 m resolution, land use from GSE Land M2.1 with 20 and 300 m resolution (Mateus et al., 2009), and soils from Portuguese Soil maps and Land use Capacity at 1:25,000 scale (Cardoso, 1965), were used. Climatic maps, including daily precipitation, temperature, relative humidity and wind speed were derived from the Portuguese National Institute of Water Resources (SNIRH) (SNIRH, 2017).

4.2.2.2. Reservoir Modelling

The present work was carried out using the hydrodynamic and biogeochemical three-dimensional MOHID Water model (Neves, 1985). This model has been applied to a variety of locations subject to different conditions since its creation (Coelho et al., 1998; Deus et al., 2013; Franz et al., 2016). The model consists of a set of modules interconnected using an object-oriented programming. Each module is responsible for the management of part of information, constituting a total of 40 modules developed over 3 decades of research work.

In this study, the MOHID Water model was applied to the Montargil reservoir. The following modules were considered for simulating water variation dynamics in this study: Atmosphere, Geometry, Hydrodynamic, Interface Water Air, Turbulence and Discharges. The model grid resolution was 100 m × 100 m, and the topography map from the SRTM with 90 m resolution was considered due to unavailability of the bathymetric map of the Montargil reservoir. As initial condition, the water level at the first day of the simulation was imposed from SNIRH (SNIRH, 2017). Meteorological data (velocity and wind direction, precipitation, solar radiation, air temperature and relative humidity) were obtained from SNIRH (SNIRH, 2017) and used as boundary conditions. The upstream river discharges computed earlier with the SWAT model were also used as boundary conditions. These were set to reach the reservoir on five locations (Figure 4.6), with the main river inflow reaching ~48 m^3/s (average of 10 years), while the four lateral smaller tributaries reached ~19 m^3/s. Finally, the effluent reservoir discharge provided from ARBVS was considered as outflow, translating the water used for irritation purposes in the downstream area.

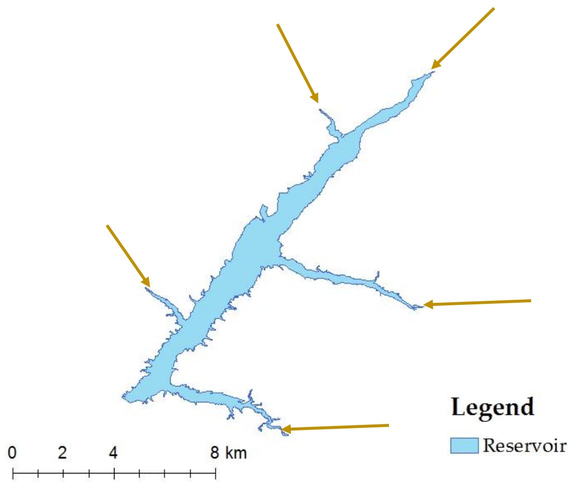

Figure 4.6. Location of the discharges from the soil and water assessment tool (SWAT) model, used as boundary condition to MOHID Water model.

4.2.2.3. Climate Models

The climate models adopted in this study were the GFDL-ESM2M (Dunne et al., 2013) and IPSL-CM5A-LR (Dufresne et al., 2013). These models followed the framework established by Nerc et al. (Nerc et al., 2018) and Birk et al. (Birk et al., 2018) during the Project "Managing Aquatic Ecosystems and Water Resources Under Multiple Stress—MARS" (Feld et al., 2016; Segurado et al., 2018), where this work is embedded. In the MARS Project, three societal scenarios were developed and implemented in the Sorraia basin (Almeida et al., 2018), based mainly on agriculture practices and on the work of O'Neill et al. (O'Neill et al., 2017)and Riahi et al. (Riahi et al., 2017). These authors defined Shared Socioeconomic Pathways (SSPs) as reference scenarios describing plausible alternative trends in the evolution of the society and ecosystems over a century timescale in the absence of climate change or climate policies. The surface air temperature and precipitation time-series were downscaled at a 0.5° resolution according to the The Inter-Sectoral Impact Model Intercomparison Project (ISI-MIP) project (Hempel et al., 2013; Warszawski et al., 2014). Differences between the GFDL and IPSL models and downscaling of variables at the basin-scale acquired from the outputs of these two models are given in Warsawski et al. (Warszawski et al., 2014) and references therein.

For the case of Montargil sub basin, this study took into consideration the storyline based on the combination of the Shared Socioeconomic Pathway-2 (SSP-2) defined as an intermediate stage in the evolution of the society and ecosystems over a century timescale (Riahi et al., 2017; Warszawski et al., 2014), and the Representative Concentration Pathways 4.5 (RCP 4.5). According to Moss et al. (Moss et al., 2010), the RCP 4.5 assumes a greenhouse gas emission with peak around 2040 followed by a decline.

Additional bias-correction for the study area was carried out in Almeida et al. (Almeida et al., 2018) and considered the temperature and precipitation historical data for the period between 2006 and 2015. The period from the last 20 years (1996–2015) was selected as a reference for the present condition (baseline simulation) and the two distinct temporal intervals were set up to run the future simulations: 2030 (defined as a 10-years average from 2025 to 2034) and 2060 (defined as a 10-years average from 2055 to 2064).

Both climate models show a decrease of precipitation when compared to the historical data from 1996 to 2015, here considered as the baseline condition (Figure 4.7), with the monthly average decreasing from ~22 to ~9 mm during the Spring/Summer season. Similar behaviour is observed during the Autumn/Winter season, with the GFDL model estimating monthly average decreases from ~59 mm to ~28 mm and ~25 mm for the 2030 and 2060 timelines, while the IPSL model shows a decrease to ~35 mm and ~34 mm during the same timelines. Concerning temperature, predictions showed fluctuations of monthly values, with more extreme maximum and minimum values being noticed (Figure 4.8).

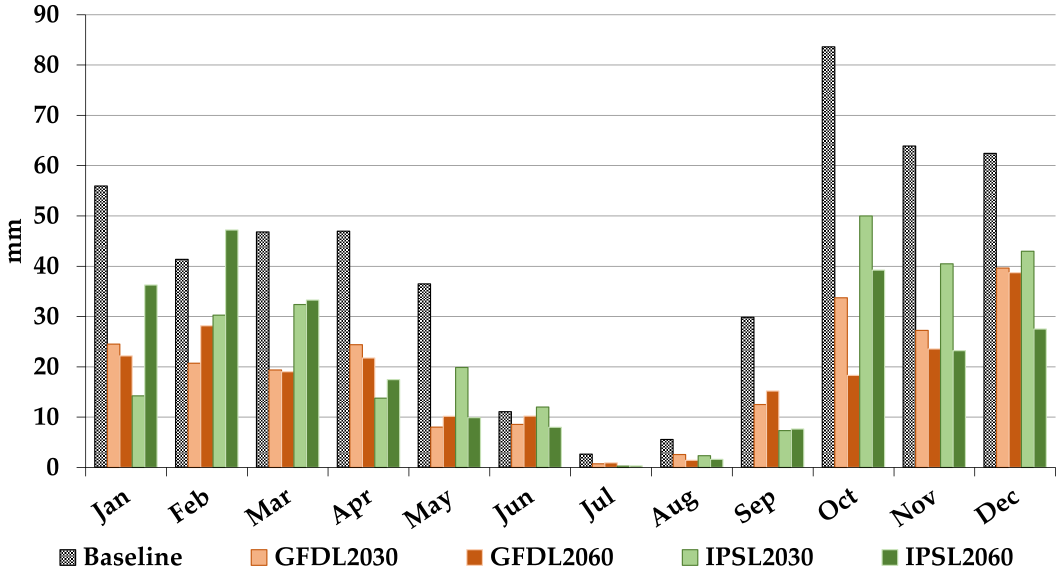

Figure 4.7. Average monthly precipitation (mm) for the baseline conditions and climate scenarios.

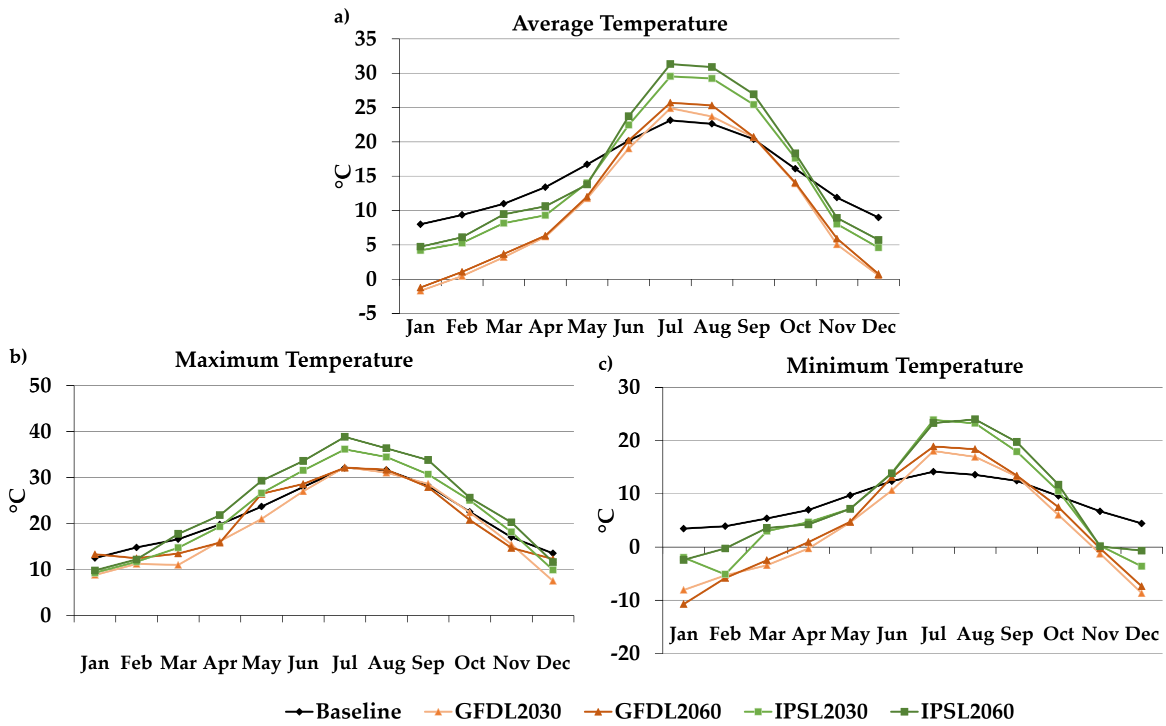

Figure 4.8. Monthly temperatures (°C) for the baseline conditions and climate scenarios: (a) average, (b) maximum and, (c) minimum.

4.2.3. Performance Indicators

Several performance indicators were adopted to evaluate the system reliability, resiliency, and vulnerability based on monthly failure events registered in the Montargil reservoir. The reliability is the oldest and widely used indicator for assessing water resources systems performance. This was defined by Hashimoto et al. (Hashimoto et al., 1982) as how often the system fails:

$$\text{Reliability} = P\{S \in NF\} \tag{2}$$

where P is the probability, *S* is the system state variable under consideration and NF is related to the non-failure state. The most recognized and applied definition uses the concept of failure which occurs when the system is unable to satisfy water needs. The time reliability can be estimated as:

$$\text{Reliability} = 1 - \frac{\sum_{j=1}^{M} d(j)}{T} \tag{3}$$

where d(j) is the duration of the failure event j, M is the number of failure events, and *T* is the total number of time intervals. The volumetric reliability is defined as the percentage of needs during the simulation period that were satisfied.

Resilience is defined as the measure how quickly the system returns to a satisfactory state once a failure has occurred. The resiliency provides an indication of the system's capability to recover from a failure. Hashimoto et al. (Hashimoto et al., 1982) define resilience as a conditional probability:

$$\text{Resilience} = P\{S(t+1) \in NF \mid S(t) \in F\} \tag{4)}$$

where $S(t)$ is the system state variable. This definition of resilience is equal to the inverse of the mean value of the time the system spends in an unsatisfactory state, i.e.,

$$\text{Resilience} = \left\{\frac{1}{M}\sum_{j=1}^{M} d(j)\right\}^{-1} \tag{5)}$$

where d(j) is the duration of the failure event j and M is the total number of failure events.

Vulnerability indicators are used to assess the severity of failure when it occurs and was defined by Hashimoto et al. (Hashimoto et al., 1982) as:

$$\text{Vulnerability} = \sum_{j=F} e(j).h(j) \tag{6)}$$

where h(j) is the most severe outcome of the failure event j and e(j) is the probability of h(j) being the most severe outcome of a failure resulting into unsatisfactory state. Hashimoto et al. (Hashimoto et al., 1982) and Jinno et al. (Jinno, 1995) estimated posteriorly vulnerability as the mean value of the deficit events v(j) as:

$$\text{Vulnerability} = \frac{1}{M}\sum_{j=1}^{M} v(f) \tag{7)}$$

4.3. Results and Discussion

4.3.1. Basin Modelling

Calibration and Validation

The SWAT model calibration and validation for the Montargil sub basin was carried out by comparing simulated and observed flows at the Moinho Novo hydrometric station (Lat. 39.228°; Long. −8.029°). The SWAT parameters CN2, ALPHA_BF, GW_Delay, SOL_AWC, SOL_ZMX, SOL_Z1 and SOL_Z2 (Table 4.1) were thus modified until deviations between simulated and observed data were minimized.

Table 4.1. Values of calibrated parameters used in the SWAT model (parameter, description and default according to Neitsch et al. (Neitsch et al., 2011)).

Parameter	Description	Default	Calibrated Value
CN2	SCS runoff curve number for moisture condition II.	25 to 92	80 to 92
ALPHA_BF	Baseflow alpha factor (1/days).	0.048	1
GW_Delay	Groundwater delay time (days)	31	3
SOL_AWC	Available water capacity of the soil layer (mm H_2O/mm soil).	0.11–0.14	−40%
SOL_ZMX	Maximum rooting depth of soil profile. (mm).	-	500
SOL_Z1	Depth from soil surface to bottom of first layer (mm).	300 to 800	slope 0–3%, to 800 slope 3–8%, to 500 slope >8%, to 300
SOL_Z2	Depth from soil surface to bottom of second layer (mm).	300 to 800	slope 0–3%, to 1000 slope 3–8%, to 800 slope >8%, to 500

The statistical indicators obtained after comparing the monthly simulated and measured flow values at the Moinho Novo monitoring station were: the coefficient of determination (R^2) of 0.71, the root mean square error (RMSE) value of 6 m^3/month, and the Nash–Sutcliffe efficiency (NSE) value of 0.71. The R^2 showed that a considerable proportion of variability of the observed data was explained by the model. The RMSE indicated a small error of model estimates. The NSE indicates that the residual variance resulted much smaller than the measured data variance (Figures 4.9 and 4.10). For the validation period, the indicators were found to be similar, indicating a reasonable calibration of model parameters when considering all uncertainties related to measurements (Figures 4.9 and 4.10). Similar performances of the SWAT model can be found in other watersheds of the same size in the Mediterranean region. For example, Briak et al. (Briak et al., 2016) simulated streamflow in the Kalaya watershed, northern Morocco, obtaining a NSE value of 0.76. Bucak et al. (Bucak et al., 2017) did the same for the watersheds of Lake Beyşehir, Turkey, producing R^2 values from 0.38 to 0.78 and NSE values from 0.37 to 0.76. Also, Dechmi et al. (Dechmi et al., 2012) obtained high R^2 and NSE values of 0.90 in the Del Reguero River watershed in northern

Spain, while Panagopoulos et al. (Panagopoulos et al., 2011) found R^2 values of 0.86–092 and NSE values of 0.51–0.68 in the Arachtos catchment, in western Greece. The SWAT model performance in the study area was particularly good ($R^2 = 0.685$) during the rainy period (autumn and winter season) when flows were higher (Figure 4.11), which is particularly relevant due to the importance of the high flow season for reservoir management.

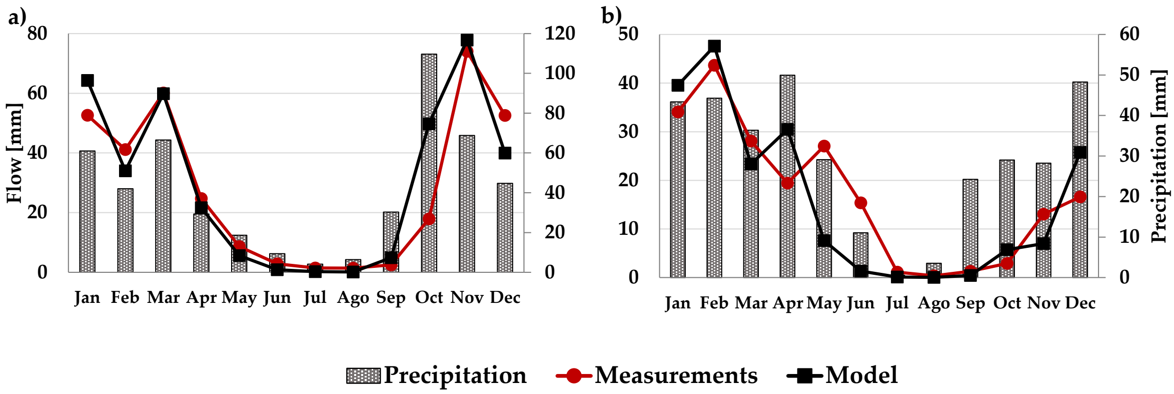

Figure 4.9. Monthly average flow (mm) in Moinho Novo: (a) calibration period; (b) validation period.

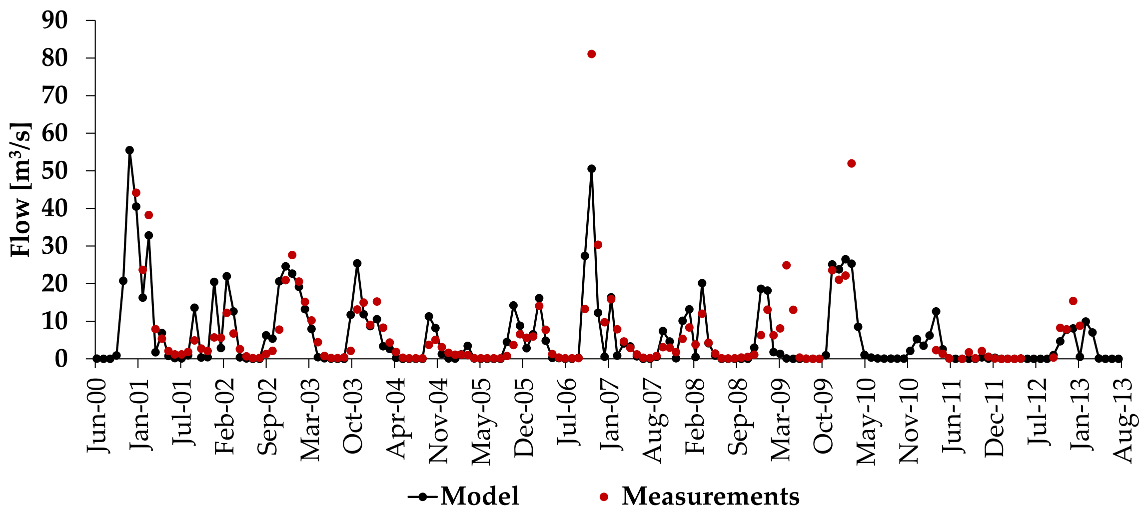

Figure 4.10. Monthly flow (m³/s) in Moinho Novo for the simulation period.

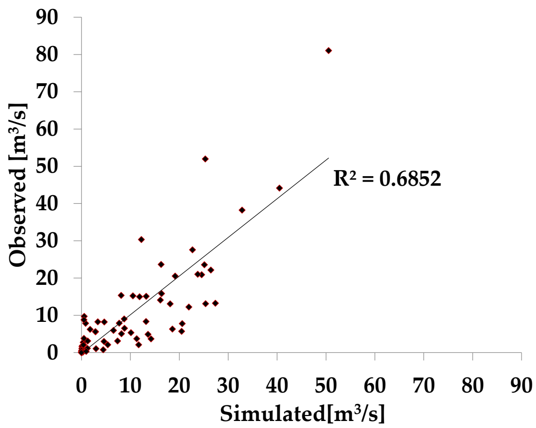

Figure 4.11. Monthly flow (m³/s) in Moinho Novo for the simulation period during the high flow season (October to March).

Water Availability

After calibration and validation, the SWAT model was used to determine the long-term water balance of the Montargil catchment for different scenarios. The monthly water balance considers precipitation, flows and actual evapotranspiration. The results indicate two distinct seasons. During autumn and winter, i.e., from October to March, precipitation and flows are high. Conversely, during spring and summer, between April and September, precipitation and flows are low (Figure 4.12).

The expected precipitation reduction for all scenarios leads to a decrease of monthly flows (Figure 4.12), in line with previous studies (Almeida et al., 2018; De Luis et al., 2009; García-Ruiz et al., 2011; Hempel et al., 2013; Warszawski et al., 2014). Higher temperatures, which result in an increase of potential evapotranspiration, also concur with this situation (Figure 4.12). The baseline monthly actual evapotranspiration values are in accordance with the detailed work developed by Simionesei et al. (Simionesei et al., 2018) to pasture and Ramos et al. (Ramos et al., 2017) to maize grown in the Sorraia basin. Vegetation growth in the region may be compromised due to higher water stress as a result of higher evapotranspiration demand and limitations in water available for irrigation.

The flow duration curves (Figure 4.13) show a decrease of flows with exceedance values Q95% from 1.7 m³/s in the baseline scenario to values of approximately 0 m³/s (Figure 4.13). The single exception is the IPSL climate model for the 2030 timeline scenario, which maintains some low flows with a Q95% (~1.2 m³/s) close to the baseline value (~1.7 m³/s). The two climate models differ when projecting high flows events. The GFDL model projects a decrease of Q10% from 20 m³/s to ~2.5 m³/s and 2.8 m³/s for the 2030 and 2060 timelines, respectively. In an opposite way, the IPSL climate model suggests a similar value of the Q10% value to 18 m³/s for the 2030 timeline and increase to 25 m³/s for 2060. This may be due to the increase of predicted high precipitation events that resulted in flow peaks as showed already in several studies in Mediterranean region (Almeida et al., 2018; Giorgi and Lionello, 2008; IPCC and IPCC5 WGII, 2014) and especially in Almeida et al. (Almeida et al., 2018) for the Sorraia basin, whose results show the impact of precipitation to water availability in the basin. Those results we mainly related to climate change projection and management practices, which are expected to affect directly the reservoir water availability and consequently its vulnerability, especially during the irrigation season when a higher water demand is expected.

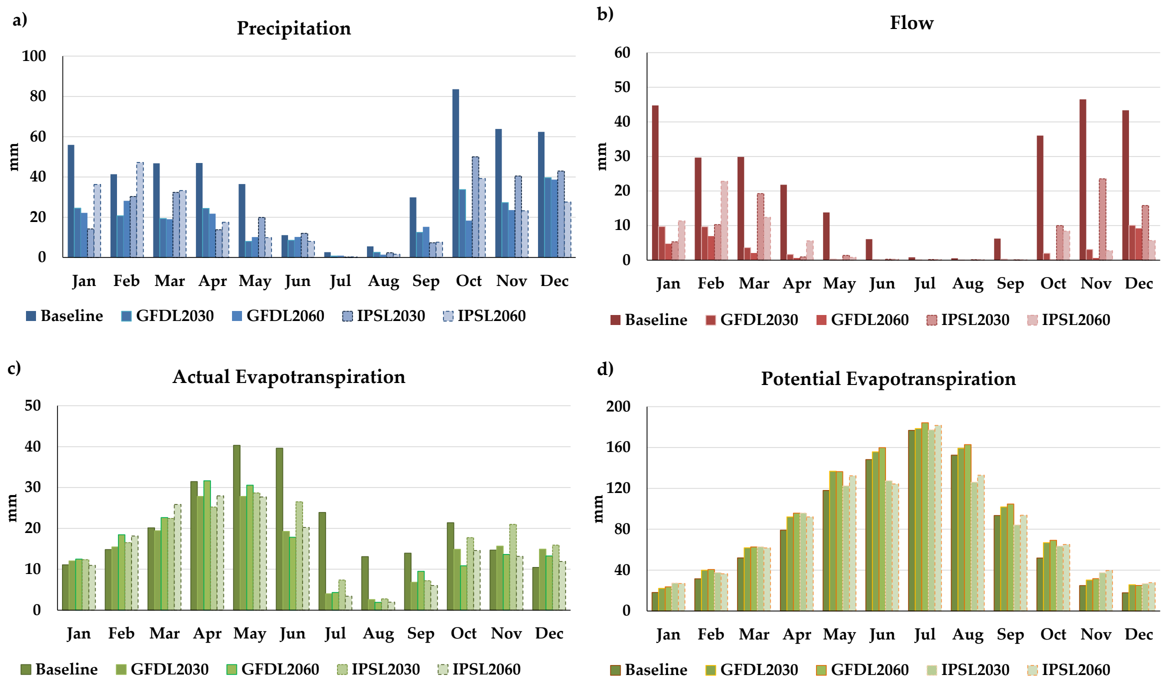

Figure 4.12. Water balance results (in mm) to the baseline and GFDL and IPSL models for each timeline simulation: (a) Precipitation; (b) Flow; (c) Actual evapotranspiration; (d) Potential evapotranspiration.

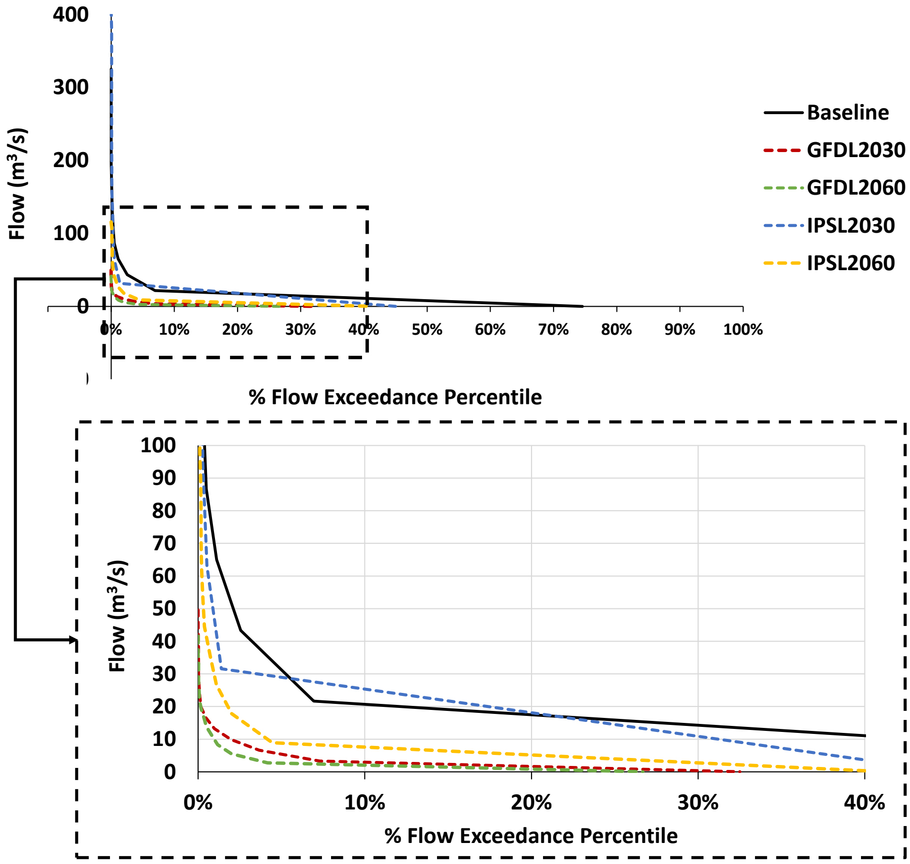

Figure 4.13. Percentage of flow exceedance percentile comparison for baseline and future simulations.

4.3.2. Reservoir Modelling

Validation

The SWAT flow estimations presented above were introduced as boundary conditions to the MOHID Water reservoir model. The baseline for simulating reservoir operation was defined from 2005 to 2014. A topography map with 90 m resolution was converted and adjusted into the 100 m resolution grid considered in the MOHID Water model using the tools available in MOHID Studio. Figure 4.14 compares the elevation–volume curve considered in the model with the one obtained from measured data. The simulation of the baseline period shows a close match between the computed and observed water surface elevation and stored volume values (Figures 4.15 and 4.16). The R^2 value obtained for the stored volumes is 0.987 while for water levels is 0.988. These results are in accordance with Brito et al. (Brito et al., 2018b), who applied a similarmodel to study the Enxoé Reservoir dynamics in southern Portugal. Similar good results were obtained by Lee et al. (Lee et al., 2018) for the Hodges Reservoir, San Diego, USA, and Noori et al. (Noori et al., 2015) for the Karkheh Reservoir, Iran, using the same model.

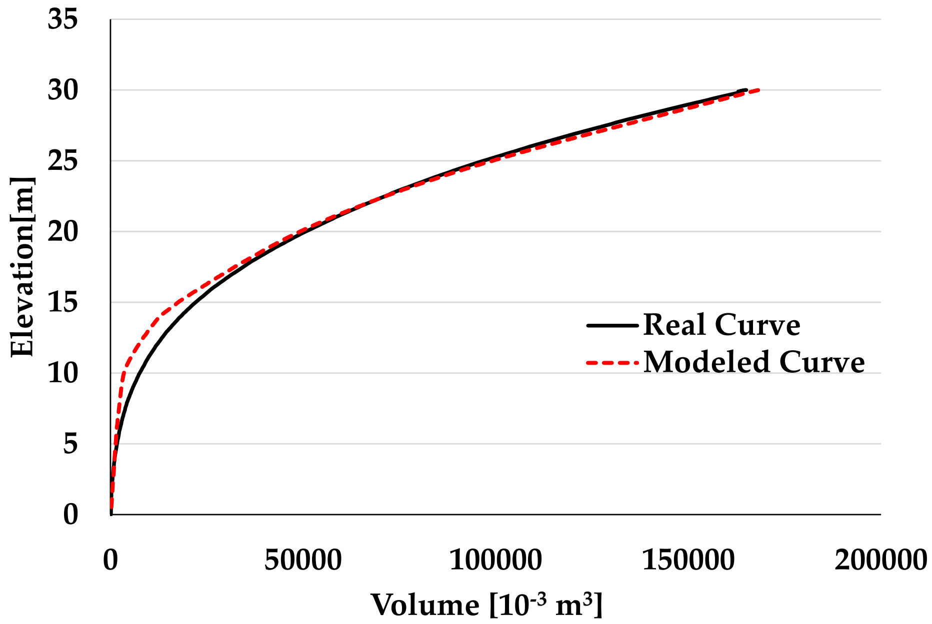

Figure 4.14. Real and modelled Elevation-Volume Curve.

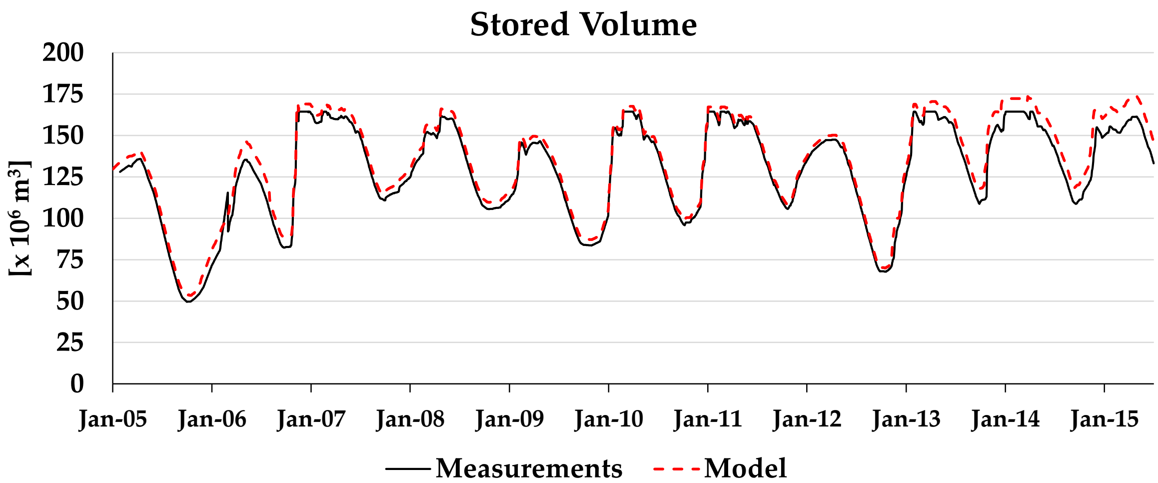

Figure 4.15. Comparison between stored volumes modelled and measurements.

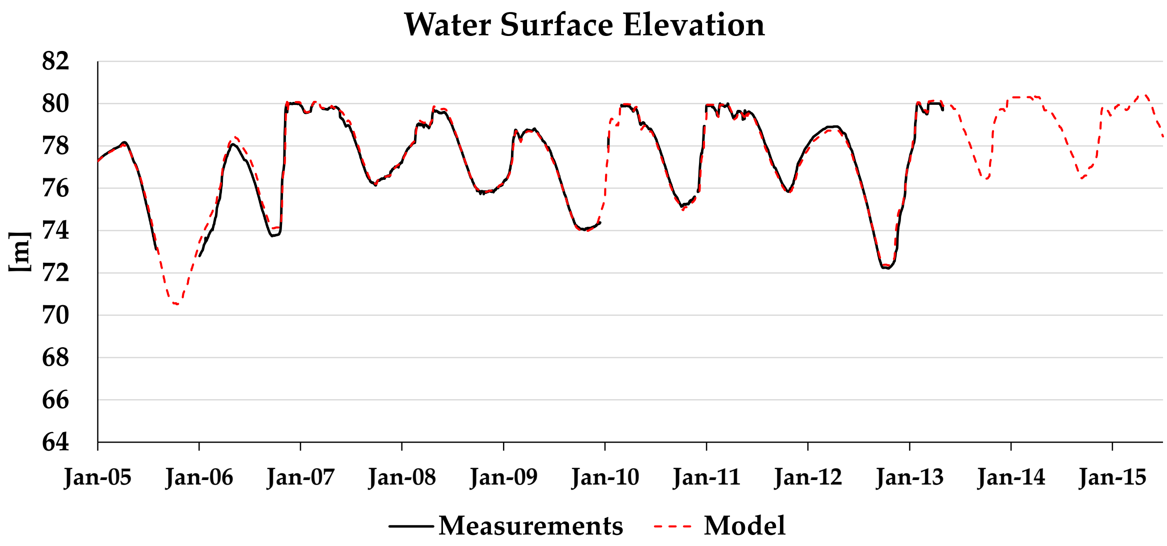

Figure 4.16. Comparison between water surface elevation modelled and measurements.

Water Availability

After validation of the MOHID Water model, results were analysed on a monthly basis to understand the future behaviour of the Montargil reservoir and assess the impact of flow reduction on the reservoir ability to meet agriculture water demand. At this stage, two demand scenarios were considered by modifying the reservoir output discharge imposed in the MOHID Water model:

- Assuming the average water demand in the past 10 years;
- Considering the year with maximum water demand in the past 10 years, which correspond to a water demand increase of ~30% when compared with the average year. The second water demand scenario reflects the increase of irrigation in the Sorraia basin since water is mainly used for this purpose.

To better understand the performance of the reservoir and its operating rules under climate change, the indicators described above were considered to determine the supply reliability, vulnerability of water needs, and the system's resilience for each simulated scenario. This approach has been applied in several reservoir studies, including the Sorraia basin where the Montargil reservoir is included (Mateus and Tullos, 2016; Simões and Oliveira, 2014; Sušnik et al., 2015). As a failure reference, the volume of ~10 hm^3 was considered in case of extreme necessity when half of the dead volume could be used.

The first water demand scenario (the average water demand in the past 10 years) resulted in an increase of monthly failures for both simulated climate scenarios and timelines (Figure 4.17 and Table 4.2). This shows that in the future, the stored volume is expected to be below the dead volume for several months, something that has never happened in the past (Figure 4.15). This is mainly due to the impact of runoff decrease in the reservoir, which is consistent with the literature as shown by Mateus et al. (Mateus et al., 2017) when studying the reliability of six reservoirs in Scotland or Afzal et al. (Afzal et al., 2015) when analysing the vulnerability of the Pong reservoir, India. Future water demand scenarios considered in both studies showed a reliability reduction and a vulnerability increase of the simulated reservoirs, advancing then with future water management strategies to cope with those predictions. The same was considered by Fiering et al. (B Fiering, 1982), proposing also mitigation strategies when vulnerability increases above 25%.

The volumetric reliability, i.e., the percentage of needs that are satisfied during the simulation period, is higher when the IPSL climate model predictions are considered, reaching about 73% in both timelines (Table 4.2). The annual reliability is only 30% and 0% when using the IPSL and GFDL climate change predictions as inputs (Table 4.2), respectively, meaning that for the IPSL scenario the time reliability is on average only 3 years (of 10 simulated years) while for the GFDL scenario the results are null. This is equally observed in the volumetric reliability results when considering the GFDL climate model predictions as inputs, with about 49% and 43% being expected during the 2030 and 2060 timelines (Figure 4.17 and Table 4.2).

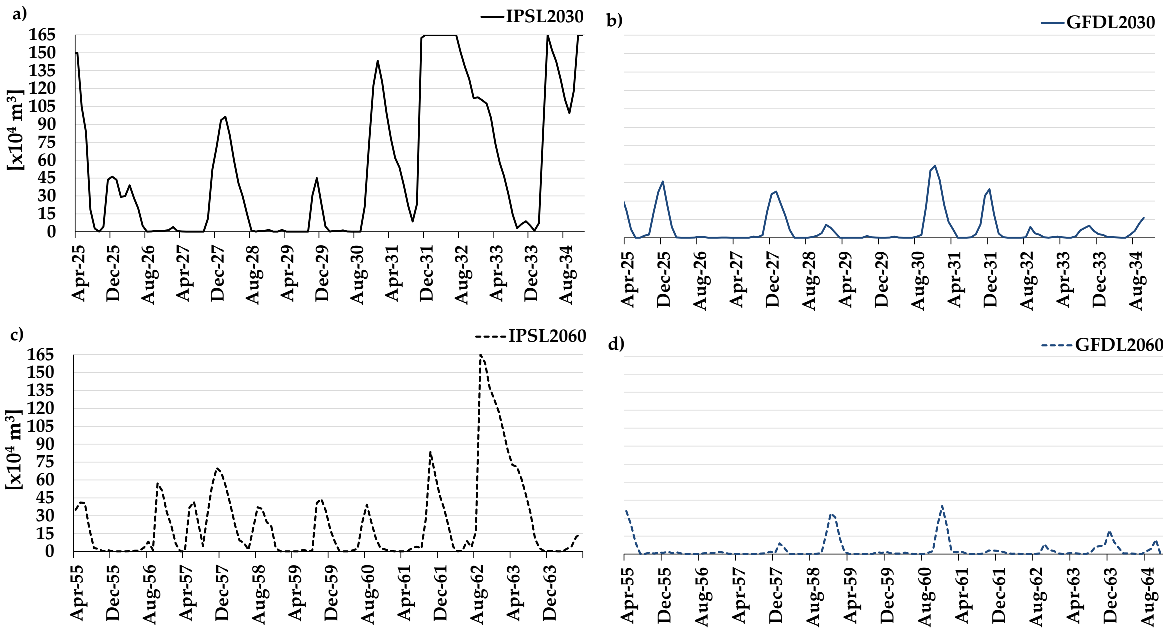

Figure 4.17. Stored volume evolution considering the average behaviour water demand: (a) IPSL2030 scenario; (b) GFDL2030 scenario; (c) IPSL2060; (d) IPSL2060.

Table 4.2. Performance indicators obtained considering the average behaviour water demand.

Scenario		IPSL 2030	IPSL 2060	GFDL 2030	GFDL 2060
Number of months without failure		88	88	59	52
Number of months with failure		32	32	61	68
Reliability	Number of annual failures	7	7	10	10
	Annual reliability (%)	30	30	0	0
Vulnerability	Volumetric reliability (%)	73	73	49	43
	Average duration of the failure (month)	5	5	6	7
Resiliency		9	9	12	14
Resiliency (%)		28	28	20	21

For the second water demand scenario, i.e., when considering the highest annual demand in the past 10 years, results show an increase of monthly failures for both simulated climate scenarios and timelines when compared with the previous water demand scenario (Figure 4.18 and Table 4.3). The volumetric reliability is expected to be higher when considering the IPSL climate model predictions, reaching about 64% and 72% during the 2030 and 2060 timelines, respectively. When adopting the GFDL climate model predictions, these only decreased to about 54% and 50% during the same period. The annual reliability is only 10% (2030 timeline) and 20% (2060 timeline) in the IPSL climate change prediction, and again 0% in the GFDL climate change prediction (Table 4.3). In other words, the time reliability averages only 1.5 year, while is null in the GFDL climate model. The resiliency for both water demand scenarios and timelines is similar, decreasing to an average of 20–35%. This value is considered not satisfactory for a basin which is highly dependent of water from the reservoir.

Model results showed a modification in the performance of the Montargil reservoir in the future which should be taken into account when improving water management at the watershed scale. The results showed the importance of analysing the metrics for improving the decision making process, especially when considering the projected changes for the Mediterranean region, as already demonstrated in Asefa et al. (Asefa et al., 2014). The decreasing trends observed in both scenarios are also observed in the literature, especially in studies addressing the impact of climate change in the water availability in rivers that drain to Mediterranean reservoirs. For example, Bates et al. (Bates et al., 2008) and the European Environmental Agency (European Environment Agency, 2005) showed that aridity is expected to increase in the Mediterranean region with climate change, increasing vulnerability in the region. More specifically, Almeida et al. (Almeida et al., 2018) reported a decrease of ~75% in the stream flows in the Sorraia basin in the 2030 and 2060 timelines. Bucak et al. (Bucak et al., 2017) estimated a reduction flow that could dry out the Beysehir reservoir in Turkey. Calbó et al. (Calbó, 2009) estimated reductions of ~34 % in water availability in Catalonia, Spain. In spite of all uncertainties described by Calbó et al. (Calbó, 2009), water availability is commonly estimated to substantially reduce in all those studies carried out in the Mediterranean region. The reduction of river discharge and the increase of extended drought periods will as expected decrease the reliability and resiliency of the water system and consequently, increase its vulnerability, similar to the Montargil basin-reservoir system.

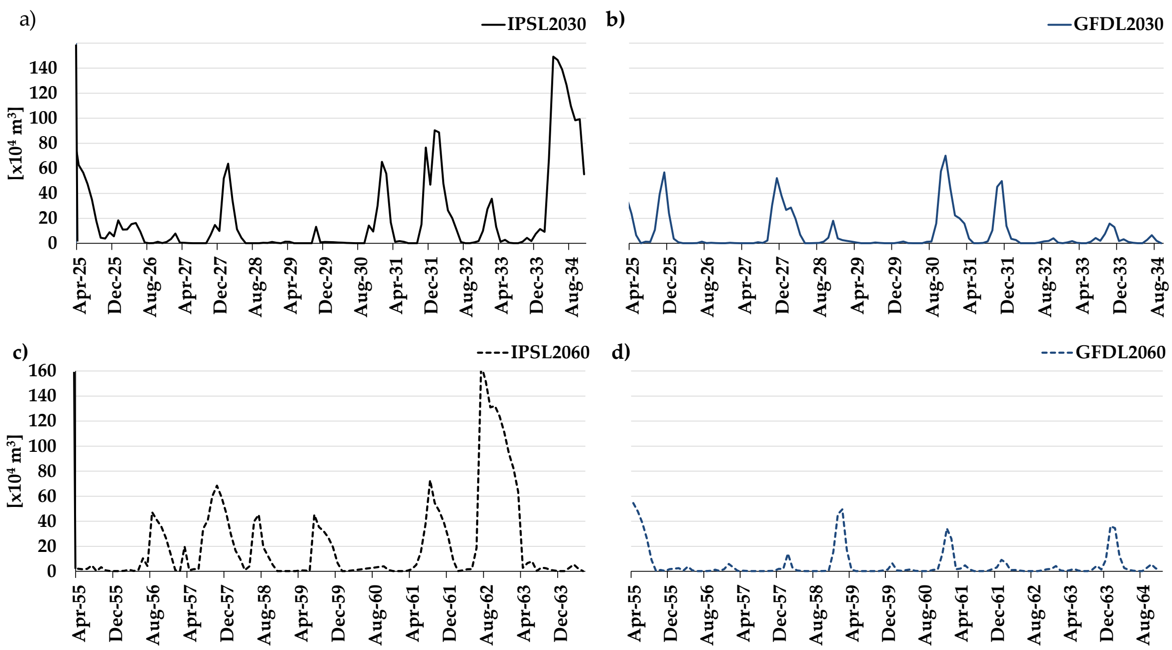

Figure 4.18. Stored volume evolution considering the maximum behaviour water demand: (a) IPSL2030 scenario; (b) GFDL2030 scenario; (c) IPSL2060; (d) IPSL2060.

Table 4.3. Performance indicators obtained considering the maximum behaviour water demand.

Scenario		IPSL 2030	IPSL 2060	GFDL 2030	GFDL 2060
Number of months without failure		77	86	65	60
Number of months with failure		43	34	55	60
Reliability	Number of annual failures	9	8	10	10
	Annual reliability (%)	10	20	0	0
Vulnerability	Volumetric reliability (%)	64	72	54	50
	Average duration of the failure (month)	5	4	6	6
Resiliency		11	12	11	16
Resiliency (%)		26	35	20	27

4.4. Conclusions and Future Research

This study presented an integrating modelling approach to quantify the availability of water resources in the Montargil basin and reservoir based on projections from two climate models and for two decades. This integrated modelling approach allowed a more comprehensive management action by providing the amount of water and the period of availability at a monthly scale.

In the results the impact of climate change on the water availability in the Montargil reservoir on a monthly basis is quite noticeable. It is notable the importance of managing outflows to prevent reduction of water resources in the region. The hydrologic changes observed in the basin simulations contributed to the failure of the reservoir in meeting its operational objectives. The reliability and timing for refill affect water availability and limited irrigation practices.

Modelling reservoir operations offered an important opportunity for mitigating hydrologic responses to climate change, which in turn could mitigate their negative impact on water availability. The findings in this work emphasize the importance of integrating modelling as a support to water managers in the decision making. This work further showed how the Montargil reservoir is particularly vulnerable to climate change, with its resilience requiring singular consideration.

This work is a first approach, which is intended to be the basis for water managers in this case study and an example to similar areas where climate change is predicted to have a similar impact. In the future it is intended to evaluate the required behaviour of water uses over the next few years so that the volumetric reliability is fulfilled, not compromising typical agricultural activity in this region. This integrated modelling approach may be used as well to test land use changes, by substituting typical crops of the regional with others with different water requirements, thus quantifying theirs impact on the water balance of the reservoir.

Author Contributions: C.A. set up the models, run the simulations, and wrote the paper. T.R, J.S, R.N. and R.P.d.O. made revisions and improvements to the draft version.

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Chapter 5 Evolution of the Trophic Status in a Mediterranean Reservoir under Climate Change: An Integrated Modelling Approach

The material on which this chapter is based has been previously submitted in ***Almeida, C.;*** *Ferreira T.; Branco, P.; Segurado, P.; Ramos, T.B.; Neves, R.; Proença de Oliveira, R. Evolution of the Trophic Status in a Mediterranean Reservoir under Climate Change: An Integrated Modelling Approach. Journal of Hydrology: Regional Studies 2019 (submitted)*

Abstract

This study describes an integrated modelling approach to better understand the trophic status of the Montargil reservoir in Southern Portugal under climate change scenarios. The Soil Water Assessment Tool and CE-QUAL-W2 models were applied to the basin and reservoir, respectively, for simulating water and nutrient dynamics while considering the climatic scenario from the IPSL Earth System Model for the 5th IPCC report and two decadal timelines (2025-2034 and 2055-2064). Model simulations showed that the dissolved oxygen concentration in the reservoir is expected to decrease in the hypolimnion by 60% in both decadal timelines. The chlorophyll-a concentration in the epiliminion is expected to increase by 25% for both future timelines. Total phosphorus concentration (TP) is predicted to increase by 63% in the water column surface and by 90% in the hypolimion during the 2030 timeline. These results are even more severe during the 2060 timeline in which TP increase is predicted to increase 118% in the hypoliminion. Under these climate change scenarios, the reservoir showed an eutrophic state during 70% of the 2030 timeline and 80% in the 2060 timeline. Even considering measures that involve decreases in 30 to 35% of water use, the eutrophic state is not expected to improve. This raises issues related with fish survival and ecosystems stability, as also the objectives outlined by EU Water Framework Directive.

Keywords: trophic status; reservoir; climate change; modelling.

5.1 Introduction

The European Water Framework Directive (WFD; 2000/60/EC) was adopted in 2000 as the main policy instrument for reaching a good ecological status of European surface waters by 2015 (WFD). However, this objective fell short, as 47% of the European surface waters still fail to meet such conditions (EC 2012b). Such outcome begs for a more sustainable and holistic approach to water management (Voulvoulis et al. 2017), particularly in the context of climate change (CEC 2009b). In a future scenario perspective, climate change is expected to impact the availability, seasonality, and variability of water resources (IPCC 2013). The adoption of climate change adaptation strategies by Member States is one of the concerns of the European Commission, who underlined the importance of an integrated analysis of impacts and a comprehensive adaptation strategy to that problem (Biesbroek et al. 2010).

In Southern Portugal, many hydro-agricultural infrastructure (reservoirs) are common and used to face water scarcity resulting from the Mediterranean climate seasonal and intra-annual variability. These aquatic systems are classified as heavily modified water bodies (HMWB) by the WFD. According to Commission of the European Communities (CEC 2015), around 30% of these heavily modified water bodies showed good ecological potential in 2015, with problems arising from difficulties in the management of riverbanks and drainage basins, and the occurrence of frequent eutrophication episodes with cyanobacteria blooms and high ichthyofauna mortality.

The use of predictive models for simulating the ecological conditions has many advantages over simple monitoring, allowing to predict the future status of a system resulting from changes of different environmental factors. The ecological status of reservoirs is inextricably linked to its drainage basin and models enable the assessment of basin-originated impacts on the reservoirs, in an integrated way according to the Driver- Force–Pressure–State–Impact–Response (DPSIR) approach (EEA 2007; Marty et al. 2014), offering also the possibility of addressing scenarios for future conditions. The integration of basin and reservoir models has been often used to study the water quality and trophic status of the Mediterranean reservoirs. For example, Saddek & Casamitjana (2018) applied a one-dimensional hydrodynamic and water quality model to study the water quality behaviour in the Boadella reservoir Catalonia, Spain. Zouabi-Aloui & Gueddari (2014) analysed three scenarios involving the impacts of severe drought season, summer rainfall and total suspended solids load on hydrodynamics and water quality, of a stratified dam reservoir in the southern side of the Mediterranean Sea. Also, Nsiri et al. (2016) applied a modelling approach to study the thermal stratification and the effect on water quality in four reservoirs in Tunisia. In Portugal, the National Water Institute (INAG) carried out an integrated modelling study to gain knowledge on the trophic levels of 30 reservoirs under the scope of the Waste Water Treatment Plant directive (INAG 2009). Several other studies were carried out to analyse water quality and consequently the trophic state of reservoirs in southern Portugal, including: those aimed at finding a solution for the constant eutrophic state of the Enxoé reservoir (Brito et al. 2018, 2017; Fontes 2010, Ramos et al. 2015a, 2015b, 2018); the water quality assessment of the Alqueva reservoir through data analysis techniques and numerical modelling (Fontes 2010); and the quantitative and qualitative assessment of the relationship between eutrophication and ground baiting on angling competition in the Maranhão reservoir (Amaral et al. 2013).

Nevertheless, there is a gap in studies including water quality status predictions in typically Mediterranean climate study cases.

Therefore the objective of this study is to analyse the present and future trophic status of a typical Mediterranean reservoir located in Southern Portugal using modelling as an integration tool of the drainage basin and reservoir. For this purpose, a climate model is used as boundary condition to a basin model, which in turn is integrated into a reservoir model. The specific objectives are: (1) to determine the trophic status of the reservoir while considering baseline conditions and future climate scenarios; and (2) to analyse possible measures to improve trophic status in future scenarios. This study is particularly relevant in performing an integrated modelling approach to analyse the trophic status of a HMWB under the context of climate change and on the sustainability of the water use in the future and its implications. Therefore, although it is a case study undertaken at a local scale, it may provide insights with a wider application to reservoirs within the Mediterranean region with similar future climatic trend.

5.2 Materials and Methods

5.2.1. Study Area

The Montargil reservoir with a drainage area of 1200 km2 is located in one sub basin of the Sorraia River, southern Portugal (Lat: 38.59° to 39.50°; Long: −8.99° to −7.24°). The climate has the typical Mediterranean behaviour with dry and hot summers, and mild and wet winters. The maximum reservoir capacity is 164 hm3; the maximum water surface elevation is 80 m; and the minimum water surface elevation acceptable for operation is 65 m, which correspond to a dead storage pool of 143 hm3. The reservoir is part of the Vale do Sorraia watering system, controlled by the local Water Board (Associação de Regantes e Beneficiários do Vale do Sorraia, ARBVS) since 1970. The Sôr River supplies most of the water to the reservoir (60-70%), with minor contributions from several ephemeral streams during winter. The water level is regulated by water demand for irrigation and meteorological conditions. Additional uses are electric power generation, fishing and recreation (water sports). The tourist potential of the location (close to Lisbon) is currently recognized in the reservoir ordinance plan (approved by the Portuguese Minister Council resolution nº 94/2002).

The use of the reservoir for recreational purposes has increased, but some bathing water quality issues have been raised at some locations, with the reservoir occasionally failing to comply with the 76/160/CEE directive due to high bacterial concentrations. The reservoir has also registered cyanobacteria blooms over the years, with reports on cyanobacteria blooms going back to 1995 (Pereira et al. 2001). The worst year was 1996 with several blooms of toxic species (Aphanizomenon flos-aquae, Aphanizomenon gracile, Anabaena spiroides, and Microcystis aeruginosa) being registered (Ferreira et al. 2009).

The main land use in the upstream catchment is forest with oak trees, covering more than 40 % of watershed area. Annual crops account for 13% of the watershed area while some irrigation cropping is present on 2% of the area. The connection between agricultural activities, point sources, and nutrient enrichment of the reservoir is an open subject for this area as is the relationship between nutrient enrichment and cyanobacteria domination over certain periods of time. These relationships are fundamental for improving both policies related to reservoir management.

5.2.2. Hydrological Modelling

5.2.2.1 The Soil and Water Assessment Tool model (SWAT)

Diffuse pollution and inflows to the Montargil drainage basin were simulated with the SWAT model (Neitsch et al. 2009) in Segurado et al. (2018) and Almeida et al. (2018, 2019). Readers are thus directed to those studies for a detailed description of the modelling approach adopted for quantifying water and nutrient yields from the watershed. In those studies, the SWAT model was applied to the Montargil basin using the ArcSWAT version. The model application relied on available GIS maps for topography from Shuttle Radar Topography Mission with 90 m resolution, land use from Earth Observation (EO) GSE Land M2.1 with 20 m and 300 m detail, and Cardoso et al. (1965) soil maps (1:25 000 scale) and properties from reference soil profiles. Climatic maps, including daily precipitation, temperature, relative humidity and wind speed were derived from the Portuguese National Institute of Water Resources, SNIRH (SNIRH 2018). Downstream the artificial reservoir, daily discharge data provided by the reservoirs' manager (ARBVS – Farmers Association from the Sorraia Valley) were considered in the model for a period from 1996 to 2015. The baseline simulation was thus defined for the period between 1996 and 2015. The SWAT model calibration and validation for the Montargil basin was carried out by comparing simulated and observed flows at the Moinho Novo hydrometric station (Lat. 39.228°; Long. -8.029°). The SWAT model was calibrated manually for the period between 1996 and 2005, while the validation covered the period from 2005 to 2015.

5.2.3 Reservoir Modelling

5.2.3.1 The Hydrodynamic and Water Quality Model (CE-QUAL-W2)

The CE-QUAL-W2 is a bidimensional model that assumes lateral homogeneity and supports vertical and horizontal gradients of all calculated properties (Cole & Wells 2015). The current version (version 4.1) simulates the systems hydrodynamics and water quality both vertically and longitudinally in both stratified and not stratified systems.

This model computes biogeochemical processes such as nitrogen, phosphorus, carbon and oxygen cycles, as well as the dynamics of algae and organic matter. In the organic matter (OM), the dissolved non-refractory OM (LDOM), the dissolved refractory OM (RDOM), the particulate non-refractory OM (LPOM) and the particulate refractory OM (RPOM) are considered in the model.

The model boundary conditions included daily river inputs of NO3−, NH4+, organic matter, orthophosphate, total suspended solids and O2 computed with the SWAT model (Almeida et al. 2018, 2019; Segurado et al. 2018). Daily weather data (air temperature, humidity, wind velocity and direction, cloud cover and solar radiation) were provided by SNIRH for the period 2005-2014 (SNIRH 2018).

Bathymetry was constructed considered the work already done in Almeida et al. (2019) where the topography map with 90 m resolution was converted and adjusted until obtain the model elevation–volume curve adjusted with the measurements. Because of the model requirements this bathymetry was defined in longitudinal and vertical segments, and cell widths. Therefore, the Montargil Reservoir was described at full capacity with a geometry consisting of 13 segments with lengths of 360–2700 m and widths of 500–3000 m at the surface (Figure 5.1). A minimum of four vertical layers upstream, and a maximum of 32 layers near the dam, all with 1 m high, were considered (Figure 5.1). Also, the effluent reservoir discharge provided from ARBVS, which translates the water used for irritation purposes in the downstream area, was used as outflow.

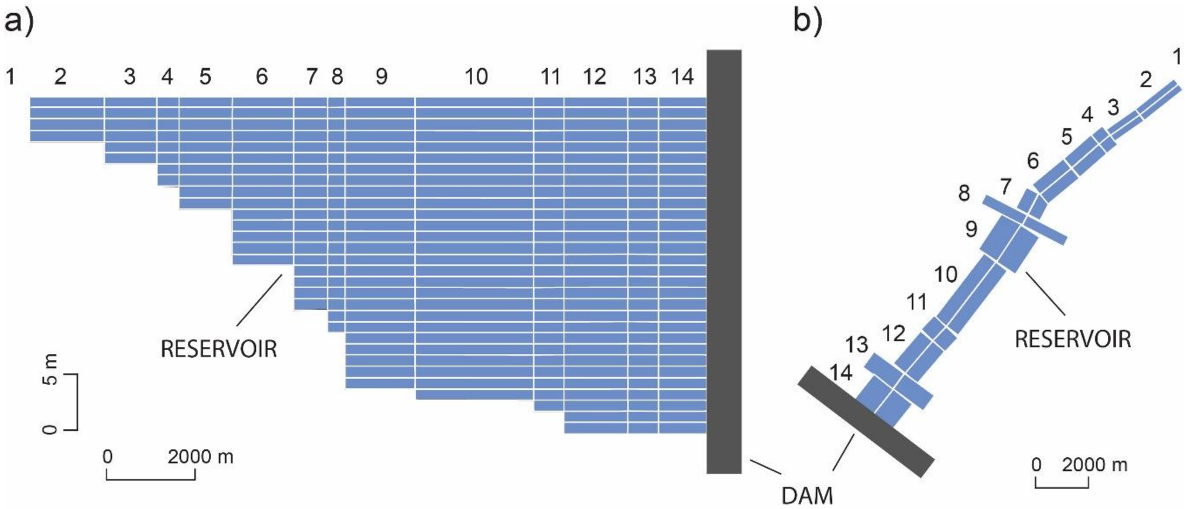

Figure 5.1 CE-QUAL-W2 grid definition of Montargil: a) plan view of the 32 layers and the 13 active segments; b) profile view along the axis.

The calibration and validation exercise was based on the comparison of in-field measurements of hydrodynamic and water quality variables against model results. The 2005-2014 period was considered as the baseline for reservoir operation simulation. The measured data used for calibration of the CE-QUAL-W2 model were: seasonal profiles of temperature and dissolved oxygen measured by Ferreira et al. (2009) during February, May and August 2006; and water surface elevation provided by SNIRH for the period 2005-2015; and for validation were: reservoir surface data of water temperature, dissolved oxygen, total N, total P, chlorophyll-a, and TSS obtained by SNIRH for the period 2005-2013.
The validation exercise considered the comparison between model and field measurements of water surface temperature, dissolved oxygen, total N, total P, chlorophyll-a, TSS, as well as the average, standard deviation and median analysis of each property.

5.2.4. Climate model and Storyline

This work followed the framework established by Grizzetti et al. (2014) and Birk et al. (2018) during the Project "Managing Aquatic Ecosystems and Water Resources Under Multiple Stress – MARS" (Hering et al. 2015), which was also adopted by Segurado et al. (2018) and Almeida et al. (2018, 2019) for the Montargil basin and reservoir. Hence, this study adopted the IPSL-CM5A-LR model (O'Neill et al. 2014) for defining the atmospheric boundary conditions. This model considers a decrease of 50% precipitation when compared to the historical data (Table 5.1), while temperature predictions show larger monthly amplitudes (Table 5.1). Historical temperature and precipitation data for the period 2005-2014 were corrected in Almeida et al. (2018), using a linear scaling bias correction method developed by Shrestha et al. (2015) based on the average difference between monthly observed and historical time series for the same period. This method is considered as having identical performance compared to complex bias correction techniques (Shrestha et al. 2017).

This 10 years period (2005-2014) was selected as a reference for the present condition (baseline simulation) and two distinct temporal intervals were set up to run the future simulations: 2030 (defined as a 10-years average from 2025 to 2034) and 2060 (defined as a 10-years average from 2055 to 2064).

This study further considered the storyline proposed by O'neill et al. (2014) and Moss et al. (2010) which results from the combination of the Shared Socioeconomic Pathway-2 (SSP-2) defined as an intermediate stage in the evolution of the society and ecosystems over a century timescale (Riahi et al. 2017; Warszawski et al. 2014), and the Representative Concentration Pathways 4.5 (RCP 4.5). It has been shown elsewhere (Almeida et al. 2019, 2018; Segurado et al. 2018) that severe impacts resulted even when considering a conservative storyline such as this. Therefore, this storyline was selected to explore the effects of managing irrigation using the most conservative approach. Thus, the underline premise in selecting this storyline is that in case substantial effects of management scenarios are predicted to occur, they will most certainly also occur if more severe scenarios would be taken into account.

The downscaling of management practices change in Montargil catchment was performed with the support of the local water board stakeholders (ARBVS), similarly as in Almeida et al. (2018, 2019). Accordingly, in the scenario here considered, the application of fertilizers was predicted to decrease by 10% and 15% in the 2030 and 2060 timelines, while irrigation needs would decrease by 20% and 25% during the same time periods (Table 5.2).

Table 5.1 Average monthly temperature (°C) and precipitation (mm) for the baseline condition and climate model timelines – 2030 and 2060.

	Temperature			**Precipitation**		
Month	**Baseline**	**2030**	**2060**	**Baseline**	**2030**	**2060**
January	8.0	4.2	4.7	56	14	36
February	9.4	5.3	6.1	41	30	47
March	11.0	8.2	9.5	47	32	33
April	13.4	9.3	10.6	47	14	17
May	16.7	14.0	13.8	36	20	10
June	20.2	22.5	23.7	11	12	8
July	23.1	29.5	31.3	3	0	0
August	22.6	29.2	30.9	6	2	2
September	20.4	25.4	26.9	30	7	8
October	16.1	17.6	18.3	84	50	39
November	11.9	8.0	8.9	64	40	23
December	9.0	4.6	5.7	62	43	28

Table 5.2 Input values used for simulating the scenario in SWAT and CE-QUAL-W2 models.

Management Practices	Baseline	Timeline	Variation (%)
Fertilization (kg/ha)	492	2030	−10
		2060	−15
Irrigation (mm)	430	2030	−20
		2060	−25

5.3. Results and Discussion

5.3.1. Water Quality of Reservoir Inflows

A good agreement was found between model and measured discharge data during the calibration period, especially on a monthly basis, resulting in a coefficient of determination (R2) value of 0.71, a Root Mean Square Error (RMSE) value of 6 m3/month, and a Nash–Sutcliffe model efficiency coefficient (NSE) value of 0.71. During the validation period the same behaviour was found, with a coefficient of determination (R2) value of 0.68, a Root Mean Square Error (RMSE) value of 7.5 m3/month, and a Nash–Sutcliffe model efficiency coefficient (NSE) value of 0.67. The SWAT model validation of N and P simulations was performed at Ponte de Coruche station (Lat. 38.956°; Long. −8.524°). For Total N, a R2 value of 0.59 and a bias of 0.22 mg.N L-1 was found. For Total P, model comparison to measured data produced a R2 value of 0.14 and a bias of -0.067 mg.P L-1. Further results of simulations of the SWAT model can be found in Segurado et al. (2018) and Almeida et al. (2019, 2018).

After calibration and validation, the model was used to estimate water quantity and quality of reservoir inflows for the baseline and climate change timelines, in order to analyse the future impacts that may result from these future changes. A decrease of 47% and 69% of reservoir inflows were estimated for the 2030 and 2060 timelines, respectively, which is in agreement with the results found by Almeida et al. (2018, 2019) in the Sorraia basin, averaging 31% for the 2030 timeline and 66% for the 2060 timeline. These decreasing in flow rivers it is expected in several Mediterranean case studies, resulting mainly from the decreasing in precipitation events, as showed by De Luis et al 2009), García-Ruiz et al. (2011), Pacual et al (2015) and Bucak et al. (2017). Nitrate concentration increased by 64% and 75% during the 2030 and 2060 timelines, as expected mostly due to the decreasing of the water flows. The difference in the orthophosphate concentration was not so pronounced, decreasing by 23% in 2030 and increasing by 11% in 2060. This slight variation may be due to the low mobility of P, which is dependent of runoff and soil erosion, when compared to N, which is mainly transported through leaching. The dissolved oxygen concentration was observed to decrease by 1% and 2% during the 2030 and 2060 timelines, respectively. The deterioration of water quality was thus noticed even though agriculture was not predominant in the Montargil basin and fertilizers application also decreased as considered in the simulated scenario. These long-term results were afterwards considered as boundary condition for reservoir model Ce-QUAL-W2.

5.3.2. Calibration and validation of reservoir model

The simulation of the baseline period showed a close match between the computed and observed water surface elevation (Figure 5.2), with a R2 of 0.92. The parameters used for calibrating the water quality model corresponded to the kinetic coefficients in the water column (Table 5.3). The calibration exercise was focused on the temperature and oxygen profiles. The parameters related to extinction coefficients that control light availability at lower depths were first reduced. The different parameters related to growth rates and optimum temperatures for the different algal species were also adjusted while considering mainly oxygen depletion.

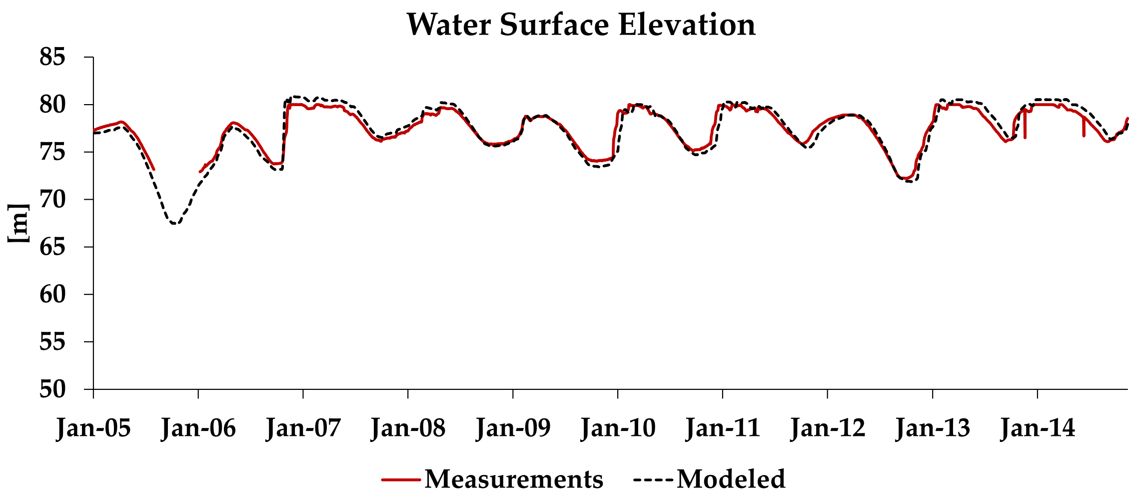

Figure 5.2 Time series of water surface elevation at the Montargil Reservoir dam (model results: black line; field data: red points).

Table 5.3 The kinetic coefficients and values for the Montargil Reservoir.:

Parameter	Description	Default value	Calibrated value
EXH2O	Extinction for pure water (m^{-1})	0.25 or 0.45	0.25
EXOM	Extinction Coefficient for organic matter (m^{-1})	0.2	0.1
EXZOO	Extinction Coefficient for zooplankton (m^{-1})	0.2	0.01
BETA	Fraction of incident solar radiation absorbed at the water surface (%)	0.45	0.55
AG-1	Algal growth rate for diatoms (day^{-1})	0.3-3.0	1
AG-2	Algal growth rate for *Chlorophyceae* (day^{-1})	0.7-9.0	0.7
AG-3	Algal growth rate for *Cyanobacteria* (day^{-1})	0.5-11	0.5

Parameter	Description	Default value	Calibrated value
AT1-2	Algal minimum temperature for *Chlorophyceae* (°C)	5	10
AT1-3	Algal minimum temperature for *Cyanobacteria* (°C)	5	15
AT2-1	Algal first optimum temperature for diatoms (°C)	25	10
AT2-2	Algal first optimum temperature for *Chlorophyceae* (°C)	25	15
AT2-3	Algal first optimum temperature for *Cyanobacteria* (°C)	25	23
AT3-1	Algal last optimum temperature for diatoms (°C)	35	20
AT3-2	Algal last optimum temperature for *Chlorophyceae* (°C)	35	25
AT3-3	Algal last optimum temperature for *Cyanobacteria* (°C)	35	25
AT4-1	Algal maximum temperature for diatoms (°C)	40	25
AT4-2	Algal first maximum temperature for *Chlorophyceae* (°C)	40	30
AT4-3	Algal first maximum temperature for *Cyanobacteria* (°C)	40	30

The model was able to describe temperature and dissolved oxygen profiles particularly during the main seasons, summer and winter (Figure 5.3). The results for the vertical temperature profiles showed a noticeable seasonality in the surface layer where the influence of solar radiation, air temperature and wind were evident. This is a typical behaviour of Mediterranean reservoirs where the seasonally is patent (Sellami et al, 2010; Tornes et al, 2014; Hassen et al, 2019). The thermocline occurred around 5-10 m depth during August, when air surface temperatures were higher and flows were reduced, with differences reaching 15°C from surface to bottom while the dissolved oxygen changed from 9 mg.L-1 to 0 mg.L-1 (Figure 5.3). During February 2006, stratification disappeared probably due to the combined action of increased wind velocity in the surface layer, cooling and increased flows. During this season, a homogeneous temperature profile was observed (Figure 5.3). The thermal stratification and mixing influenced the dynamics of primary production, controlling light and nutrients availability. During winter, the decreased stratification effect created a homogeneous profile of temperature, while nutrients availability existed from the bottom to surface layers.

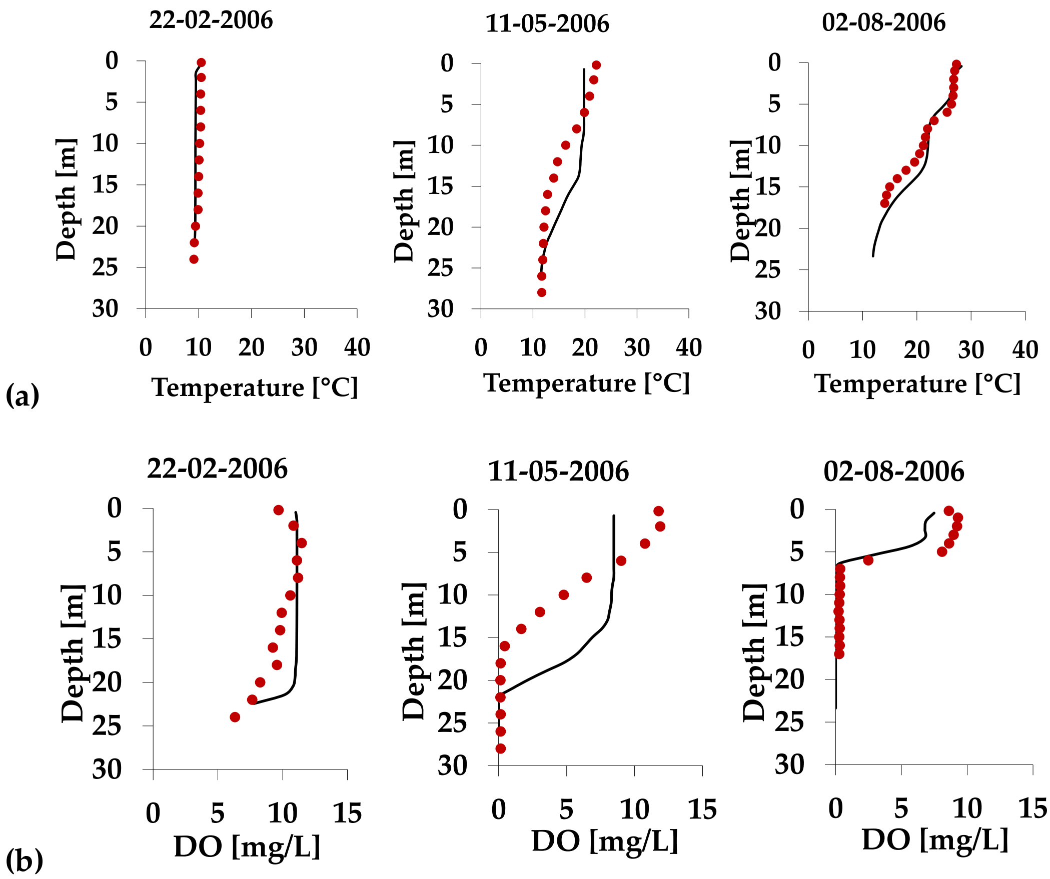

Figure 5.3 Temperature (a) and dissolved oxygen (b) profiles at the Montargil Reservoir dam on different dates (model results: black line; field data: red points).

In the validation exercise it should be taken into consideration, as a cumulative uncertainty, that the model results are mean daily values, contrary to the measured values, which are hourly instant values.

The comparison made for simulated and measured surface water temperature showed that the model was able to represent the seasonality of the reservoir as well as minimum and maximum values for the period considered. The average temperature was 18°C (Table 5.4), ranging from 10°C in winter, to 25°C during the warmer season (Figure 5.4). The model was able to reproduce the trend of surface dissolved oxygen (average 9 mg.L-1 and a standard deviation of 1.6 mg.L-1 modelled and 1.9 mg.L-1 in the field data) (Table 5.4), including oversaturation, resulting mostly from the rapid increase/accumulation of algae (algae bloom). In general, the dissolved oxygen concentration in the Montargil reservoir did not vary below the limit value of 5 mg.L-1 below which the potential ecological state may be compromised as stated by Ferreira et al. (2009) and INAG (2009). The few field data of total nitrogen concentration do not allow for an adequate statistical analysis, only being observed that the mean values are within the same order of magnitude (average 1.4 mgN.L-1 and range from 0.5 mgN.L-1 to 5 mgN.L-1, and a standard deviation of 0.8 mg.L-1 modelled and 0.3 mg.L-1 in the field data) (Table 5.4 and Figure 5.4). Total phosphorus concentration was acceptably reproduced (average 0.2 mgP.L-1), despite producing a slight overestimation of the measured values. Likewise, the chlorophyll-a data in the reservoir was in agreement with the measured data, averaging 22.0 μg.L-1 (Table 5.4), and revealing maximum concentrations reaching values above 50 μg.L-1 during the simulated time period. In general, the concentration values related with algae blooms are above the limit of eutrophication when higher than 10 μg.L-1 (Chapra 1997). The measured data presented significant variation, with the model reproducing well the seasonal pattern (Figure 5.4). The CE-QUAL-W2 model was also able to reproduce the trends of TSS during the period (average of 11 mg.L-1 modelled and 9 mg.L-1 in the field data, and a standard deviation of 8.9 mg.L-1 modelled and 7 mg.L-1 in the field data), which were consistent with the inflows from the drainage basin.

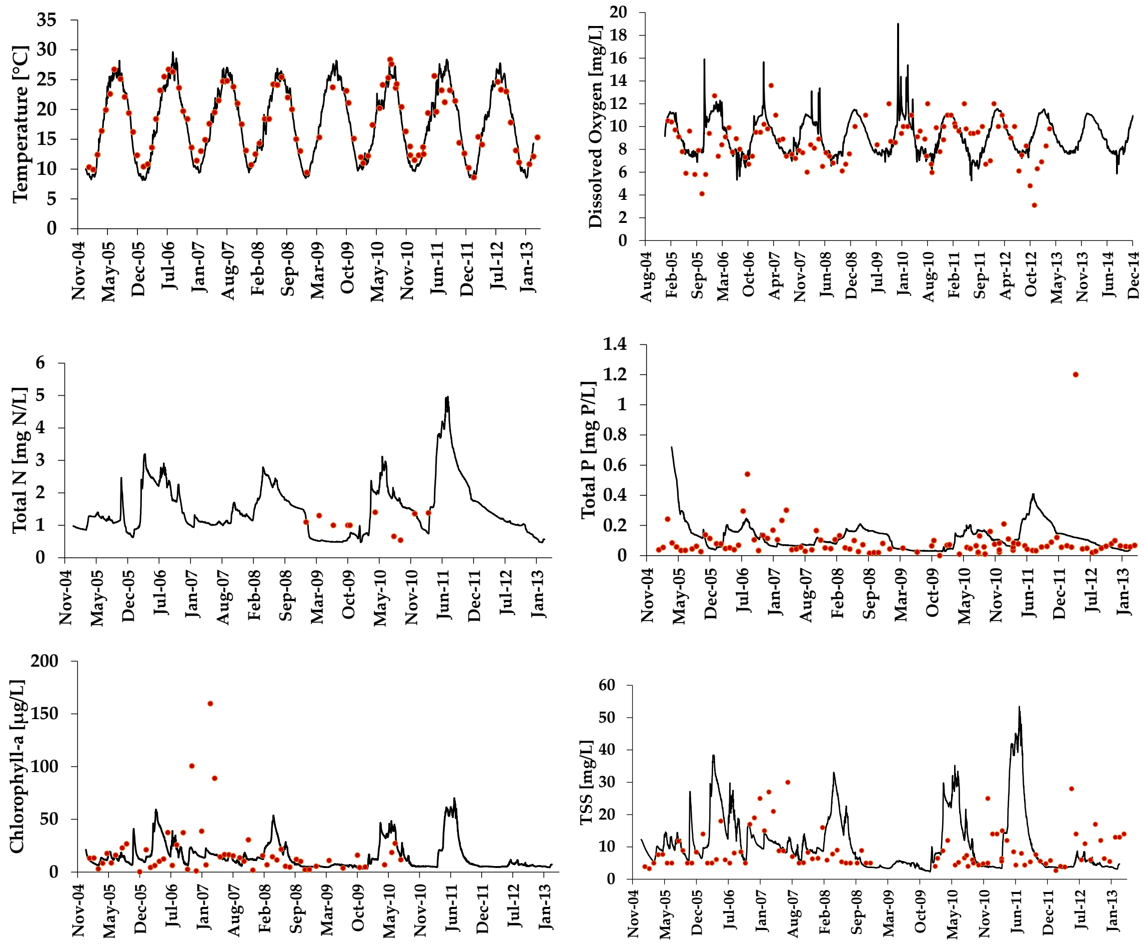

Figure 5.4 Time series of surface properties (temperature, dissolved oxygen, total N, total P, chlorophyll-*a*, TSS) at the Montargil Reservoir dam (model results: black line; field data: red points).

Table 5.4 Statistical analysis of measured field data and model estimates.

		Average	Standard Deviation	Median
Water Level	Model	77.3	2.9	77.7
	Data	77.6	1.9	77.9
Temperature	Model	17.8	6.1	18.1
	Data	18.2	5.4	18.4
Dissolved Oxygen	Model	8.9	1.6	8.9
	Data	8.7	1.9	8.9
Total N	Model	1.4	0.8	1.3
	Data	1.1	0.3	1.1
Total P	Model	0.2	0.1	0.1
	Data	0.1	0.1	0.1
Chlorophyll-*a*	Model	22.0	23.7	13.8
	Data	18.6	27.2	11.7
TSS	Model	11.0	8.9	8.3
	Data	9.4	7.0	6.5

5.3.3. Assessment of climate change impact on reservoir water quality under SSP-2/RCP 4.5 scenario

After the CE-QUAL-W2 model calibration and validation, the baseline and scenarios results were analysed on an annual, monthly and daily basis to understand and evaluate the evolution of Montargil's trophic state.

The predicted decrease of reservoir inflows in both timelines (2030 and 2060) led to a decrease of water levels by 10% even when assuming a decrease of 20 and 25% in future irrigation needs (Table 5.2). This is in accordance with Almeida et al. (2019), who considered more severe climate scenarios for the Montargil basin which limited even more water availability in the reservoir. Also, Milly et al. (2005) predicted a decrease by 10-30% in runoff in the Mediterranean region; and Bucak et al. (2017) predict the possibility in the future, of drying out of the Lake Beyşehir, catchment in Central Anatolia, Turkey.

The decrease in the inflows to the reservoir will increase residence time, which lead to an increase in the nutrients concentration and in turn a decrease in dissolved oxygen concentration. This decrease water inflow will thus decrease the dilution and flushing effect which will increase the biomass of plankton algae by increasing the nutrients concentration (Bartoszek & Koszelnik 2015).

The dissolved oxygen concentration in the water surface layer epilimnion (considered at 0.8 m depth) showed a minor decrease for both timelines, with reductions reaching 4% when compared to the baseline mean value (Table 5.5). The highest reduction is observed in the hypolimnion (considered at 20 m depth), with the model predicting a reduction of 58% and 62% for the 2030 and 2060 timelines (Table 5.5).

Table 5.5 Variation (Var.) in temperature, dissolved oxygen, chlorophyll-*a* and total P, in the different layers and scenarios, comparing with baseline, in %; and respectively standard error (Std. Err.), in %.

Scenario	**Layer**	**Temperature**		**DO**		**CHLA**		**TP**	
		Var.	Std. Err.	Var.	Std. Err.	Var.	Std. Err.	Var.	Std. Err.
2030	Epilimnion	+3	1.93	-4	0.49	+25	2.65	+63	0.16
	Hypolimnion	-8	1.10	-58	1.36	-13	1.95	+90	0.19
2060	Epilimnion	+3	1.91	-4	0.47	+20	2.80	+62	0.16
	Hypolimnion	-14	1.03	-62	1.28	-46	1.20	+118	0.27

The monthly averages of the dissolved oxygen concentration for the 30 years considered (baseline, 2030 and 2060 decades) revealed, as expected, the decrease of this parameter during months with higher temperature and lower inflow rate. In the epilimnion layer, values did not vary considerably and were maintained above the minimum limit considered for a water body to be classified as having good ecological potential which is above 5 mg.L-1 according to INAG (2009). Nonetheless, for dissolved oxygen the focus of the analysis should be the hypolimnion where the dissolved oxygen registered values close to 0 mg.L-1 for several months for both timelines. A daily basis analysis showed that DO concentration was lower than 5 mg.L-1 in 36% of the baseline simulated days; contrarily that condition was predicted to occur in 66% and 69% of the simulated days for the 2030 and 2060 timelines, respectively, thus clearly indicating a tendency for the Montargil reservoir to evolve to a hypereutrophic state.

In addition to DO concentration, chlorophyll-a and total phosphorus concentration parameters are essential for trophic analysis. Chlorophyll-a is a pigment common in most primary producers and appears as a biological variable of easy determination, indicative of plant biomass. This is the reason why it has been used in different water classification systems, namely in the classification of the trophic state by OECD (Caspers 1984).

Chlorophyll-a concentration increased in the epilimnion layer during both timelines, averaging more 25% and 20% when compared to the baseline mean value (Table 5.5). In contrast, a reduction of 13% in the 2030s and 46% in the 2060s was observed in hypolimnion layer (Table 5.5). This decrease was mainly due to photosynthesis and DO limitation. Monthly chlorophyll-a concentration values increased mainly during the spring months. The reservoir was considered as oligotrophic (chlorophyll-a <2.5 μg.L-1) during most part of the baseline period (55%), yet presenting an eutrophic state (chlorophyll-a > 10 μg.L-1) during the remaining period. Model simulations showed that for the 2030 and 2060 timelines, there is a tendency for an increase of the number of days registering an eutrophic state, covering 69% and 81% of the days in the 2030 and 2060 periods, respectively, and a decrease of the number of days predicted to register an oligotrophic state was only noticed on 15% and 31% of the days. Total phosphorus concentration increased in both layers during the period under analysis. In the epilimnion layer, total phosphorus concentration increased by 62% in both scenarios when compared with the baseline mean value (Table 5.5). In the hypolimnion layer, that increase reached 90% and 118% during the 2030 and 2060 timelines (Table 5.5), being mostly explained by the availability of phosphorus in the sediment bottom (Jouni 2011) and the lower percentage of oxygen saturation. This is in line with the studies in the Mediterranean lakes and lagoons which reported nutrient release from the bottom sediment (Gikas et al. 2006; Chamoglou et al. 2014; Beklioglu 2007). Considering the maximum limit established by INAG (2009) to maintain the good ecological status of a reservoir (0.07 mg.L-1), the annual average of total phosphorus concentration in the Montargil reservoir indicates mostly an eutrophic state. Model simulations show that the trophic status is expected to deteriorate due to climate change, similarly as in the Karla's Lake in Greece where phosphorus concentration far exceeded the limit of good ecological status (Chamoglou et al. 2014). Several studies showed already unacceptable ecological status in many reservoirs, such as the eutrophic Enxoé reservoir in southern Portugal, according to Brito et al. (2017), where only with structural measures trophic state may improve; Molina-Navarro et al. (2014) also predicted a deterioration of trophic conditions in the Pareja limno-reservoir, Spain, in most of the future scenarios considered; and the same in the study of Chang et al. (2015), which related the thermal stratification caused by the rising temperature in the future, with the higher risk of eutrophication.

5.3.4. Assessment of climate change impact on reservoir water quality under an improved SSP-2/RCP 4.5 scenario

Considering the previous results where the impact of climate change especially related to the precipitation decrease resulted in a decrease of water quality in the reservoir is evident, it was considered an improvement of the scenario. Both considered scenarios may be treated as measures to be implemented in the future. There are two main types of measures to be applied in reservoirs: preventive and corrective. Preventive measures act mainly in the drainage basin (such as: land uses management, improvement of agricultural practices or reduction of water abstraction). Corrective measures act in a mechanical method, biological or chemical. Preventive measures should be studied in a context of future scenarios in order to avoid the implementation of corrective measures, which are considered costly and could have negative impact on the environment and aquatic life. Moreover, in an integrated mathematical modelling approach such as the presented in this study, the measures implementation is restricted to management practices related to the water quantity and quality.

Based on the results found in this study as well as in previous studies in this location (Almeida et al. 2018, 2019; Segurado et al. 2018), where the major impact was shown to be mainly related to water scarcity, as a result of precipitation decrease, scenarios considering decreasing irrigation needs (by 30% and 35%, respectively for 2030 and 2060) equivalent to decreasing water abstraction measure, were defined in order to explore whether a less abrupt decrease in water level would result in an improvement of the future trophic state.

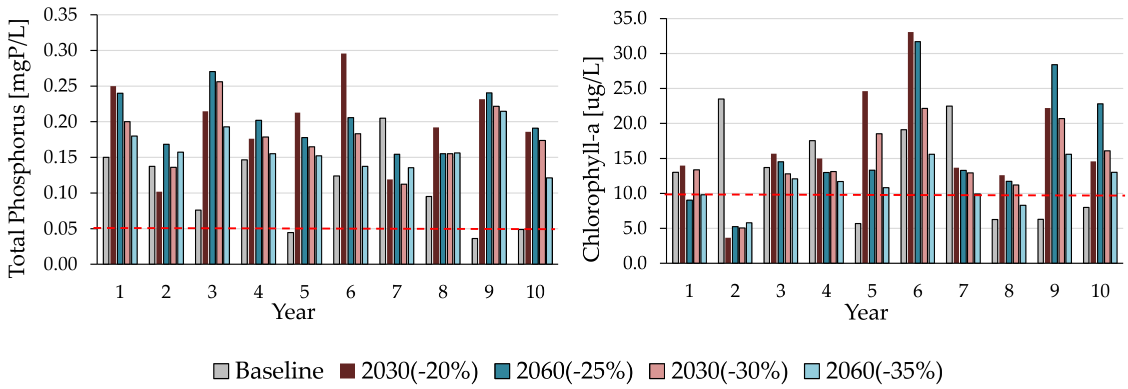

Figure 5.5 Annual comparison of total phosphorus and chlorophyll-a, in epilimnion. Dashed red line is the national official limit for the boundary of good status.

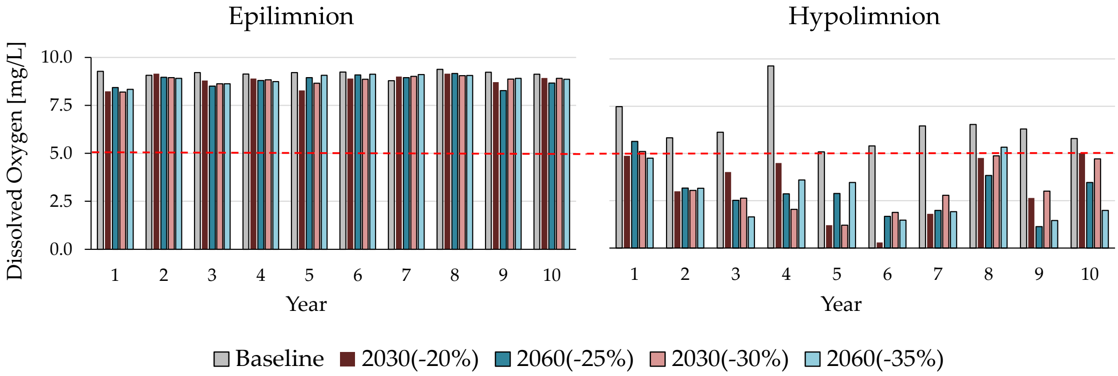

Figure 5.6 Annual comparison of dissolved oxygen, in epilimnion and hypolimnion. Dashed red line is the national official limit for the boundary of good status.

With the implementation of a 30% and 35% reduction in water abstraction for irrigation, a small improvement in the reservoir water quality concerning total phosphorus (on average -10% in 2030 and -20% in 2060) and chlorophyll-a (on average -14% in 2030 and -31% in 2060) (Figure 5.5) was observed. On average, the dissolved oxygen concentration has remained constant, although in the years where the concentration is predicted to increase, the reservoir does not reach an acceptable good quality status (Figure 5.6).

Concerning the impact of these water quality indicators on aquatic life, additional measures should be tested, considering the limitations on the implementation of these models: These include reduction on water abstraction for irrigation by an improved adaptation to seasonal changes, or through incentives to encourage land use transition from irrigated crops to rainfed crops.

5.4. Conclusions and Future Research

The integrated modelling used here proved to be an asset for management purposes, since it allowed to continuously analyse the inflow to the reservoir and its changes in the water quality under the influence of climate change. It is concluded that the case-study reservoir, as a consequence of the decrease of the inflows and increase of nutrient concentrations, as well as consequence of the decrease of precipitation observed in the region, will suffer an increase in nutrient and chlorophyll-a concentrations and a decrease in dissolved oxygen. In general, and considering all parameters here analysed, the tendency for the trophic status in the studied reservoir in the future is to an increasing eutrophic state, even considering a scenario of decreasing water abstraction. These results suggest that the ecological status of this reservoir in the future will be strongly impacted, compromising the survival of many fish species, mainly due to the high variation of dissolved oxygen with low levels during long periods of time.

Measures should be implemented to counteract more efficiently the predicted effects of climate change and should be preferably preventive, in opposition to corrective, to reduce both financial and environmental costs. Alternative management scenarios could be incorporated within the integrated modelling approach developed in the present study to predict their outcomes and anticipate cost-effective measures. Because similar climatic future tendencies are foreseen across the Mediterranean region (Chamoglou et al. 2014; Chang et al. 2015; Molina-Navarro et al. 2014), the trophic status trends under climate change scenarios predicted by this study, as well as the outcomes of the management scenarios, might be generalized to similar Mediterranean basins. These studies should provide tools to water managers allowing them to act timely without compromising the ecosystem, and in this way accomplishing more effectively the community objectives established by WFD.

Author Contributions: C.A. set up the models, run the simulations, and wrote the paper. T.F, P.B, P.S., T.R., R.N. and R.P.d.O. made revisions and improvements to the draft version.

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Chapter 6 General Conclusions

The central objective of this thesis was to develop and test an integrated modelling approach to access the impacts of climate change and societal scenarios on water quantity and quality in the Sorraia River basin. The achievement of this objective was confirmed through the application of the selected models and the different analyses described. These analyses were based on the socio-economic scenarios of evolution of the society that are expected in the future and the results of this evolution at the climatic level, as well as the analysis of the changes in the precipitation and drainage regimes, water quality status in the river and reservoir, mainly concerned with nutrient concentration, water temperature and dissolved oxygen.

These analyses allowed therefore, answering the following questions:

✓ Is modelling an effective approach to access the impacts of future climate and societal scenarios on a basin water quantity and quality?

The first modelling approach developed in this work was focused on the Sorraia River basin in order to estimate water flows and nutrients concentrations, which will be determinant on the downstream impact. The main finding in the results showed in Chapter 3, was that in the future and considering the scenarios studied, the Sorraia river basin will have poor water quality and low water availability. In the river, it is expected an increase of nitrogen and phosphorus concentration, and a severe decrease of the river flows.

This study shows the capability of the hydrological modelling in predicting changes in flows and nutrients concentrations, resulting from different scenarios and its possible cumulative impacts on the future. The results show how the mathematical models can be considered as a starting point for defining appropriate management plans to counteract such negative impacts.

✓ Is integrated modelling an effective approach to access the future water demand vulnerability in a reservoir?

The integration of the basin and reservoir models considered was focused on water quantity and allowed to analyse vulnerability and resiliency of the Montargil reservoir - one of the main Sorraia river reservoir - in the future under different management scenarios. The results found in Chapter 4 showed that it is expected a marked decrease on the water level during most of the period studied in the future, causing an extremely high difficulty to respond to water needs observed over the years. It has also been observed that even after a significant reduction in water consumption, the reservoir remains at very low levels, and thus water needs will not be guaranteed over long time periods. The impacts found, indicate the importance of an integrated management system to avoid the decrease of the water resources in the region and to increase the system's reliability and resilience, and subsequently reduce its vulnerability.

Furthermore, this approach showed the possibility to implement a more comprehensive management action by providing the amount of water and the period of availability at a monthly scale, especially in a region such as the Mediterranean where the importance of managing outflows to prevent reduction of water resources is crucial. This methodology, applied on a different time scale, will thus allow reservoir managers to decide, for example, what the minimum flow should be considered to not compromise the reservoir ecosystem and to meet users' needs.

- ✓ Is integrated modelling an effective approach to access to access the future trophic status under climate change?

The integration of the basin and reservoir models showed in Chapter 5, was focused on water quality issues in the reservoir. This study could be a basis for the trophic status classification of water bodies, extremely important for the European Members in order to meet the objectives of the Water Directive Framework. The integration of the basin and reservoir models allowed analysing continually the trophic status, which is critical to investigate the behaviour of each water body, especially reservoirs. In the Montargil reservoir, the results obtained showed that it is expected an increase of the nutrient concentration and a marked decrease of dissolved oxygen. These results showed that the Water Framework Directive objectives will not be accomplished in this reservoir and by continuing these practices it is unlikely that the good water body status will be achieved, as would be desirable. This approach is thereby quite acceptable to predict present trophic status of reservoirs which are poorly monitored, such as the Montargil reservoir, as to analyse its behaviour, considering future inflows from its drainage basin, and the expected climate change in the region.

Beyond the integrated modelling approach showed in Chapter 3, 4 and 5, complementary studies were carried out under this thesis. In both studies, presented in Appendixes 1 and 2, the results obtained with the hydrological model SWAT from the Chapter 3 were considered and some scenarios related to land use changes were considered. These studies allowed to answer the question:

- ✓ Are process-based models able to be integrated in the empirical models?

The purpose of the study developed by Segurado et al. (2018) (Appendix 1) was to provide a wide scale approach to basin management by interpreting the effect of isolated and interacting factors in several biotic elements. The combination of the hydrological modelling (with SWAT) to simulate hydrological and nutrient enrichment stressors and empirical modelling to relate these stressors with biotic indicators, was applied. This study demonstrates the potentialities of coupling process-based modelling with empirical modelling within a single framework, allowing relationships among different ecosystem states to be hierarchized, interpreted and predicted at multiple spatial and temporal scales.

Also Navarro et al. (2019) (Appendix 2) aimed to develop a Bayesian Belief Network (BBN) framework for modelling the ecological quality of rivers and streams in two European river basins located in two distinct European climatic regions: The Odense Fjord basin (Denmark) and the Sorraia basin (Portugal). The results obtained with the SWAT model were thus integrated with field measurements and empirical models in Bayesian Belief Networks (BBNs), to model the effect of multiple stressors on several biological indicators of the Sorraia river water quality and, subsequently, on their ecological status to model the ecological status. This study showed small impacts of climate and socioeconomic changes on the biological quality elements analysed. This yield a final ecological status similar to the baseline in the Odense case, and slightly worse in Sorraia. Results also showed that macrophytes and fish indices were the main responsible for a non-desirable global ecological status in Odense and Sorraia, respectively. By encompassing two case studies of very different characteristics, these BBN may be more easily adapted as decision-making tools for water management of other river basins.

In any of these approaches here investigated and their principal advantage, is the possibility to test management measures in order to respond to these increased pressures that are predicted in the future. This approach allow also to study the aquatic system in a more comprehensive way (considering abiotic and biotic indicators), with the integration of the results from the watershed model with empirical models.

Considering the results founded in this work it is noticeable the need to implementation of more drastic measures. These measures can range from upstream actions at the river basin scale, such as changes in agricultural practices by change of irrigated to rainfed crops, no-till practices or use of cover crops; to actions at the reservoir scale, for example by changing the amount of water available for irrigation by changing the irrigation source to groundwater. These measures can be implemented using the integrated modelling methodology here studied efficiency, and may be thereby replicable for case studies with the same climatic and agricultural characteristics.

In these studies it is crucial to take into consideration the uncertainties that may be associated with the models itself and its implementation. In addition, the projections obtained from the climate models are also subject of uncertainties which are still difficult to quantify, largely due to being recently developed and only now are being further investigated. Notwithstanding the uncertainties associated with mathematical modelling, this methodology remains quite effective given its continuous, simplified and integrative approach in the study complex processes of nature such as those occurring in soils related to nutrients (mineralization, nitrification, denitrification , leaching, etc.), erosion, water balance of the river basins, in the water column, among others.

Therefore, this work showed that on a local scale, the Sorraia watershed and the Montargil reservoir in particular, will be strongly affected in terms of water quality and quantity in its water bodies, and the Water Directive Framework objectives will be extremely difficult to achieve. However, it is also concluded that the scenarios studied here should be adapted to this case study to better characterize the future conditions. Thus, the storylines studied and developed under the European FP7 project, should be adjusted in order to have more realistic results, or to confirm the projections founded in this work.

Considering the high amount of details taken into account, future research is needed to confirm these projections or to formulate answers to questions that may arise in the future given the uncertainties in climate changes.

APPENDIXES

APPENDIX 1 - UNDERSTANDING MULTIPLE STRESSORS IN A MEDITERRANEAN BASIN: COMBINED EFFECTS OF LAND USE, WATER SCARCITY AND NUTRIENT ENRICHMENT

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Understanding multiple stressors in a Mediterranean basin: Combined effects of land use, water scarcity and nutrient enrichment

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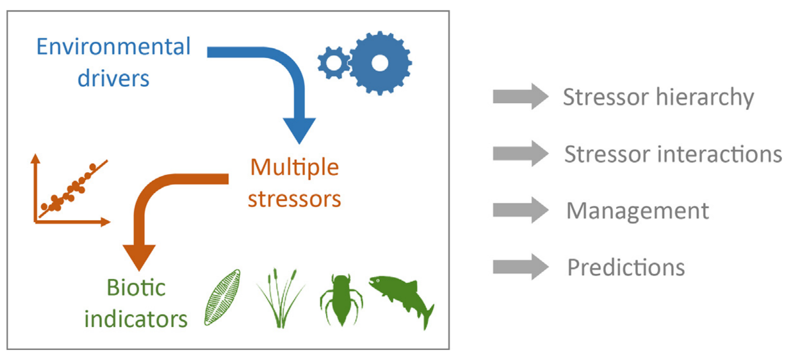
HIGHLIGHTS

- The interplay of water scarcity and nutrients in river biotic state is addressed.
- Stressors were simulated through process-based modelling.
- Stressors, land use and environmental background were used to model biotic state.
- Agriculture and nutrient enrichment showed major effects on biotic state.
- Interactions should be carefully examined to avoid wrong conclusions for management.

GRAPHICAL ABSTRACT



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ABSTRACT

River basins are extremely complex hierarchical and directional systems that are affected by a multitude of interacting stressors. This complexity hampers effective management and conservation planning to be effectively implemented, especially under climate change. The objective of this work is to provide a wide scale approach to basin management by interpreting the effect of isolated and interacting factors in several biotic elements (fish, macroinvertebrates, phytobenthos and macrophytes). For that, a case study in the Sorraia basin (Central Portugal), a Mediterranean system mainly facing water scarcity and diffuse pollution problems, was chosen. To develop the proposed framework, a combination of process-based modelling to simulate hydrological and nutrient enrichment stressors and empirical modelling to relate these stressors - along with land use and natural background - with biotic indicators, was applied. Biotic indicators based on ecological quality ratios from WFD biomonitoring data were used as response variables. Temperature, river slope, % of agriculture in the upstream catchment and total N were the variables more frequently ranked as the most relevant. Both the two significant interactions found between single hydrological and nutrient enrichment stressors indicated antagonistic effects. This study demonstrates the potentialities of coupling process-based modelling with empirical modelling within a single framework, allowing relationships among different ecosystem states to be hierarchized, interpreted and predicted at multiple spatial and temporal scales. It also demonstrates how isolated and interacting stressors can have a different impact on biotic quality. When performing conservation or management plans, the stressor hierarchy should be considered as a way of prioritizing actions in a cost-effective perspective.

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1. Introduction

Riverine environments have been increasingly imperilled by human activities and have become one of the most degraded systems in the world (Sala et al., 2000; Gleick, 2003). Degradation of rivers is caused by a multitude of individual stressors, originating from drivers such as agriculture, urbanization and climate change, which affect ecological patterns and processes through a highly and increasingly intricate cause-effect chain (Hering et al., 2015; Gieswein et al., 2017). The implementation of effective river management actions and appropriate ecological restoration actions greatly relies on the ability of researchers to disentangle this complex cause-effect chain into simple models that are capable of providing guidance for managers (Hering et al., 2015). For example, modelling frameworks that project multiple stressor effects on biological components of ecosystems under scenarios of changes in drivers and measures may provide especially useful tools to support decision making. Although there are several examples of such attempts (e.g. Fernandes et al., 2016; Segurado et al., 2016), these are still major challenges that river ecologists and managers are currently facing.

Rivers, because of their particular nature, pose additional challenges to assess and model the effects of multiple stressors. Multiple stressor combinations vary deeply along river longitudinal gradients and among different ecoregions (Schinegger et al., 2012), causing difficulties in disentangling their effects on biotic components from natural causes because of the co-variability of environmental conditions (Alahuhta and Aroviita, 2016). Moreover, very often the effect of single stressors may depend on the environmental and biotic settings where they are acting. Several studies show biotic alterations associated with human-induced disturbances (Branco et al., 2013) that have a strong regional pattern in terms of the degree of impact imposed on streams. Another challenge posed by rivers comes from their particular network structure. Rivers have a directionality imposed by flow but they are more than “ribbons of aquatic habitat” (Fausch et al., 2002) because they form hierarchical dendritic network structures (Cote et al., 2010). These hierarchical, dendritic, directional networks are heterogeneous and continuous, with longitudinal, lateral, vertical, temporal (Ward, 1989) gradients that change at different scales (Frissell et al., 1986) and regions (Hering et al., 2015). This complexity severely hampers the ability to implement effective management actions in a river basin, especially if the goal is to achieve holistic targets e.g., taking into account all biotic quality elements and not do an over-“ribbon-like”-simplification.

The Water Framework Directive (WFD - European Commission, 2000) enforced the use of several biotic elements as indicators of surface water quality as an alternative to just water quality (Moss, 2007). The WFD involves defining biotic indicators of specific stresses, and their aggregation in the so-called one-out-all-out principle, but does not necessarily reflect a reliable indication of multiple stressors that recognize an integrated assessment of ecosystem health and mal-functioning (Hering et al., 2010). Additionally, most studies analyse solely the effect of individual stressors - a change in the environment that forces a response by the biological group of interest (Underwood, 1989) – on biotic indicators (Birk et al., 2012), notwithstanding the fact that often the response of an indicator to an isolated stressor is “wedge-shaped” – a clue that there are additional pressures at work that are expressed when the intensity of the isolated studied stressor is relatively low (Thomson et al., 1996; Friberg, 2010). It seems thus apparent that stressors interact, and, by doing so, create complex non-linear impacts. River systems are chiefly altered by hydromorphological degradation and diffuse pollution (EEA, 2012), which are themselves composed of several individual components. River regulation is widespread and severely alters flow velocity and water depth, creates vertical outflow drops that modify thermal and hydrology regimes of river systems and promotes the loss of original habitat which reduces heterogeneity and hampers the movement of river species (Segurado et al., 2013; Branco et al., 2014). Additionally, water quality is increasingly being deteriorated through urban, industrial and agricultural waste water. The combined impact of all these alterations has changed dramatically the constitution of river biotic communities (Allan, 2004).

Nowadays, increased water demand and climate change are likely to increase the magnitude and number of stressors acting upon river ecosystems and increase possible interactions. The interaction of different stressors can be manifold: additive when the response is predicted by the sum of the responses to isolated stresses; synergistic when the combined effect is greater than the sum of the effects of isolated stresses; or even antagonistic by creating responses smaller than those predicted (Underwood, 1989, but see Piggott et al., 2015 for an extensive review of the concepts). Deviations from additive effects among stressors tend to dominate, as shown by several studies (Côté et al., 2016; Nõges et al., 2016; Schinegger et al., 2016; Teichert et al., 2016; but see Gieswein et al., 2017 for opposing conclusions). Although studies focused on multiple stressors in aquatic environments are increasingly found in the literature (e.g. Ormerod et al., 2010; Côté et al., 2016; Feld et al., 2016; Jackson et al., 2016; Leal et al., 2016; Schinegger et al., 2016; Teichert et al., 2016), there is still a generalized lack of mechanistic understanding of stressors' interactive effects, which is a barrier for the prediction of responses to changing environments, risk assessment, management, impact mitigation and restoration of ecosystems (Vinebrooke et al., 2004). The use of models facilitates the prediction of management and conservation actions and by doing so facilitates cost-effective measures to be selected for future application. But, models are just a simplification of reality. This is more evident for models applied to river networks given their intrinsic complexity. Although there are large numbers of unforeseeable eventualities, the use of models in river systems is accepted as a standard practice with relevant knowledge arising from them (Feld et al., 2016).

The main goal of this work is to understand the interplay between the effects of multiple stressors, land use, reach scale attributes and climate on several biotic quality indicators in the Sorraia Basin, a typical Mediterranean basin located in SW Portugal. The Sorraia River is mainly affected by water scarcity - both as a consequence of its Mediterranean nature and an extensive water abstraction for irrigation - and nutrient enrichment from diffuse pollution from agriculture. This case study is part of one of the modelling framework approaches developed within the MARS project (Managing Aquatic Ecosystems and Water Resources Under Multiple Stress; Hering et al., 2015; Feld et al., 2016) that aims to predict effects of multiple stressors at the basin scale under different future climate change models, storylines and management scenarios. For this purpose, a process-based approach is used to estimate several stressors related to the hydrological regime and nutrient loads which is then coupled with an empirical modelling framework to calibrate models relating these stressors and other sources of variability with four common WFD biotic quality elements: fish, macroinvertebrates, macrophytes and phytobenthos. This work specifically looks at the stressors and gradients at play in this basin, identifies the stressor hierarchy and tests interactions among stressors in their effects on the biotic indicators. By doing so, this work, besides highlighting some specificities of working under a multi-stressor framework towards managing entire river basins that will predictably be affected by future alterations, advances knowledge and provides a theoretical basis that will facilitate management and conservation planning.

2. Materials and methods

2.1. Study area

The case study focused on the Sorraia Basin (Fig. 1), which has an area of 7730 km^2 and a length of 155 km. It flows towards the Tagus River estuary (outlet - latitude 38.83 and longitude −8.99) and is the Tagus tributary with the largest basin area.

The Sorraia Basin is characterized by a Mediterranean climate with an average annual air temperature of 15.2 °C that ranges from 21,6 °C in the summer to 9.4 in the winter. The average annual precipitation is about 600 mm, from 400 mm in dry years to up to 900 mm in wet years. The average monthly precipitation is 50 mm, ranging from 25 mm in summer months to 70 mm in winter months. Approximately 41% of the Sorraia's basin area is forest, 28% range-grasses, 17% agriculture, 9% pine, 2% orchard, 2% urban and industrial and 1% pasture (Mateus et al., 2009). The two reservoirs in the basin affect runoff at the gauging stations. Natural flow is substantially reduced by water abstraction for irrigation. The Sorraia Basin has a total of 153,099 inhabitants with a density of 20 hab/km^2, mainly concentrated in three core areas: Ponte de Sôr (16,722 inhabitants), Samora Correia (17,123 inhabitants) and Coruche (19,944 inhabitants) (INE, 2012).

According to the Tagus River Basin Management Plan (APA, 2012), the main pressures on the basin are: (1) hydromorphological changes, (2) diffuse pollution, (3) municipal discharges, (4) flow regulation and (5) extraction of water. Key ecosystem services identified by the RBMP are: (1) water for irrigation, (2) recreation services and (3) waste water treatment. The ecological status of 122 water bodies, in which the biotic component was based on the four biotic quality elements (phytobenthos, macrophytes, macroinvertebrates and fish) considered in the present work, is: 54 good (44%), 15 moderate (12%), 12 poor (10%), 2 bad (2%) and 39 (32%) unclassified. The main causes of poor or failing status in the basin are mainly related to the water demand for agricultural purposes, which in the Sorraia basin is the highest within the Tagus River Basin (26% of total need). Nutrient loads from agriculture, livestock and urban origin, mainly in the alluvial valley, are also important potential causes of poor status in the basin.

2.2. Process based modelling - deriving stressor variables

To simulate daily variation of stressors related to hydrological processes and nutrient loads, the Soil and Water Assessment Tool (SWAT; Neitsch et al., 2005) model was used through its ArcSWAT interface for ArcGIS (ESRI, Redlands, CA, USA). SWAT is a process-based semi-distributed watershed model focused on land management at the reach or basin scale. It has growth parameters for about 100 plant species with crop interest and a vegetation growth model developed by the Grassland Laboratory of the USDA (United States Department of Agriculture). Topologically, SWAT divides the basin into subareas that are assumed to be homogeneous in their hydrologic response units (HRU) and infiltration or groundwater flow is computed based on empiric or semi-empirical formulations (as the SCS rainfall-runoff curves or soil-shallow aquifer-river transfer times). The hydrology of the model is based on the water balance equation, which includes runoff, precipitation, evaporation, infiltration and lateral flow in the soil profile.

The calibration procedure entails adjustments to the model parameters to obtain the best possible adherence of the modelled data to the measured data. To a priori determine which parameters should be adjusted in the model, flows modelled and observed in the same location and during the same period are compared and deviations interpreted. Model results were compared with data available from two monitoring stations from the Sorraia Basin: Moinho Novo and Ponte Vila Formosa (SNIRH; http://snirh.apambiente.pt/; accessed 30 July 2017). The period considered for the calibration and validation analyses was between 1996 and 2015. The coefficient of determination between the monthly mean flow modelled and observed was $R^2 = 0.69$ for Moinho Novo and $R^2 = 0.32$ for Ponte Vila Formosa; bias was -0.56 for Moinho Novo and 0.24 for Ponte Vila Formosa; the Nash-Sutcliffe efficiency (NSE) coefficient was 0.68 for Moinho Novo and 0.02 for Ponte Vila Formosa. For Total N, only the Moinho Novo had sufficient time series of data available for a proper estimation of model performance. For the mean annual mean of this parameter, the coefficient of determination was $R^2 = 0.59$, bias was 0.22 and NSE was -0.98.

Available GIS maps of topography, land use, soil type and climate, in the study area were used as inputs to the SWAT model. Topography was derived from the Shuttle Radar Topography Mission, with 90-m resolution (Jarvis et al., 2008). Soil physical properties were derived from the Portuguese Soil maps and Land use Capacity (http://www.dgadr.pt/cartografia; accessed 30 July 2017). Land use classification, adapted to the SWAT classification, was derived from the GSE Land M2.1 (Mateus et al., 2009), with 20 and 300-m resolution. Climatic maps, including daily or hourly precipitation, temperature, relative humidity and wind speed were derived from SNIRH (http://snirh.apambiente.pt/; accessed 30 July 2017).

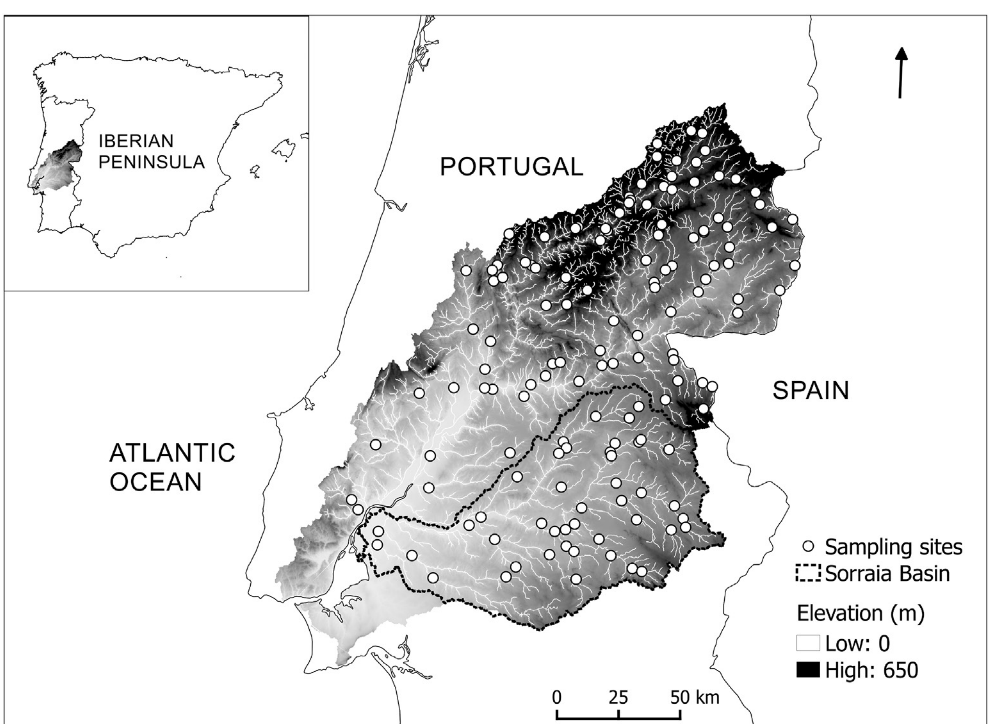

Fig. 1. River Tagus Basin, with a highlight of the study area (Sorraia Basin) and the location of sampling sites.

2.3. Empirical modelling - linking stressors to biotic indicators

To encompass a wider environmental and stressor gradient, we used data from the whole Tagus River Basin, where the Sorraia Basin is included, to fit empirical models relating biotic quality indicators, derived from biological monitoring data, with stressors. The dataset comprised 141 sites (Fig. 1) from the WFD biomonitoring program (Portuguese Environmental Agency, APA), with two sampling occasions (2010–11). Site selection included a set of least-disturbed sites used as reference sites. Remaining sites were selected to cover, as much as possible, different river types and the whole gradient of global disturbance measured in ordinal categories and based on hydromorphological alteration, water quality degradation and connectivity disruption.

The dataset included information on national biotic quality indices for four biotic quality elements: fish, macroinvertebrates, macrophytes and phytobenthos. For phytobenthos the national biotic quality index is the diatom metrics IPS (Indice de Polluosensibilité Sécifique) (Cemagref, 1982; Almeida et al., 2014). This index takes into account individual counts and species richness of all diatom taxon and it is an indicator of eutrophication, organic matter, acidification and salinity (Almeida et al., 2014). The national biotic quality index for macrophytes is the IBMR (Macrophyte Biological Index for Rivers), which is based on species abundance, ecological amplitude and trophic indicator value (Haury et al., 2006; Aguiar et al., 2014). It is considered a good indicator of nutrient inputs and/or heavy organic pollution (Haury et al., 2006). The macroinvertebrate national biotic quality index is the IPtI (Rivers Biological Quality Assessment Method — Benthic Invertebrates) (Ferreira et al., 2008; Feio et al., 2014). This index is based on the following metrics: number of taxa, species evenness, number of EPT (Ephemeroptera, Plecoptera, Trichoptera) families, evenness, IASPT (Iberian Average Score per Taxon index = IBMWP / number of families), log (selected ETD + 1) or EPTCD (log abundance of selected families of Ephemeroptera, Plecoptera, Trichoptera, Diptera, Coleoptera) (Feio et al., 2014). The index was developed using reference conditions based on land use, riparian condition, sediment load, hydrological regime, acidification and toxicity, morphological condition, nutrient enrichment and river continuity (Feio et al., 2014). The national biotic quality index for fish fauna is the F-IBIP (Fish-based Index of Biotic Integrity for Portuguese Wadeable Streams) (INAG and AFN, 2012; Segurado et al., 2014). The F-IBIP is a multimetric index based on parameters derived from fish assemblage composition and ecological functional groups (guilds) which differ among six fish-based river types. The index is based on twelve metrics scored separately by fish-type: number of native species, number of intolerant and intermediate species, % alien individuals, % intolerant individuals, % intolerant and intermediate individuals, % intolerant and intermediate Cyprinid species, % omnivorous individuals, % invertivorous individuals (excluding tolerant species), % potamodromous individuals, % reproductive generalist and “non-spawner” individuals, % lithophilic individuals and % water column individuals. The index was shown to be mainly responsive to water abstraction, presence of dams, presence of weirs, toxic risk and water quality (Segurado et al., 2014). The biotic quality indices were transformed into an ecological quality ratio (EQR) computed as the ratio between the original value of biotic quality index for a site and the value for reference or least disturbed sites of the same typology. An EQR close to zero indicates a site with a biological community that strongly deviates from those found in reference conditions.

The sampling protocol for phytobenthos followed European standard methods (CEN, 2003a). Most samples were collected in spring/summer. At least 5 pebbles covering in total at least 100 cm^2 of colonized surface were sampled per site. Diatoms were used as proxies for phytobenthos and counting of the cells followed standard procedures (CEN, 2004), with a minimum of 400 valves identified and counted. Macrophytes were sampled according to the European standards EN14184:2003 (CEN, 2003b) and EN14996:2006 (CEN, 2006). One-shot surveys per site were performed in spring–summer season (April to September). The sampling of macroinvertebrates followed the standard protocol established by Instituto da Água for the implementation of the Water Framework Directive in Portugal (INAG, 2008). A 50 m reach representing habitat diversity was defined for each site. Macroinvertebrates were sampled with a hand-net (0.25 m opening and 500 nm mesh size), each sample comprising six composite collections. Identification was performed mainly at the genus level. Fish sampling was performed by electrofishing following standard procedures (CEN, 2003c) for assessing fish species composition and abundance. Each site was sampled during spring–summer base flow. The fishing team progressed upstream in a zigzag pattern with single passes covering all present habitats (riffles, pools). Minimum sampled length was 20 times the mean wetted width of the channel.

Fifteen predictor variables were selected, including four land use pressure variables, two nutrient stressors, four hydrological stressors and five variables describing natural environmental variability (Table 1). Environmental variables were compiled from the CCM2 river network database (Vogt et al., 2007) for all river segments (river stretch between confluences). Land use pressures were derived from the CORINE landcover database (European Environmental Agency, 2010) as the percentage of area derived from a wide spatial scale corresponding to the whole upstream catchment. These pressure variables were used as a proxy of different environmental stressors (e.g. nutrient enrichment, water abstraction, sediment pollution, damming, flow regulation) rather than a stressor in itself. We considered it important to include these variables as predictors to control for the effects of other sources of variability that were not measured or modelled. The four land use variables were selected based on their potential effects on rivers. Agricultural land may be considered essentially a proxy for many different kinds of diffuse pollution in the form of nutrients (e.g. fertilizers, organic wastes from livestock activities) and toxic substances (e.g. pesticides). In addition, irrigation crops are a proxy of several hydrological alterations (e.g. water abstraction, patterns of extreme flow events). Urban areas are mainly a proxy for different types of point source pollution (e.g. from domestic and industrial wastes). Forests are essentially a proxy of several processes that contribute to reduce sediment in rivers and filter water pollutants. The percentage of area in the upstream catchment was computed with the RivTool software v1.0.0.1 (Duarte et al., 2016).

Table 1
List of candidate predictor variables. VIF – Variation Inflation Value with a threshold value of 3.

Predictor variables	Units	Range	VIF selection
Land use pressures			
Agriculture in the upstream catchment	%	0–96	Yes
Irrigated crop in the upstream catchment	%	0–19	Yes
Forest in the upstream catchment	%	0–83	Yes
Urban in the upstream catchment	%	0–12	Yes
Nutrient stressors			
Total phosphorus annual mean	mg/l	0.00–1.46	No
Total nitrogen annual mean	mg/l	0.95.69	Yes
Hydrological stressors			
Mean annual Flow	m3/s	0.13–129.01	Yes
Low flow pulse – number of events	.	0–40	Yes
Low flow pulse – mean duration (days)	Number of days	0.00–106.00	Yes
Mean annual flow alteration	%	0–35.56	Yes
Natural environmental variability			
Distance from source	km	2–981	No
River slope	%	0.01–75.01	Yes
Size of the upstream catchment	km^3	8–67,051	Yes
Mean annual temperature	°C	9.9–17.2	Yes
Mean total annual precipitation	mm	628–1552	No

The nutrient-related variables included two commonly used indicators of nutrient stress: total nitrogen and total phosphorus. Both stressors are main causes of eutrophication effects such as phytoplankton blooms and accelerated plant growth which results in low dissolved oxygen. The selected hydrological stressor indicators - mean annual flow, mean annual number of low flow events, mean annual duration of low flow events and mean annual flow alteration - are four uncorrelated measures of water scarcity. Low pulses were defined as periods during which the daily mean flow falls below the 10th percentile of the mean annual flow.

Because biotic indicators are affected by natural environmental gradients, it is crucial to control this effect when testing relationships with stressor variables. For the Tagus Basin we considered two main natural environmental gradients as the most relevant: a climatic gradient and a river longitudinal gradient. These gradients, expressed in our datasets by five environmental variables (Table 1), were included as candidate predictors in the empirical modelling framework to control as much as possible for the effect of natural background.

We found skewness problems in almost all predictors and therefore all explanatory variables were transformed using Box-Cox transformation (Box and Cox, 1964) followed by variable centering (mean $= 0$) and standardization (SD $= 1$), to express regression coefficients as standardized effect sizes. Collinearity among predictor variables was assessed through the use of VIFs (Variation Inflation Value) with a threshold value of 3 (Zuur et al., 2010). We used this criterion to exclude predictors in a stepwise fashion, by starting to remove the predictor with the highest VIF and repeating the VIF computation until all variable's VIFs were <3. We used the function vifstep of the package usdm that automatically performs the stepwise deletion based on a VIF threshold defined by the user (Naimi, 2015). Twelve variables were retained as candidates for inclusion in models (Table 1).

We ran several alternative empirical approaches following the overall procedure proposed by Feld et al. (2016) to analyse the impacts of multiple stressors in aquatic biomonitoring data. We performed a first exploratory analysis by running two machine learning techniques, Boosted Regression Trees (BRT; Elith et al., 2008) and Random Forests (RF; Breiman, 2001). After selecting the most relevant predictor variable candidates from the previous analyses, we quantified and tested both individual and multiple stressor effects through Linear Mixed Models (LMM; Zuur et al., 2009) using site as a random effect. Model selection was based on a multi-model inference procedure (Grueber et al., 2011) using the Akaike weight as a measure of the probability of the same model to be selected as the best approximating model using an independent dataset (Burnham and Anderson, 2002). We ran all combinations of models with no more than six predictor variables, to avoid selecting overly complex models. Pairwise interaction terms between hydrological and nutrient stressors were also included as candidate variables in the model selection procedure. Finally, the best approximating model, i.e. with the highest Akaike weight, was selected. LMM was also used to test pairwise interactions, i.e., to test significant deviations from additive effects and identify the interaction type (synergistic, antagonistic and opposing) based on the direction and intensity of such deviations. We included a year variable in all models to control for annual variability. In LMM we included year as a fixed factor because the number of classes (2 years) was not sufficient to use the variable as a random factor.

To allow comparisons of the goodness-of-fit among the three modelling techniques, we computed the correlations between observed and fitted EQR values for each biotic quality element. We also computed correlations between observed and predicted values using validation data. The validation procedure varied among the modelling technique. For BRT, the correlations were computed as the mean correlation of a 10-fold cross-validation procedure (see e.g. Elith et al., 2008 for further details). For RT, average predictions of "out-of-bag" samples used in each tree development were used to compute the correlations with observed EQR values. For LMM, we used a jackknife-based, or leave-one-out, cross-validation procedure to compute correlations of validation predictions with the observed response.

We used the three modelling approaches to rank the relative importance of stressors, land use, climate variables and stream attributes for each biotic indicator. In BRT, the importance of each variable in the model was estimated by averaging the number of times each variable was selected for splitting a tree as well as the squared improvement resulting from these splits (Friedman, 2001). The importance in RF models was based on Breiman-Cutler permutations in which, for each tree, the prediction errors are computed for "out-of-bag" data using both original and randomly permuted cases. Variable importance is then defined as the difference between the error rate of the original and permutated data averaged over all trees in the forest (Ishwaran, 2007). Because in this case low values of importance may take a negative sign, all negative values were truncated to zero. The relative importance of predictor variables in LMM was assessed based on the probability of each variable to be included in the best approximating models, estimated by summing the Akaike weights of all candidate models where the variable was included (Burnham and Anderson, 2002). For comparison purposes, values of importance were transformed in percentages in relation to the sum of importance values. The variables were then ranked for each modelling technique and biotic quality element and a mean rank was computed for each variable. Inconsistency among models in the rank of importance was then computed as the percentage of the difference between maximum and minimum position in the rank in relation to the maximum possible difference (equal to total number of variables). By checking the consistency across modelling techniques of the importance of predictor variables we assessed the uncertainty of predictions driven by the choice of the modelling technique.

All the analyses were performed with R version 3.3.2 (R Core Team, 2017) using packages gbm (Ridgeway, 2007) and dismo version 1.1-4 (Elith et al., 2008; Hijmans et al., 2013) for running BRT, randomForestSRC (Ishwaran and Kogalur, 2017) for running RF, lmerTest (Kuznetsova et al., 2014) and lme4 (Bates et al., 2015) to run LMM and MuMIN (Bartoń, 2016) to perform multimodel inference. We used R codes similar to those provided by Feld et al. (2016).

3. Results

3.1. Performance of empirical models

The empirical models relating the EQR of each biotic quality element with environmental, land use and stressor variables showed an overall good adjustment to the data (Fig. 2). Models fitted with LMM tended to show the best explanatory power. With BRT and RF, especially for phytobenthos, macrophytes and macroinvertebrates, fitted values tended to be biased towards an overestimation of EQR, especially for lower response values. These tendencies are confirmed by the correlations between fitted and observed EQR values (Fig. 3). Correlations using training data ranged from 0.81 for macrophytes using BRT and 0.99 for Fish using LMM. Correlations using validation data were lower, ranging from 0.27 for macrophytes using R and 0.81 for Fish using LMM. These validation correlations showed that models fitted with LMM also tended to show the best predicted power for the four biotic quality elements.

3.2. Relative importance of variables

Among all four biotic quality elements and modelling techniques, the variables most frequently ranked in the first three positions of relative importance (Tables 2 to 5) were % of agriculture (for phytobenthos, macroinvertebrates and fish), and the annual mean temperature (for macroinvertebrates and fish). The variables most frequently ranked in the last three positions of relative importance were Flow alteration (all biotic quality elements) and Number of low flow events

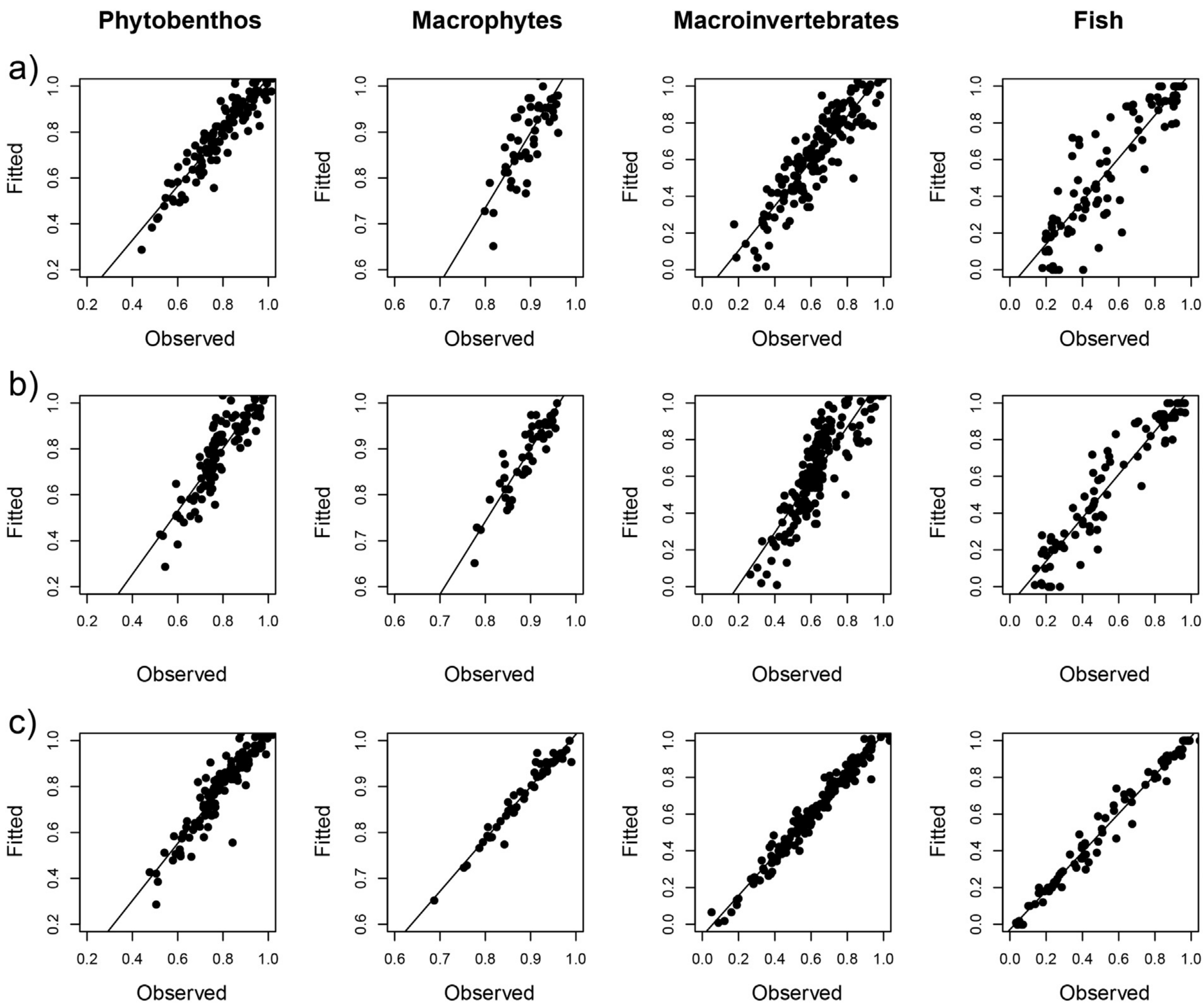

Fig. 2. Fitted versus observed values for each model and biotic quality element. a) Boosted Regression Tree; b) Random Forests; c) Linear Mixed Models.

(phytobenthos and macroinvertebrates). The variable year was the variable that was ranked more inconsistently among modelling techniques. Partial responses of each biotic indicator in each model are shown in Supplementary data (Appendix Aces).

For phytobenthos EQR (Table 2), two land use variables, % agriculture and % urban, were consistently the most important predictor variables among the three models. A stressor variable related to water scarcity (mean duration of low flow events) was ranked in the third position, followed by river slope and mean annual temperature. The % forest, number of low flow events and flow alteration were consistently the least important variables. Year was the variable that showed the most inconsistent rank of importance among the three models, ranked in the fourth position in LMM and in the 2 last positions in BRT and RF models.

The most important predictor variables affecting macrophytes EQR (Table 3) were a river segment attribute (river slope), a land use variable (% forest, mostly cork-oak land) and a hydrological stressor (mean annual flow), although inconsistently ranked in first, second or third place among the three models. Mean annual temperature, % irrigated croplands and flow alteration were consistently ranked in the last three positions among the models. Again, year showed the most inconsistent rank of importance among the three models.

For macroinvertebrates EQR (Table 4), the predictor variables ranked in the first three positions were % agriculture, mean annual temperature and % of irrigated croplands. In this case, outputs from LMM showed an overall inconsistency with those from BRT and RF. For example, year was ranked in the first position in LMM but in the last three positions in BRT and RF models. Size of catchment, flow alteration and number of low flow events were ranked in the last three positions, although their ranking showed weak consistency among methods.

Mean annual temperature, total N and % agriculture were the variables that had the highest rank of importance for fish EQR (Table 5). Mean duration of low flow events was the second most important stressor, although showing the highest inconsistency among models, ranked in the third from the last position according to the BRT model. Mean annual flow, year and flow alteration were ranked in the last three positions, but their rank order showed weak consistency among methods.

3.3. Effects sizes and interactions

The variables included in the best approximating LMM for each biotic quality element are shown in Table 6. Mean annual temperature, river slope, % agriculture and total N were the most frequent selected variables, all included in two of the four models. The predictor variables selected in the best approximating model and their effect sizes are not necessarily consistent with the ranks found in Tables 2–5 because these ranks take into account a large number of models with different combinations of variables.

The variables included in the phytobenthos model were river slope with a positive effect, two land use variables, % agriculture and % urban, both with a negative effect, and year. Percent agriculture and the % urban showed the highest effect size.

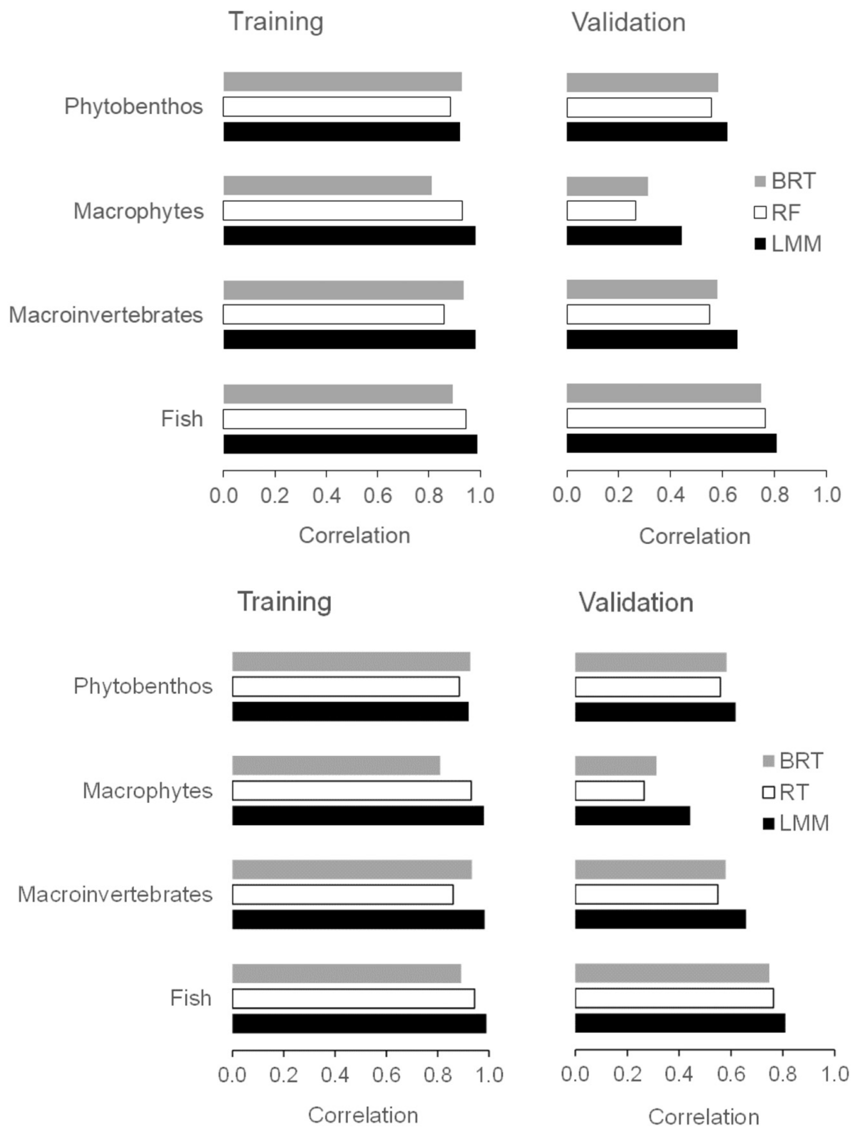

Fig. 3. Correlation between fitted and observed values for each model type and biotic quality element, based on the training dataset (left graph) and a validation procedure (right graph).

Table 2
Relative importance of variables as predictors of phytobenthos EQR in each model (BRT – Boosted Regression Trees; RF - Random Forests; LMM - Linear Mixed Models), mean rank of importance among models and inconsistency among models in the rank of importance (percentage of the difference between maximum and minimum position in the rank in relation to the total number of variables). Red indicates higher ranking and blue indicates lower ranking.

Variable	BRT	RF	LMM	Mean rank	Inconsistency (%)
% agriculture	23.13	35.91	17.35	1.00	0.00
% urban areas	15.61	19.60	16.99	2.00	0.00
Mean duration of low flow events	6.42	8.57	6.44	5.33	38.46
River slope	6.80	4.28	10.97	5.67	30.77
Mean annual temperature	7.29	3.57	6.13	6.00	30.77
Mean annual flow	10.49	5.49	4.64	6.00	46.15
Size of catchment	7.25	6.35	4.65	6.33	23.08
% irrigated croplands	7.26	3.55	5.84	7.00	30.77
Total N	5.59	7.44	4.53	7.67	46.15
Year	1.49	0.00	9.38	9.67	69.23
% forest	4.39	3.17	4.47	10.33	7.69
Number of low flow events	4.27	1.91	4.35	11.33	7.69
Flow alteration	0.00	0.15	4.27	12.67	7.69
Mean inconsistency (%)					26.04

Table 3
Relative importance of variables as predictors of macrophytes EQR in each model (BRT – Boosted Regression Trees; RF - Random Forests; LMM - Linear Mixed Models), mean rank of importance among models and inconsistency among models in the rank of importance (percentage of the difference between maximum and minimum position in the rank in relation to the total number of variables). Red indicates higher ranking and blue indicates lower ranking.

Variable	BRT	RF	LMM	Mean rank	Inconsistency (%)
River slope	17.80	22.95	15.56	2.33	15.38
% forest	18.76	31.63	8.06	2.67	30.77
Mean annual flow	24.05	30.12	8.02	3.00	38.46
% urban areas	15.82	10.08	7.39	5.00	23.08
Number of low flow events	4.66	0.16	11.45	6.33	61.54
Total N	5.51	0.51	6.52	6.67	23.08
% agriculture	2.41	2.49	5.18	7.33	30.77
Mean duration of low flow events	5.22	1.17	5.09	7.33	30.77
Size of catchment	1.77	0.43	8.95	7.67	46.15
Year	0.53	0.46	10.28	7.67	69.23
Mean annual temperature	1.99	0.00	4.46	10.67	23.08
% irrigated croplands	1.48	0.00	4.78	11.67	15.38
Flow alteration	0.00	0.00	4.26	12.67	7.69

The macrophyte model included also river slope with a positive effect, two stressor variables, total N and number of low flow events, both with a negative effect, and year. A significant interaction between total N and number of low flow events was found. The positive sign of the interaction regression coefficient, which goes in the opposite direction of the individual effects, indicates an antagonistic interaction between the two stressors, i.e., one stressor attenuates the effect of the other. This is confirmed by the 2D plot representing the co-effect of the two stressors on macrophytes EQR (Fig. 4). This plot also shows an opposing interaction, i.e., when one of the stressors is above a certain level, the effect of the other is inversed. However, most cases are located in the third quadrant of the plot, which indicates that an antagonistic interaction dominates.

The variables included in the best approximating model for macroinvertebrates were mean annual temperature, with a negative effect, two land use variables, % agriculture and % irrigated cropland, both with a negative effect, flow alteration, with a positive effect, and year. Percent agriculture and year showed the highest effect size.

The fish model included also mean annual temperature, with a positive effect, and two stressor variables, total N and mean duration of low flow events, both with a negative effect. A significant interaction between total N and mean duration of low flow events was found. Similarly to the macrophytes model, the positive sign of the interaction regression coefficient, with an opposite sign of the individual effects, indicates an antagonistic interaction between the two stressors. This is indicated by the 2D plot representing the co-effect of the two stressors on fish EQR (Fig. 4), showing that the colour change pattern along one variable axis changes along the other variable axis. This plot also shows an opposing interaction, although most cases are located in the third quadrant of the plot, which indicates a dominant antagonistic interaction.

4. Discussion

Managing such heterogeneous complex environments like river systems is a mammoth task that has to deal with a high degree of system-specificity and with mixed gradients of different nature (e.g. climatic, hydromorphological, biotic) that change the effect of a stressor along them. This translates into an impossibility of applying static measures with a homogeneous effectiveness throughout the stressor gradient, as the stressor itself changes its effect along other stressor gradients or even along environmental gradients. Scientists and managers should then understand how the response changes along these isolated or combined gradients, to adapt management actions to tackle stressors according to the specific gradient found in the basin of interest. The

Table 4
Relative importance of variables as predictors of macroinvertebrates EQR in each model (BRT – Boosted Regression Trees; RF - Random Forests; LMM - Linear Mixed Models), mean rank of importance among models and inconsistency among models in the rank of importance (percentage of the difference between maximum and minimum position in the rank in relation to the total number of variables). Red indicates higher ranking and blue indicates lower ranking.

Variable	BRT	RF	LMM	Mean rank	Inconsistency (%)
% agriculture	23.88	31.63	18.42	1.33	7.69
Mean annual temperature	9.69	9.39	9.11	3.00	15.38
% irrigated croplands	9.21	12.49	7.89	3.33	23.08
% urban areas	7.85	7.31	6.72	5.33	23.08
Total N	7.35	9.98	4.15	6.33	46.15
River slope	4.70	5.47	8.70	7.33	53.85
Year	6.18	2.68	18.74	7.33	76.92
Mean annual flow	7.83	4.77	3.67	8.67	53.85
% forest	7.50	4.58	3.99	8.67	30.77
Mean duration of low flow events	6.58	6.35	3.47	9.00	53.85
Size of catchment	6.55	5.00	3.96	9.33	23.08
Flow alteration	0.95	0.36	7.00	10.33	53.85
Number of low flow events	1.73	0.00	4.18	11.00	38.46
Mean inconsistency (%)					38.46

Table 5
Relative importance of variables as predictors of fish EQR in each model (BRT – Boosted Regression Trees; RF - Random Forests; LMM - Linear Mixed Models), mean rank of importance among models and inconsistency among models in the rank of importance (percentage of the difference between maximum and minimum position in the rank in relation to the total number of variables). Red indicates higher ranking and blue indicates lower ranking.

Variable	BRT	RF	LMM	Mean rank	Inconsistency (%)
Mean annual temperature	57.92	45.82	21.67	1.00	0.00
Total N	12.44	14.73	16.41	2.67	7.69
% agriculture	14.12	16.44	6.57	3.33	30.77
% forest	6.20	3.77	6.70	4.67	15.38
Mean duration of low flow events	0.26	4.64	8.41	6.00	61.54
River slope	2.14	3.02	5.15	7.00	15.38
% irrigated croplands	0.84	3.90	5.13	7.67	30.77
Number of low flow events	0.48	2.19	6.62	8.33	38.46
% urban areas	2.56	2.37	4.52	8.33	46.15
Size of catchment	1.33	2.57	4.36	9.67	38.46
Mean annual flow	1.63	0.54	4.42	10.00	38.46
Year	0.08	0.00	5.25	10.67	46.15
Flow alteration	0.00	0.00	4.79	11.67	23.08
Mean inconsistency (%)					30.18

work presented herein had the purpose of identifying difficulties and providing means to understand stressor importance and response variation along interacting stressor gradients.

4.1. Relative importance of variables

In the addressed case study there was a high impact of land use in the upstream drainage area on biotic indicators (see Liuzzo et al., 2015; Santos et al., 2015 and Sellami et al., 2016 for concurring previous findings). This was evident for all the studied biotic elements, and it is a consequence of the fact that land use variables tend to be a proxy for multiple stressors (Feld et al., 2016). For example, the presence of croplands is a proxy for very distinct single stressors, such as diffuse pollution, water abstraction and riparian habitat degradation that even may act synergistically. Additionally, both hydrologic and climatic variables were deemed important predictor variables, although for different biotic elements. This is understandable (Biggs et al., 2005), expected (Bonada and Resh, 2013; Gasith and Resh, 1999; Hershkovitz and Gasith, 2013; Wada et al., 2011) and previously demonstrated (Segurado et al., 2016). Water abstraction effects can severely affect lotic systems (Dewson et al., 2007; Wooster et al., 2016; Benejam et al., 2010; Lange et al., 2014), especially in Mediterranean regions and under the effect of climate and socioeconomic changes.

Albeit the aforementioned commonalities, all biotic elements varied in terms of the top ranking variables. Specifically, macrophytes were structured according to river slope, a variable that reflects the natural gradient between headwaters and lowland rivers – it was the only biotic element for which a “structural” variable ranked high in terms of importance. This is because of the ecology of this biotic element and the multiple effects of river slope – e.g. water velocity, sediment transport and residence time – that creates a very marked longitudinal variation in both the composition and structure of the aquatic and riparian vegetation communities (Manolaki and Papastergiadou, 2013). Fish, on the other hand, were the only element to rank a stressor (total N) among the most important variables. This is because total N is related to the surrounding land use and those are also closely linked to known changes in the fish assemblage following structural “along-the-river” alterations. An increase in nutrient concentration may lead, in high insolation areas, to the proliferation of submerged macrophytes and to consequent severe impacts on freshwater fish (Pusey and Arthington, 2003). Branco et al. (2016) also found that, using dissolved oxygen as a proxy in an experimental setup, the input of organic pollution and subsequent degradation seemed to affect fish activity levels. It is known that in some cases the biotic quality status indicators give clear and expectable responses to human induced disturbances, but for other indicators there are weak responses to human stressors, with the strongest responses related to natural environmental variability and spatial processes (Alahuhta and Aroviita, 2016).

Apart from pure biological factors, other causes related to methodological options may also contribute to the observed differences among biotic quality elements in their responses to predictor variables.

Table 6
Summary of the best approximating LMM model, including the standardized effect size (SES), the standard error of the estimate (SE), the degrees of freedom (df), the *t*-test value of the coefficient and its associated p-value.

Variable	SES	SE	df	*t*-Value	p-Value
Phytobenthos					
(Intercept)	−58.150	39.805	57.300	−1.461	0.150
River slope	0.029	0.016	87.320	1.883	0.063
% agriculture	−0.046	0.017	85.760	−2.712	0.008
% urban	−0.042	0.016	82.680	−2.562	0.012
Year	0.029	0.020	57.300	1.481	0.144
Macrophytes					
(Intercept)	−72.876	32.106	20.430	−2.270	0.034
River slope	0.037	0.014	45.370	2.744	0.009
Number of low flow events	−0.031	0.012	55.000	−2.559	0.013
Total N	−0.023	0.014	47.360	−1.692	0.097
Year	0.037	0.016	20.430	2.298	0.032
Number of low flow events × total N	0.027	0.015	41.750	1.768	0.084
Macroinvertebrates					
(Intercept)	−279.103	36.871	50.990	−7.570	<0.001
Mean annual temperature	−0.043	0.023	132.600	−1.885	0.062
% agriculture	−0.100	0.021	132.250	−4.726	<0.001
Flow alteration	0.035	0.019	131.810	1.853	0.066
% irrigated croplands	−0.039	0.022	130.940	−1.748	0.083
Year	0.139	0.018	50.990	7.587	0.000
Fish					
(Intercept)	0.560	0.028	79.960	20.283	<0.001
Mean annual temperature	−0.212	0.029	79.960	−7.306	<0.001
Mean duration of low flow events	−0.012	0.026	86.130	−0.438	0.662
Total N	−0.086	0.029	81.880	−2.928	0.004
Mean duration of low flow × total N	0.060	0.028	62.190	2.156	0.035

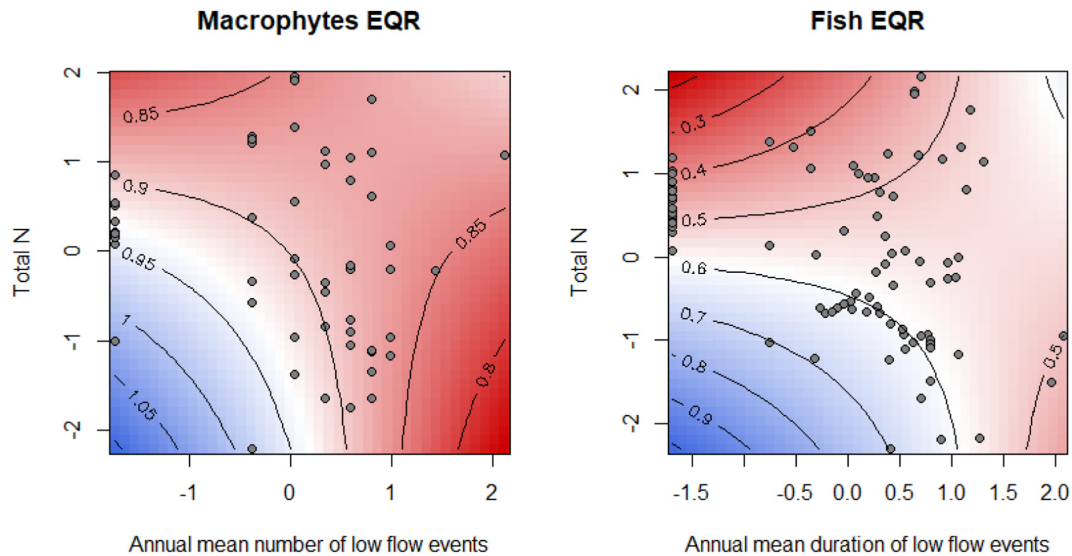

Fig. 4. Plots showing the pairwise interactions in the LMM model for macrophytes (left) and fish (right). Response variables are expressed by colour intensity, varying from low EQR values (red) to high EQR values (blue). Dots represent the true observations and may be used to check which portion of the plot is more supported by data. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Differences may arise because of distinct rates of assemblage change in the presence of stressors, i.e., they might be attributed to the temporal resolution at which predictor variables were compiled. Phytobenthos and macroinvertebrates, given their shorter life cycles in comparison to macrophytes and fish, are expected to respond more promptly to environmental change and hence to respond to shorter time windows. This might explain why selected LMM included more land use variables and fewer individual stressors in the case of phytobenthos and macroinvertebrates. The time window (annual mean) to derive individual stressors may not be the most adequate for these organisms. Responses may also be influenced by the spatial scale at which variables were compiled or simulated (e.g. HRU size in SWAT simulations), mainly because of different dispersal abilities among organisms. For example, fish are known to be more responsive to stressors acting at wider spatial scales than other organisms (Harris, 1995) because they can easily move to more favourable environments in face of local disturbances. Therefore, differences found among biotic quality elements in their response to predictor variables may have been partially driven from the use of common temporal and spatial resolutions in the modelling framework.

The influence of sampling protocols and site selection in model precision and accuracy, and hence in their generality and predictive power, cannot be discarded (Stevens & Olsen, 2004; Hughes & Peck, 2008; Hughes et al., 2000, 2012). Even scientifically informed sampling designs involved in biomonitoring program are necessarily constrained by funding resources (limiting the number of samples), logistics (e.g. site accessibility) and subjective human decisions (Hughes & Peck, 2008). Sampling decisions that originated data used in the present work are no exception and their effects on models are inevitable. On the other hand, the global disturbance gradient that considered for sampling site selection of the biomonitoring database might not totally reflect the gradient of stressors that were dealt with in this work. Additionally, because the case study basin is dominated by a Mediterranean landscape which has been shaped from centuries of human activities, there is an overall lack of minimally disturbed catchments (Segurado et al., 2011) which necessarily shortens stressor gradients, with implications on modelling results (Feld et al., 2016; Leitão et al., 2017). Despite all the potential methodological effects on the results of the several modelling approaches, a certain degree of confidence is ensured given that the biomonitoring data used in this work was originated from sampling protocols that strictly followed European standards. In addition, sampling protocols for the four biotic quality elements were all WFD compliant which allowed the biotic quality indices to be subjected to the WFD intercalibration process to harmonize quality class boundaries with other European indices (Aguiar et al., 2014; Almeida et al., 2014; Feio et al., 2014; Segurado et al., 2014).

4.2. Stressor interactions

The present paper also aimed at identifying and understanding stressor interactions at play in the Sorraia Basin. Significant stressor interactions (LMM) were found for two biotic elements, macrophytes and fish. In both cases the interactions were found to be opposing (see Feld et al., 2016). But, if there is a focus on the data supported portion of the stressors gradients, it becomes evident that, in fact, the stressor interaction taking place is mostly antagonistic (see Feld et al., 2016). So, the interaction along the full gradient of the two interacting stressors is opposing but it changes along the gradient. When looking at partial gradients the interaction may differ from opposing. This highlights the need to analyse the full gradient of the stressors (Branco et al., 2016; Schinegger et al., 2016). Furthermore, the resulting opposing interaction might be a mathematical artefact of the model in the portion of the gradient under-represented by data. This is most likely to be the case of the interactions detected in this study. In fact, the plots representing interactions in a model must be interpreted very carefully. Original data must always be projected in the plot to check if there are regions of the modelled relationship that are not well supported by the data.

A synergistic interaction between hydrological stressors and nutrients, rather than the observed antagonistic interaction, was expected. This is because water scarcity would expectedly amplify the effects of nutrient loads by decreasing the natural diluting property of rivers (Blasco et al., 2015). An important aspect to be considered in the particular case of pairwise interactions in the context of regression-based modelling, which is the typical approach when analysing biological monitoring data, is that significant deviations from additive effects occur when one variable affects the slope of the response to the second variable. This peculiarity is very distinct from interactions inferred from typical factorial designs of controlled experiments, which do not involve estimates of response rates, but usually simple comparisons between stressed and unstressed conditions. So, one possible explanation for antagonistic interactions among stressors is that when stressor 1, e.g. total

N, is acting alone, the slope of the increase of the effect along the stressor gradient is expectedly steeper because at low stressor intensity, the biotic quality is at its maximum (low values of both stressors), i.e., for a small increase of the stressor there is a more pronounced decrease in the biotic quality. When stressor 2, e.g. duration of low flow events, is acting the rate of the increase of the effect along the stressor 1 gradient might be weaker because even at low values of stressor 1, the biotic quality is already being affected by stressor 2. Additionally, it is expected that when a single stressor dominates, the biotic response may reach a level beyond which it will not decrease even in the presence of a second stressor. In fact, a recent meta-analysis found that antagonistic effects among stressors prevail in the literature focused on freshwater ecosystems (Jackson et al., 2016). The antagonistic effect found between hydrological and nutrient stressors does not necessarily mean that the presence of one stressor attenuates the effect of the other uniformly along the stressors' gradient (Brown et al., 2014). It is often claimed that efforts to mitigate stressors are least effective in systems where antagonistic interactions prevail (Brown et al., 2013; Piggott et al., 2015) but this is very contingent on the position of the data along stressor gradients, which determines whether antagonistic effect deviates more or less from the additive effect.

4.3. Implications for management

The results of this work clearly highlight the importance of having more than one biotic element as a management/conservation goal, or as an indicator for management/conservation prioritization, as each element responds very differently to the diverse categories of environmental variables. Additionally, it is important to consider several environmental variables of each category (e.g. hydrology, climate, land-use), as for some elements some variables of the same category can either rank high or low in terms of importance in explaining the registered variability, and their relative positions may drastically change between biotic elements. The overall image is important to fully ascertain a basin status and to define management/conservation practices as each biotic element is differently affected by the natural background and stressors. Even if a stressor is considered as an important variable for two biotic elements, their responses to stressor levels may be different as the subsidy-stress thresholds change (or not) between elements (Odum et al., 1979).

The high degree of inconsistency that was attained for the results of the three modelling techniques for all studied biotic elements shows that, although all the pursued techniques are adequate for the data and questions at hand, the impact of the choice of the modelling technique on the results is large. This is even more evident when focusing on the importance of the year that only ranked high, in terms of importance, for the LMM approach. The high degree of inconsistency between modelling techniques demonstrates that any management or conservation decisions that immerge from distinct modelling technique outputs may originate dramatically distinct results. This work clearly shows that such a basin-wide management endeavour, cannot be properly fulfilled looking to just one or two biotic elements and by conducting analysis based on a single technique. The approach to basin-wide management has to be done holistically.

The way how modelled stressor effects behave along other gradients suggest that scale effects must be taken into account when dealing with stressor gradients and interactions. If in a given basin a certain stressor only expresses a portion of its full gradient, only that portion should be considered if the goal is basin management. The scope of the analysis must be in line with the scale of the task ahead. If not, management and conservation decisions may be skewed and not fully effective because they were thought in a way to be effective in portions of the stressor gradient that are never expressed in that particular river basin. Some ecological and biological traits have been shown to disentangle the effects of interacting stressors. So, the response variables elected for analysing multiple stressors should be mechanistically relevant to the stressors (Townsend and Hildrew, 1994; Poff, 1997; Statzner and Beche, 2010; Doledec and Statzner, 2008). Additionally, when looking at several biotic elements with different dispersion abilities, the effect of spatial processes should be considered, although most often they are not reflected in the large spatial scale at which bioassessments are undertaken (Frimpong et al., 2005; Aroviita et al., 2009; Heino, 2013; Alahuhta et al., 2013). Even though standard field protocols have been proved to be able to be used across very large areas (Paulsen et al., 2008), it may be valuable to use concepts such as “extent” and “risk” (for further details see: Paulsen et al., 2008 and Sickle and Paulsen, 2008) that present stressor effects as relative magnitudes or importance across a region.

Because nutrient enrichment stressors and land uses associated with agriculture were shown to have a major overall impact on the target biotic indicators, a big effort should be focused on limiting nutrient loads into aquatic ecosystems in future river management plans of the case study basin. This may be accomplished for example by increasing the efficiency of fertilization practices. A future increase of extreme low flow events are expected in Mediterranean regions according to most global and regional circulation models (IPCC, 2001), with an expected negative impact on biotic quality of rivers. Agriculture may exacerbate this effect through water abstraction and therefore an effort centered on the implementation of more effective irrigation schemes is also recommended.

4.4. Concluding remarks

This work demonstrates the potentialities of coupling process-based modelling with empirical modelling within a single framework that, through model projections under hypothetic scenarios, may help decision making at the basin scale. This is accomplished without loss of spatial resolution because predictions of biotic state may be computed for all river segments in a freshwater system network – while taking into account the effect of the upstream drainage area to all segments, merging Allan (2004) and Fausch et al.'s (2002) view on “riverscapes”. Such an approach facilitates plans of measures to be tested under several climatic and socioeconomic future scenarios, ensuring a cost-effective efficient basket of measures to be deployed depending on future developments, but also to detect best-practices and measures to increase the system resilience to the perceived future changes – acting as a prophylactic against forthcoming threats by present stressors. It further highlights how stressor interaction is still a difficult problem to tackle and how not looking at the full gradient of the stressors while looking at an appropriate response might lead to erroneous conclusions (Branco et al., 2016) and then to disastrous management decisions. Whereas interacting stressors are extremely important, one should not focus management solely on dealing with them, as there are often strong effects rising from isolated stressors. The understanding of the importance of the stressor is paramount. One should look at the effect size, either isolated or interacting, and prioritize management actions according to it.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.scitotenv.2017.12.201.

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APPENDIX 2 - PREDICTING ECOLOGICAL STATUS OF RIVERS AND STREAMS UNDER DIFFERENT CLIMATIC AND SOCIOECONOMIC SCENARIOS USING BAYESIAN BELIEF NETWORKS

Predicting the ecological status of rivers and streams under different climatic and socioeconomic scenarios using Bayesian Belief Networks

*The material on which this chapter is based has been previously submitted in Eugenio Molina-Navarro, Pedro Segurado, Paulo Branco, **Carina Almeida**, Hans E. Andersen Predicting the ecological status of rivers and streams under different climatic and socioeconomic scenarios using Bayesian Belief Networks. Limnologica 2019 (submitted)*

Abstract

Freshwater systems have increasingly been subjected to a multitude of human pressures and the re-establishment of their ecological integrity is currently a major worldwide challenge. Expected future climate and socioeconomic changes will most probably further exacerbate such challenges. Modelling techniques may provide useful tools to help facing these demands, but their use is still limited within ecological quality assessment of water resources due to its technical complexity.

In this work, we aimed to develop a Bayesian Belief Network (BBN) framework for modelling the ecological quality of rivers and streams in two European river basins located in two distinct European climatic regions: the Odense Fjord basin (Denmark) and the Sorraia basin (Portugal). This method enabled us to integrate different data sources into a single framework to model the effect of multiple stressors on several biological indicators of river water quality and, subsequently, on their ecological status. The BBN provided a simple interactive user interface with which we simulated combined climate and socioeconomic changes scenarios to assess their impacts on river ecological status.

According to the resulting BBNs the scenarios demonstrated small impacts of climate and socioeconomic changes on the biological quality elements analysed. This yield a final ecological status similar to the baseline in the Odense case, and slightly worse in Sorraia. Since the present situation already depicts a high percentage of rivers and streams with moderate or worse ecological status in both basins, this means that many of them would not fulfil the Water Framework Directive target in the future. Results also showed that macrophytes and fish indices were the main responsible for a non-desirable overall ecological status in Odense and Sorraia, respectively. The approach followed in this study is novel, since BBN modelling is used for the first time for assessing the ecological status of rivers and streams under future scenarios, using an ensemble of biological quality elements. An important advantage of this tool is that it may easily be updated with new knowledge on the nature of relationships already established in the BBN or even by introducing new causal links. By encompassing two case studies of very different characteristics, these BBN may be more easily adapted as decision-making tools for water management of other river basins.

Keywords: Bayesian Belief Network; Ecological Status; Global change; Rivers; Scenarios; Streams.

1. Introduction

Improving the ecological quality of freshwaters is one of the main environmental challenges. In Europe, waters are affected by an increasing number of pressures (e.g. water abstraction, morphological modifications and diffuse pollution). Climate change may pose an additional threat to waterbodies augmenting the effect of pressures (Kristensen, 2012). The European Union (EU) has shown a strong determination to address this problem, and several policies such as the Nitrates Directive (The Council of the European Communities, 1991) and the Water Framework Directive (WFD) (European Parliament and Council, 2000) have been launched to guarantee the availability of good quality water. Initially, the WFD committed all EU member states to achieve "good" ecological status in all surface waterbodies by 2015. Based on the information reported by Member States in the first River Basin Management Plans (reporting was due at the end of 2009), Kristensen (2012) demonstrated that 56% of rivers and 44% of lakes in the EU had less than good ecological status. Concurrently, Grizzetti et al. (2017) estimated that only 38% the rivers were in a good or high ecological status, using data compiled from these plans compiled by the European Environment Agency from 2004 to 2009. Additionally, environmental monitoring shows that the situation has remained largely unchanged during the last years (Barton et al., 2016). Several authors have thus shown that many water bodies failed to achieve a good ecological status due to multiple stressors, which compromises the integrity of water resources and ecosystems (Grizzetti et al., 2017; Hering et al., 2015; Schinegger et al., 2016). Although some progress has been made, agricultural diffuse pollution and hydromorphological pressures are still threats to many waterbodies (Grizzetti et al., 2017; Tsakiris, 2015). To better address these problems the EU has planned a revision of the WFD by 2019 and postponed the deadline to achieve the ecological status targets by 2027 to give more time to implement the revised WFD version (Hering et al., 2015). This allows for new measures to be discussed in the current river basin management plan cycle (2016-2021), which, in addition, has to consider the potential effects of climate change.

Modelling tools have become essential to assist water managers in the context of bioassessment programmes (Trolle et al., 2012). Empirical modelling is often applied to describe relationships between biotic metrics and stressors with the purpose of finding adequate indicators (Feld et al., 2016). On the other hand, process-based models are important to predict patterns resulting from well-known processes (most often abiotic indicators) (Arnold et al., 1998). Their ability to mechanistically describe and incorporate various ecological processes from different disciplines and their interdependencies, makes them particularly interesting to simulate multiple stressors under different environmental conditions. However, their use is limited within ecological quality assessments: i) they require advanced technical skills and large training effort, and thus are not always appealing to water managers (Kragt, 2009; Phan et al., 2016); ii) they usually require a large data input, especially for calibration, so their application is limited to sites with such data availability (Qian and Miltner, 2015); and iii) most process-based models do not include biological elements, which are required as biotic status indicators by the WFD (Moe et al., 2016).

The incorporation of expert judgment is limited in the abovementioned modelling approaches (Kragt, 2009; Phan et al., 2016). However, it may be useful in some situations, for instance when mechanisms are not well known or when data are not sufficient to run empirical models. Consequently, in recent years, researchers have been working on developing simple but effective modelling approaches to integrate information from different sources (empirical, process-based, expert judgment) and nature (quantitative and qualitative). Among them, there has been a rising interest in the use of Bayesian Belief Networks (BBNs) as tools for ecological and water resources modelling (Barton et al., 2008; Kragt, 2009; Phan et al., 2016).

BBNs, which rely on Bayes' theorem of probability theory to propagate information, are acyclic graphical models representing relationships (links) among variables (nodes) using an underlying probabilistic structure in the form of conditional probability tables (CPTs) that link a given variable (defined in terms of different states) to one or more variables in the system. More information about Bayesian network theory can be found in Kragt (2009). BBNs are able to handle problems associated with high levels of uncertainty and complexity due to their data integration capability. This helps to overcome data limitations, and makes them useful for management purposes (Kragt, 2009; McDonald et al., 2015; Phan et al., 2016). Other advantages of BBNs for water quality modelling include a relatively simple graphical representation, the explicit incorporation of uncertainties, the ability to handle incomplete datasets, and the fact that they can be easily created, updated, modified and extended (Barton et al., 2008; Kragt, 2009; McDonald et al., 2015; McDonald et al., 2016). Furthermore, when compared to existing process-based models, BBN approaches allow to integrate biological elements in ecological status assessment (Moe et al., 2016). Nonetheless, BBNs have some caveats: the inability to model feedback loops, the need for discretising continuous variables, and their validation (Barton et al., 2008; McDonald et al., 2015; Qian and Miltner, 2015). Despite these disadvantages, BBN modelling may prove meaningful to a broad range of users within management of water resources due to the ability to integrate science and management goals as well as to easily communicate complex information, which might facilitate decision-making (Kragt, 2009; McDonald et al., 2015; Phan et al., 2016).

BBN applications for water resources management started in the late 1990s and since then many scientific studies involving this approach have been published. However, despite the continuing advances in BBNs research and development, their actual use remains limited, used mainly by aquatic ecologists and managers for the assessment of river and stream water quality (McDonald et al., 2015). In a systematic review discussing BBN applications in water resources management, Phan et al. (2016) found 111 peer-reviewed research papers on the topic the majority of which (42%) dealing with water quality management. Besides, the authors pointed out a lack of BBN studies on international scales and only a few explicitly designed to explore the potential impacts of climate change on water quality. Among them, Dyer et al. (2014) aimed to determine the effects of climate change and river regulation on water quality; Nojavan et al. (2014) modelled eutrophication in an estuary under climatic and nutrient pollution management scenarios; and Couture et al. (2018) and Moe et al. (2016) have assessed the combined effect of land use and climate changes on lake ecological status. To the best of our knowledge, BBN modelling has not yet been used to evaluate the impact of combined climate and socioeconomic scenarios on the ecological status of streams and rivers.

Our study aims at developing a BBN framework for stream and river water quality modelling (in the following referring to as river), taking as case studies two climatically different river basins that share commonalities in the typology of stresses potentially interacting to affect their ecological quality: the Odense Fjord basin (Denmark) and the Sorraia basin (Portugal). Climate and socioeconomic changes are likely to interact with the stressors present at these basins with uncertain consequences (Kristensen, 2012). We believe that a BBN approach will be valuable for converting large datasets into a simple and fast prognostic tool for supporting river basin managers in decision making processes focused on river ecological status, providing a user-friendly graphical tool to assess the impact of climate and socioeconomic scenarios on river ecological status.

To achieve these goals, we designed a BBN model for both basins based on their characteristics, main pressures and previous knowledge, following a Scenarios – Stressors – Indicators – Status approach. Different data sources (measured, modelled and expert knowledge) were integrated to simulate the effect of multiple stressors on the ecological status of rivers, using several indices to provide a complete status assessment. Within the BBN, we integrated several modelling tools (process-based and empirical), achieving a more holistic outcome (Phan et al., 2016). Subsequently, we simulated climate and socioeconomic scenarios demonstrating their impact on river water quality, specifically on its ecological status.

2. Methods

2.1 Case-study areas

2.1.1 Odense Fjord basin

The Odense Fjord basin is located in the island of Funen (Denmark), with an area of approximately 1,100 km^2 (Fig. 1A**Fig**). The climate is oceanic with an annual mean temperature of 8.7 °C (2000–2010), with monthly mean temperatures ranging from 1 °C in January and 17 °C in July. Mean annual precipitation is 812 mm (2000-2010), with no pronounced seasonality. Agriculture is the main land use (68%), followed by urban areas (16%) and forest (10%). The main city in the basin is Odense with 187,000 inhabitants. Aquatic ecosystems in the basin include lakes, rivers and transitional waters. In spite of several action plans, many of these waters fail to meet the Water Framework Directive targets, having 58% of the streams (km) and 82% of the lakes (larger than 5 ha) a moderate or worse status (Table 1, data for streams have to be seen with caution because for most of the streams only one biotic indicator was considered). Water quality in the basin is conditioned by urbanization, hydro-morphological modifications (including channelization and tile draining in about half of the agricultural area), occasional summer droughts and groundwater abstraction drying out headwater streams, and fertilizers and pesticides from agriculture. More details on the study area characteristics can be found in Thodsen et al. (2015) and Molina-Navarro et al. (2018).

2.1.2 Sorraia basin

The Sorraia basin occupies an area of 7,730 km^2 in Central Portugal and flows along a length of 155 km (Fig. 1B). It merges with the river Tagus at the estuary and is the Tagus tributary with the largest basin area. The climate is Mediterranean with an average annual air temperature of 15.2 °C that ranges from 21.6 °C in the summer to 9.4 °C in the winter. The mean annual precipitation is around 600 mm, ranging from 25 mm in summer months to 70 mm in winter months. Approximately 41% of the basin area of the Sorraia is forest, 28% range-grasses, 17% agriculture, 9% pine, 2% orchard, 2% urban and industrial and 1% pasture (Mateus et al., 2009). It includes one of the largest area of irrigated crops in Portugal, with a total area of 15,500 ha. The presence of two large reservoirs in the basin affects flow patterns and runoff downstream. Additionally, the natural flow is substantially reduced by water abstraction for irrigation. The Sorraia watershed has a total of 153,000 habitants (INE, 2011) with a density of 20 hab/km^2, mainly concentrated in three core areas: Ponte de Sôr, Samora Correia and Coruche. It has only minor issues regarding urban pollution and urban wastes. Among 122 water bodies (essentially rivers), the ecological status in 24% of them is moderate or worse (Table 1). The main cause of poor or failing status in the basin is the water abstraction for agricultural purposes. On average, 16,500 hectares are irrigated with a total water volume of $120 \cdot 10^3$ m^3 per year. Water abstraction for irrigation in the Sorraia basin is the highest within the Tagus River basin region (26% of total need). Nutrient loads from agriculture, livestock and urban origin, mainly in the alluvial valley, are also important potential causes of poor status in the basin.

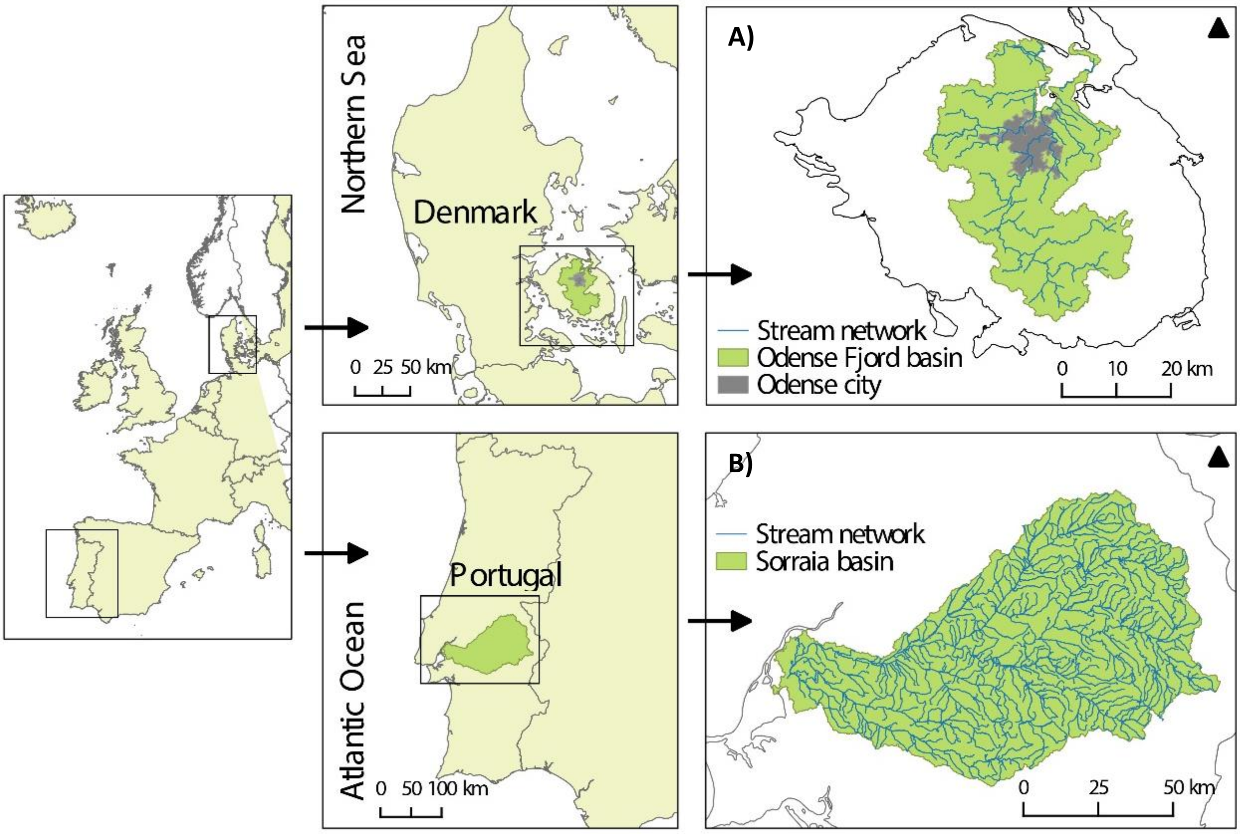

Fig.1. Location of the (A) Odense Fjord and (B) Sorraia basins and their river networks

Table 1. Ecological status reported in the Odense Fjord (Miljø- og Fødevareministeriet, 2017) and in the Sorraia basins (APA, 2012) (H: High, G: Good, M: Moderate, P: Poor, B: Bad, U: Unclassified).

	Ecological status (num. and % of water bodies)					
	H	**G**	**M**	**P**	**B**	**U**
Odense basin (streams*)	40 (7%)	173 (29%)	210 (35%)	104 (17%)	35 (6%)	38 (8%)
Odense basin (lakes)	0 (0%)	2 (12%)	3 (18%)	5 (29%)	6 (35%)	1 (6%)
Sorraia basin	0 (0%)	54 (44%)	15 (12%)	12 (10%)	2 (2%)	39 (32%)

* Numbers and % refer to km of streams.

2.2 Data sources and pre-processing

Data used to feed the BBN came from both process-based models and from national biomonitoring programmes, collected in the context of the implementation of the Water Framework Directive. To simulate stressors related to hydrology and nutrients, process-based catchment models already implemented with the Soil and Water Assessment Tool (SWAT; Neitsch et al., 2005) were used (for further details see Almeida et al., 2018; Molina-Navarro et al., 2017, 2018; Segurado et al. 2018). Additionally, SWAT was also employed to simulate stressors under different future climatic and socio-economic scenarios.Other stressors in the Sorraia case included land use, which was derived from the CORINE landcover database (European Environmental Agency, 2010) as the percentage area in the whole upstream catchment; river slope, derived from the CCM2 river network database (Vogt et al., 2007); and mean annual temperature, derived from the same climatic models used in the scenario settings (see next section).

Empirical or statistical models (Feld et al., 2016) were used prior to this study to identify and quantify the statistical relationships between the stressors and the biotic indicators. Empirical models developed for the Odense Fjord case study used data from a national Danish streams dataset, which contains measured data from 131 streams (Ferreira et al., 2016). For the Sorraia River case study, to encompass a broader environmental gradient, the empirical modelling was based on a database for the whole Portuguese Tagus basin comprising 240 records from the Water Frame Directive biomonitoring program (Portuguese Environmental Agency, APA), corresponding to 141 sampling sites with two sampling occasions for most sites (2010-11) (Segurado et al., 2018). Results obtained with both process-based and empirical models assisted in the construction of the BBNs, as described in section 2.4.

2.3 Scenarios settings

In both study cases, scenarios were developed under the socio-economic storylines adopted in the MARS Project (www.mars-project.eu). The storylines adopted were the following (Faneca-Sanchez et al., 2015): (1) a "Techno World" (TW) that represents a rapid global economic growth, enabling technological development but with high energy demands and no real drive to specifically enhance or ignore natural ecosystem health; (2) a "Consensus World" (CW) representing a world where current policies continue after 2020, economy growing at the same pace as now, with awareness for environment preservation; (3) a "Fragmented World" (FW) world represents "survival of the fittest" world driven by countries own interests, with fast economic growth in NW Europe but decrease in other regions, with minimal or no investment and effort in environmental protection, conservation and restoration.

Storylines were incorporated in SWAT to run the future climatic and socio-economic scenarios. First, they were downscaled for each basin by applying expert judgement while taking into account their specificities in terms of dominant land use and socio-economic contexts (Table 2). In the Odense basin, downscaling was focused on farming, since agriculture is the dominant land use (68% of the area). In the Sorraia basin, minor changes in urban areas were also considered. More information on the storylines' downscaling regarding land use and socio-economy and how it was applied within the SWAT model can be found in Almeida et al. (2018) and Molina-Navarro et al. (2018). Regarding climate, different Representative Concentration Pathways (RCPs) were assigned to each storyline: the RCP 8.5 (rising scenario with very high greenhouse gas emissions) was assigned to storylines TW and FW, since both consider fast growing economies and fossil-fuelled development; and the RCP 4.5 (stabilization emission scenario) was assigned to the storyline CW, which considers regulations to save energy in favour of reducing emissions (Faneca-Sanchez et al., 2015).

Climate scenarios produced by the ISI-MIP project (www.isi-mip.org) were applied in this study, namely the IPSL-CM5A-LR model in the Odense case-study and the GFDL-ESM2M model in the Sorraia case-study, considering both the RCP 8.5 and RCP 4.5 emission scenarios. These models were selected because they yielded the best median output regarding cumulative precipitation relative to observations in each study area (MARS internal document "Choice of the Climatic Model for MARS case studies", unpublished). The future time horizons for scenarios simulations were 2030 (interval 2025-2034) and 2060 (2055-2064) (Faneca-Sanchez et al., 2015). Baseline scenarios were produced for the period 2011–2020 using the same climatic models to allow a comparison among the different time periods. ISI-MIP climate data at a 0.5º resolution was downloaded for the grid points closest to each basin and bias-corrected with measured data (temperature and precipitation in both study areas, and additionally solar radiation, humidity and wind speed in the Odense basin). Then, data was used as input in SWAT to run the scenarios previously described (Table 2). More details can be found in Almeida et al. (2018) and Molina-Navarro et al. (2018).

Besides the abovementioned future time horizons and baseline period, additional scenarios were run with recorded climatic variables for the period 2001-2010 (OBS) to account for the isolated effects of land use changes (LUC), including a fourth baseline scenario with present land use (PLU). For the Sorraia basin we only considered the changes set for 2060 time horizon.

Table 2. Future scenarios considered in the Bayesian Belief Network models and downscaling of storylines for the two case studies. For land use, the values correspond to the predicted percentage of the total basin area. For the remaining parameters, the percentage change is shown (except temperature in °C change) (PLU: Present Land Use, TW: Techno World, CW: Consensus World, FW: Fragmented World, RCP: Representative Concentration Pathway, IPSL: IPSL-CM5A-LR climate model, GFDL: GFDL-ESM2M climate model).

Scenarios	Baseline (PLU)	TW 2030	TW 2060	CW 2030	CW 2060	FW 2030	FW 2060
a) Both basins							
Emission scenarios	RCP4.5 RCP8.5	RCP8.5	RCP8.5	RCP4.5	RCP4.5	RCP8.5	RCP8.5
Years	2011-2020	2026-2035	2056-2065	2026-2035	2056-2065	2026-2035	2056-2065
b) Odense Fjord basin							
Climatic Model	IPSL	IPSL	IPSL	IPSL	IPSL	IPSL	IPSL
Precipitation	-	+5.6%	+13.2%	+0.6%	+1.9%	+5.6%	+13.2%
Temperature	-	+1.0°C	+2.7°C	+0.8°C	+1.6°C	+1.0°C	+2.7°C
Animal manure*	-	-0.2%	-0.2%	-0.5%	-0.5%	+15.0%	+15.0%
Artificial fertilizer*	-	-3.7%	-3.7%	-3.5%	-3.5%	+44.0%	+44.0%
Pig farms	44%	35%	35%	29%	29%	52%	52%
Cattle farms**	15%	12%	12%	11%	11%	15%	15%
Mixed farms	15%	11%	11%	9%	9%	15%	15%
Permanent grass	2%	5%	5%	15%	15%	2%	2%
Forest	10%	10%	10%	21%	21%	2%	2%
Willow	-	13%	13%	-	-	-	-
c) Sorraia basin							
Climatic Model	GFDL	GFDL	GFDL	GFDL	GFDL	GFDL	GFDL
Precipitation		-39%	-42%	-37%	-43%	-39%	-42%
Temperature		+0.8°C	+1.0°C	-0.9°C	+0.3°C	+0.8°C	+1.0°C
Fertilization	-	+10%	+15%	-10%	-15%	+30%	+35%
Irrigation	-	-10%	-15%	-20%	-25%	+30%	+35%
Agriculture	33.62%	37.9%	41.4%	29.6%	25.60%	39.9%	41.4%
Irrigated crops	4.26%	5.1%	5.9%	3.7 %	3.0%	5.1%	5.9%
Urban areas	0.51%	0.51%	0.52%	0.50%	0.49%	0.51%	0.52%

**Changes applied in manure and fertilizer application rates for Odense are averages weighted by farm type area. More details can be found at Molina-Navarro et al. (2018)*

***Total surface of cattle farms does not change in the FW storyline in Odense, but the surface of cattle farms with low fertilization decreases, while the surface of those with high fertilization increases (see Molina-Navarro et al. (2018) for further details)*

2.4 Construction of the Bayesian belief network

2.4.1 Structure of the model

The BBN models were based in a multiple stress cause-effect framework, evaluating the impacts of land use, agricultural management and climate change on both physical and chemical variables. These variables acted in turn as stressors for the biological variables that indicate the ecological status of the rivers in the basins, expressed by biotic quality indices following the EU Water Framework Directive criteria (WFD - European Parliament and Council, 2000). The BBN models comprised five main components, from parent to child nodes: (1) climate change scenarios and socio-economic storylines, (2) stressors (modelled data) or proxies (land use), (3) natural environmental background (measured data, only for Sorraia basin), (4) biotic indicators (measured data) and (5) biotic state (model output) (Fig. 2). The BBN models were designed with the software GeNIe, created by BayesFusion and freely available for academic and scientific use (bayesfusion.com/genie, BayesFusion LLC, 2019).

In both case studies, stressors related with the hydrological regime and nutrient loads were considered as the most relevant to be included in the BBN model. For the Odense Fjord basin case study, four hydrological and two nutrient stressors were included, while for the Sorraia basin case study, three hydrological and one nutrient stressors were considered (Table 3, Fig. 2). All hydrological and nutrient stressor variables were derived from SWAT simulations for each scenario at the sub-basin level. Output variables such as total flow, groundwater flow or nutrient concentrations at a daily time-step were extracted from the reach output file (output.rch) and the stressors were calculated as described in Table 3. Hydrological stressors were mainly descriptors of low or high flow events, although each case study used different metrics because of inherent river basin specificities. In the BBN model for the Sorraia basin, given an overall stronger environmental gradient in comparison to the Odense Fjord basin, there was the need to consider the variability in the data induced by land use, climate and hydromorphology. Therefore, three land use variables, temperature and river slope were also included in the BBN model (see section 2.2 for data sources). Values of these stressors for future scenarios were obtained as described in Table 2, except for river slope which does not change in future storylines. Indeed, in the Sorraia basin, land use variables were previously shown to have a strong effect on biotic quality, probably acting as proxies of several interacting individual stressors (Segurado et al., 2018). In the Odense Fjord basin case, total nitrogen concentration was included as an output node even though it was not identified as a significant stressor for predicting biotic status in the Odense Fjord basin. Thus, it is not linked with the indicators level in the BBN model, but we consider it relevant since it might serve as a chemical water quality proxy.

Table 3. Variables selected in the Bayesian Belief Network modelling for (a) the Odense Fjord basin and (b) the Sorraia basin, and (c) both basins.

Stressor/variable	Description
a) Odense Fjord basin	
BFI	Baseflow index, defined as baseflow volume divided by total volume
Q90	Flow below the 90^{th} percentile* of the flow-duration curve divided by median flow (Q_{50})
FRE25	Annual frequency of flow events above the 25^{th} percentile of the flow-duration curve**
DUR3	Annual duration of extreme flow events three times above the flow at Q_{50} (days)
TP	Annual mean concentration of total phosphorus (mg/L)
b) Sorraia basin	
AGRIC	% area of agriculture in the upstream basin
IRRIG	% area of irrigated crops in the upstream basin
URBAN	% area of urban areas in the upstream basin
LFLOWD	Mean annual duration of low flow events - periods during which the daily mean flow falls below the 10th percentile of the mean annual discharge (days)
LFLOWN	Mean annual frequency of low flow events (number of events)
FLOWA	% of change in flow in relation to the free running river (no barriers)
SLOPE	River slope (%)
TEMP	Mean annual temperature (ºC)
c) Both basins	
TN	Annual mean concentration of total nitrogen (mg/L)

* 90^{th} percentile = the flow value that is exceeded 90 % of the time, i.e. a low flow indicator.

** 25^{th} percentile = the flow value that is exceeded 25 % of the time, i.e. a high flow indicator.

Regarding indicators, biotic quality status indices were included and expressed as Ecological Quality Ratios (EQR, observed index divided by its value in reference conditions) and then translated into ecological status classes (bad, poor, moderate, good or high), following the WFD. Each EQR was represented by a node in the BBNs. For Odense Fjord basin, the DFFV for fish (Danish Fish Index for Streams; Kristensen et al., 2014), DVPI for macrophytes (Danish Stream Plants Index; Larsen and Baattrup-Pedersen 2015), and DVFI for macroinvertebrates (Danish Stream Fauna Index; Larsen et al., 2014) were the indices selected; whereas for Sorraia river basin the indices were: IPS for phytobenthos (Indice de Polluosensibilité Sécifique; Almeida et al., 2014; Cemagref, 1982), IBMR for macrophytes (Macrophyte Biological Index for Rivers; Aguiar et al., 2014; Haury et al., 2006), IPtI for macroinvertebrates (Rivers Biological Quality Assessment

Method - Benthic Invertebrates; Feio et al., 2014; Ferreira et al., 2008) and F-IBIP for fish (Fish Index of Biotic Integrity for Portugal; INAG and AFN, 2012; Segurado et al., 2014). A final node combining the ecological status classes given by the biotic quality indicators, following the "one out all out" principle established in the EU Water Framework Directive (Van de Bund and Solimini, 2007), closed the network. Using this principle, the final overall ecological status class is assigned according to the poorest ecological status class among the different biotic quality indicators. The link structure between stressors/land use/environmental background nodes and biotic indicator nodes were defined essentially according to the relationships found in the corresponding empirical models (Ferreira et al., 2016; Segurado et al., 2018). A node with all scenarios used to run SWAT was used as the parent node of each stressor and as the parent node for the climatic scenarios node and the storylines node (Fig. 2).

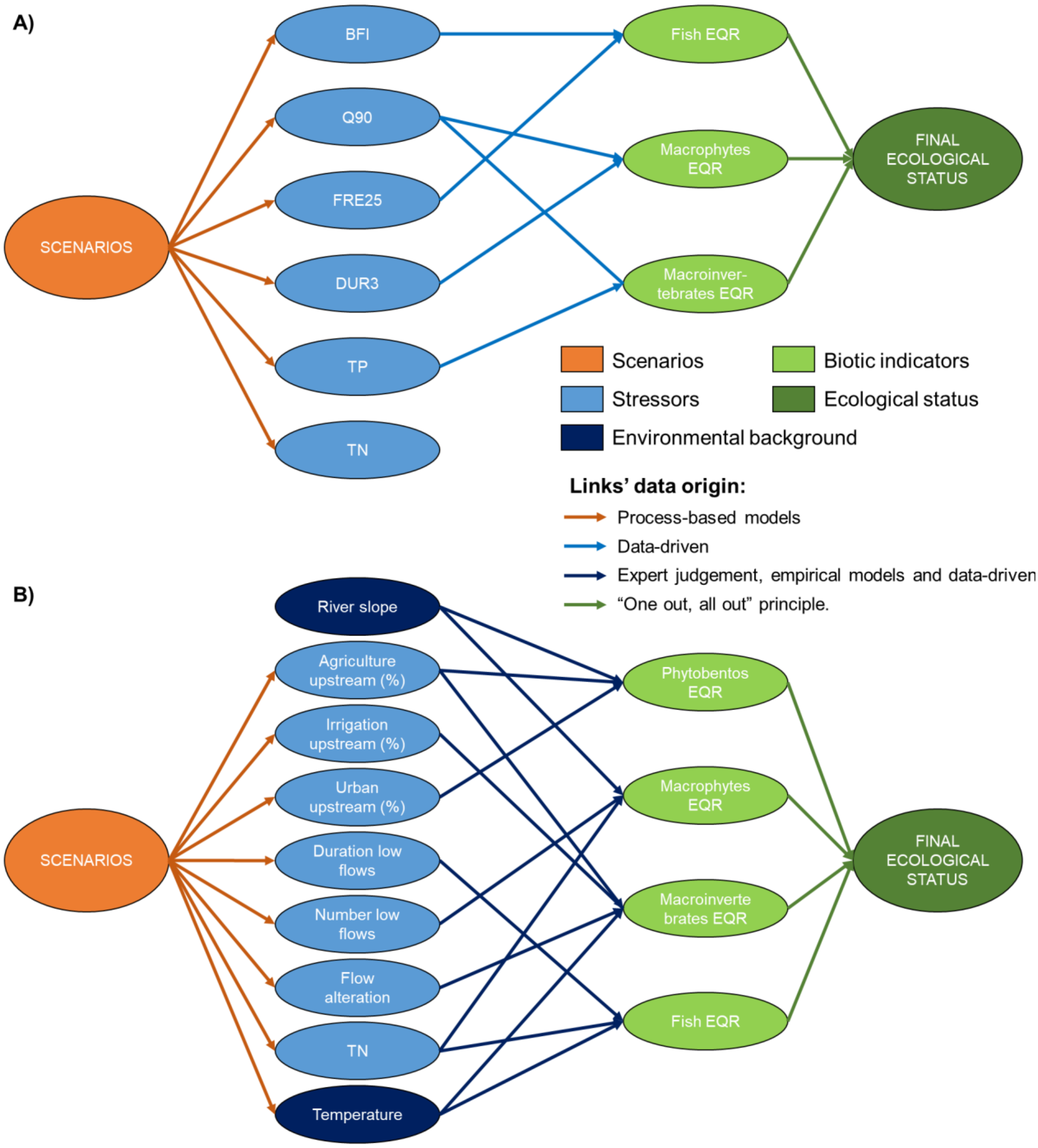

Fig. 2. Bayesian Belief Network scheme for the Odense Fjord basin (A) and the Sorraia Basin (B) (EQR: Ecological Quality Ratio, for other acronyms please see Table 3).

2.4.2 Class boundary definition

Once the structure of the network was designed, the variables represented in network nodes needed to be discretized. Three levels, "Low", "Medium" and "High", were defined for every stressor (Appendix A, Table S1). The absolute boundaries (lower boundary for "Low" and higher boundary for "High") were determined taking into account the whole dataset for each basin. In this way, the boundaries represent a whole range of field conditions that can determine the subsequent indicator values (conditional probabilities between stressors and indicators are also obtained from the national dataset, due to lack of observed data in the Odense basin, as explained later). Then, the discretization into three clases was done using the "Uniform counts" tool in GeNIe, which creates three classes with the same number of cases each. In the case of the Sorraia Basin the class borders were further adjusted towards the inflection points of EQR partial response curves derived from the empirical models. The class boundaries of biotic indicators were based on the official quality boundaries of the biotic quality indices (Aguiar et al., 2014; Almeida et al., 2014; Feio et al., 2014; Kristensen et al., 2014; Larsen et al., 2014; Larsen and Baattrup-Pedersen, 2015; Segurado et al., 2014) between the "poor" and "moderate" classes and between this and the "good" class. We therefore considered three classes: "Poor/Bad" (PB), "Moderate" (M) and "High/Good" (HG). The same classification was adopted for the overall biotic status classification in the final node.

2.4.3 Conditional probability tables

Conditional probability tables (CPT) define the links or dependencies of each child node to parent nodes. The CPT linking scenarios to stressors were based directly on the outputs from SWAT simulations. The correspondence between each biotic quality indicator (EQR) classes and the overall biotic status classes was also deterministic, based on the "one out all out" principle. In the Odense case-study conditional probabilities linking stressors with biotic indices were derived from the national Danish streams dataset (see 2.2). Denmark as a whole is a lowland country (Windolf et al., 2011), hence with a relatively narrow environmental gradient, so the use of a national dataset might represent no concern in this sense. For the macrophytes index, two stressor-indicator classes combinations had no data available (low DUR3 -Annual duration of extreme flow events three times above the flow at Q_{50}- and low Q90 - flow below the 90th percentile* of the flow-duration curve divided by median flow (Q_{50})-; high DUR3 and high Q90). Probabilities of the closest neighbour combination were assigned in these cases, following Moe et al. (2016). The ecological status classes had a 1:1 correspondence with the indicator classes. In the Sorraia case-study the construction of the conditional probability tables linking stressors, land use and environmental background to biotic indicators were based on an expert judgement partially informed by the effect sizes and partial responses given by empirical models. The parameters were then learned with biomonitoring data from the year 2010. All the CPTs are available in Appendix A, Tables S2-S4.

2.4.4 Model validation

Probability predictions of stressors from scenarios rely on process-based SWAT models that were already calibrated and validated (Ferreira et al., 2016; Molina-Navarro et al., 2017; Segurado et al., 2018). Similarly, the choice of which stressors are influencing each indicator was based on their statistically significance within empirical models (Ferreira et al., 2016; Segurado et al., 2018). However, these empirical models included more stressors than the BBNs, which are more simplistic, so an additional validation of BBN probability results is desirable. Data-driven validation was done in both study cases, but different approaches were followed due to different availability of independent real data to validate with.

In the Odense Fjord basin, real data for validation was available from the latest Odense Fjord basin management plans, but only as ecological status classes in the rivers, not EQR values. The first basin plan only provides ecological status for macroinvertebrates (Miljøministeriet, 2011), while the second one provides classes for the three Biotic Quality Elements (BQE; Miljø- og Fødevareministeriet, 2016, 2017). The BBN was validated comparing the probability distribution for ecological status classes calculated by the BBN for the present land use (PLU) scenario run with observed (2001-2010) climate data (PLU_OBS) with the data published in those management plans.

In the Sorraia basin case study, however, measured data for the year 2011, not used in the BBN construction, were available for both stressors and BQE´s and EQRs. Data driven validation was performed by using 2011 data to construct new CPTs for the stressors nodes and predict class probabilities of the EQR for each BQE and the final biotic quality. These predictions were then compared with real EQR classes and resulting biotic quality from the 2011 biomonitoring data.

2.5 BBN modelling

The BBNs allowed to model the resulting class probability distributions for the overall biotic status and for each BQE for each scenario by first setting the corresponding evidence in the scenarios node and updating the beliefs. First, the effects of isolated LUC were evaluated comparing the present land use scenario (PLU_OBS) with the three storylines (techno world LUC, consensus world LUC and fragmented world LUC), all of them ran with observed climate (2001-2010). Running these scenarios allows addressing the next step, modelling combined land use and climate change scenarios, and guarantees an appropriate discussion of the future storylines results, since when analysing combined climate and LUC scenarios, the signals of the first are often masked by the effects of the second (Dyer et al., 2014). Then, in both case studies, the effects of future storylines were analyzed comparing the probabilities obtained in the scenarios with their respective baselines. For both case studies, the response of biotic indicators were modelled for the years 2030 and 2060 under different combinations of climate scenarios and storylines, comparing the probabilities obtained for each scenario with their respective baselines. Additionally, BBNs were kept as simple as possible to present the simplest form (Marcot, 2012; McDonald et al., 2015) as a large number of model nodes does not necessarily guarantee a lower uncertainty (Barton et al., 2008). Marcot et al. (2006) recommend keeping the number of parent nodes to three or fewer to limit the size of the CPTs.

3. Results

3.1 BBNs Validation

Figures 3 and 4 show the validation results for Odense and Sorraia cases, respectively. For both case studies, BBN predictions tend to underestimate the High/Good class probability and overestimate the Poor/Bad in most cases. The exception in both case studies is an underestimation of the Poor/Bad class in the case of the fish indices.

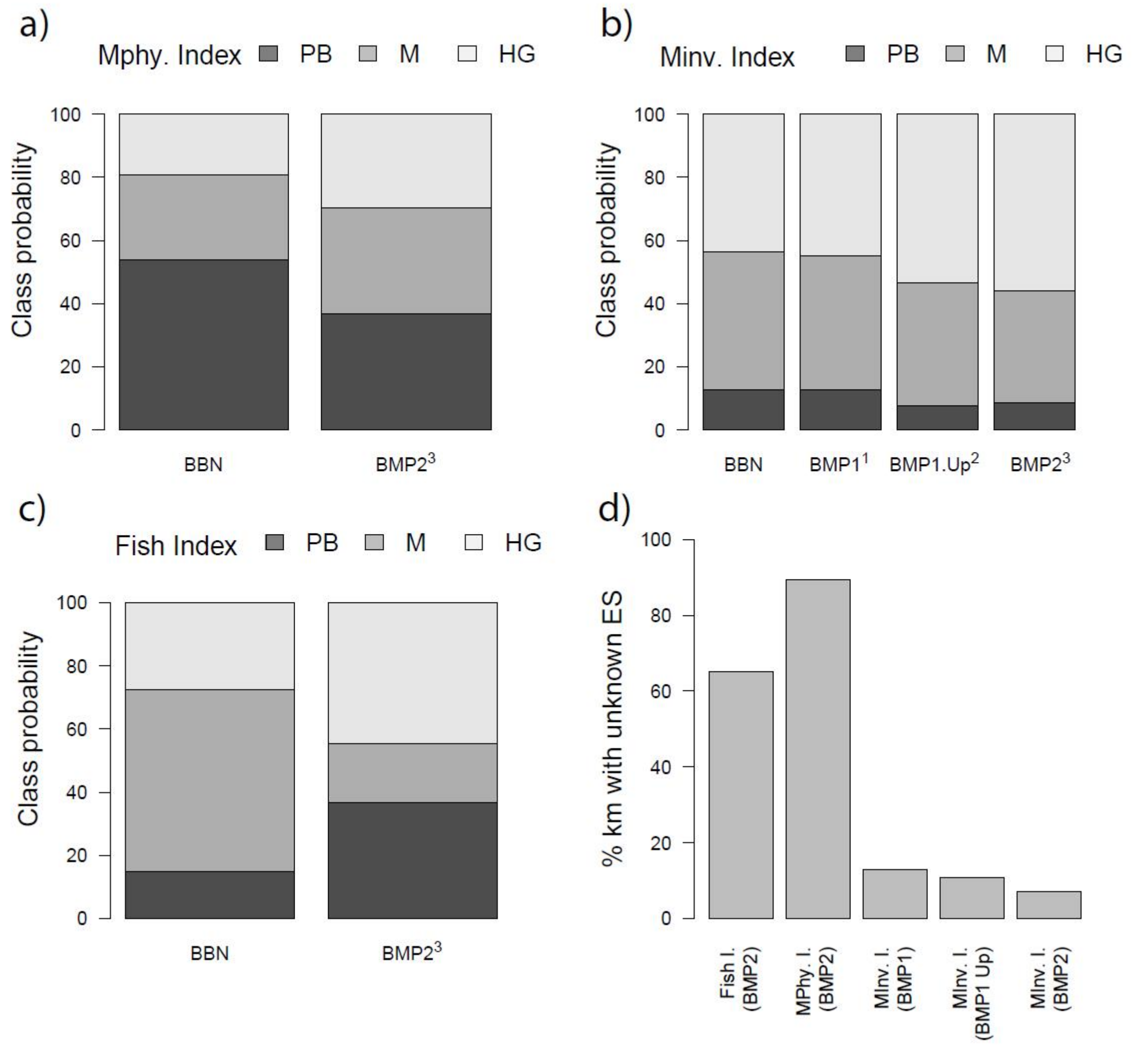

Fig. 3. Modelled (Bayesian Belief Network, BBN) and observed (BMP, Basin Management Plan) probability distribution of biotic status classes (PB: Poor/Bad, M: Moderate, HG: High/Good) in the Odense Fjord basin for fish (a), macrophytes (Mphy., b) and macroinvertebrates (Minv., c) indices, and percentage of river length without information for the observed data (d) (I.=index). [1] Data from the first Odense Basin Management Plan (2010-15, includes data from 2003-10, Miljøministeriet, 2011). [2] Data from the first Odense Basin Management Plan updated in 2013 (median from 01-2008, GIS corrected for the SWAT delineated basin; Miljø- og Fødevareministeriet, 2017). [3] Data from the second Odense Basin Management Plan (2015-2021, includes latest data up to 2012 -2013 for fish-, GIS corrected for the SWAT delineated basin; Miljø- og Fødevareministeriet, 2016, 2017).

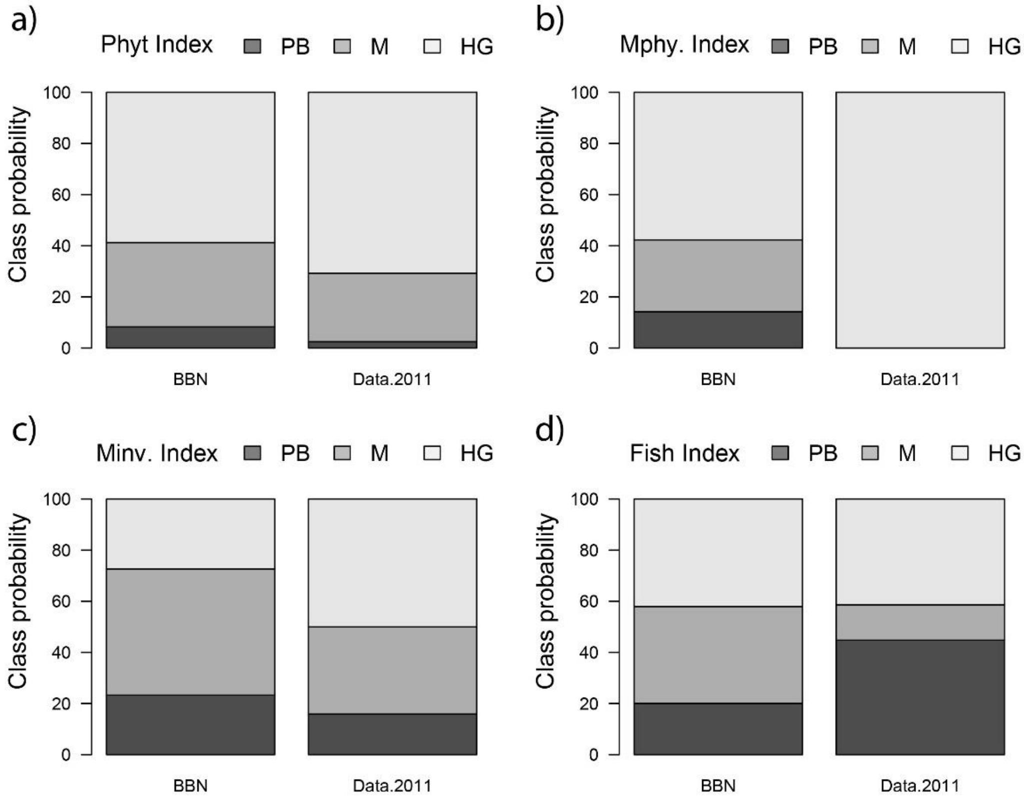

Fig. 4. Probability distribution of biotic status classes (PB: Poor/Bad, M: Moderate, HG: High/Good) estimated by the Bayesian Belief Network (BBN) using probability distributions of stressors derived from the 2011 biomonitoring data vs. observed biotic status classes in 2011 for phytobentos (Phyt., a), macrophytes (Mphy., b), macroinvertebrates (Minv., c) and fish (d) indices in the Sorraia basin.

3.2 BBN modelling: Scenario´s simulation results

Isolated Land Use Change (LUC) scenarios

The probability distributions of different biotic status across LUC scenarios were very similar in both basins, showing very subtle variations (Figs. 5 and 6). In the Odense basin, the macrophyte index showed slight differences: the probability of Poor/Bad status decreased in the techno world LUC scenario, increasing the probabilities of Moderate and High/Good status. Changes in other scenarios, however, were minor (Fig. 5a). For the macroinvertebrate index, probability distributions across scenarios were similar (Fig. 5b). Regarding the fish index, the biotic status slightly moved towards the extreme classes in techno world LUC (mainly towards High/Good) and in consensus world LUC (mainly towards Poor/Bad), while it moved to the moderate status in fragmented world LUC (Fig. 5c). Probability distributions for the final ecological status classes remained very similar across scenarios (Fig. 5d).

Regarding stressors, isolated LUC scenarios showed a very noticeable impact on TN (Annual mean concentration of total nitrogen (mg/L)) probability distribution. Probabilities of low and, especially, medium TN levels increased in techno world LUC and consensus world LUC, decreasing drastically the probability of high TN (Appendix A, Figure S1-A). The opposite trend was observed in fragmented world LUC, in which high TN probability became 100%.

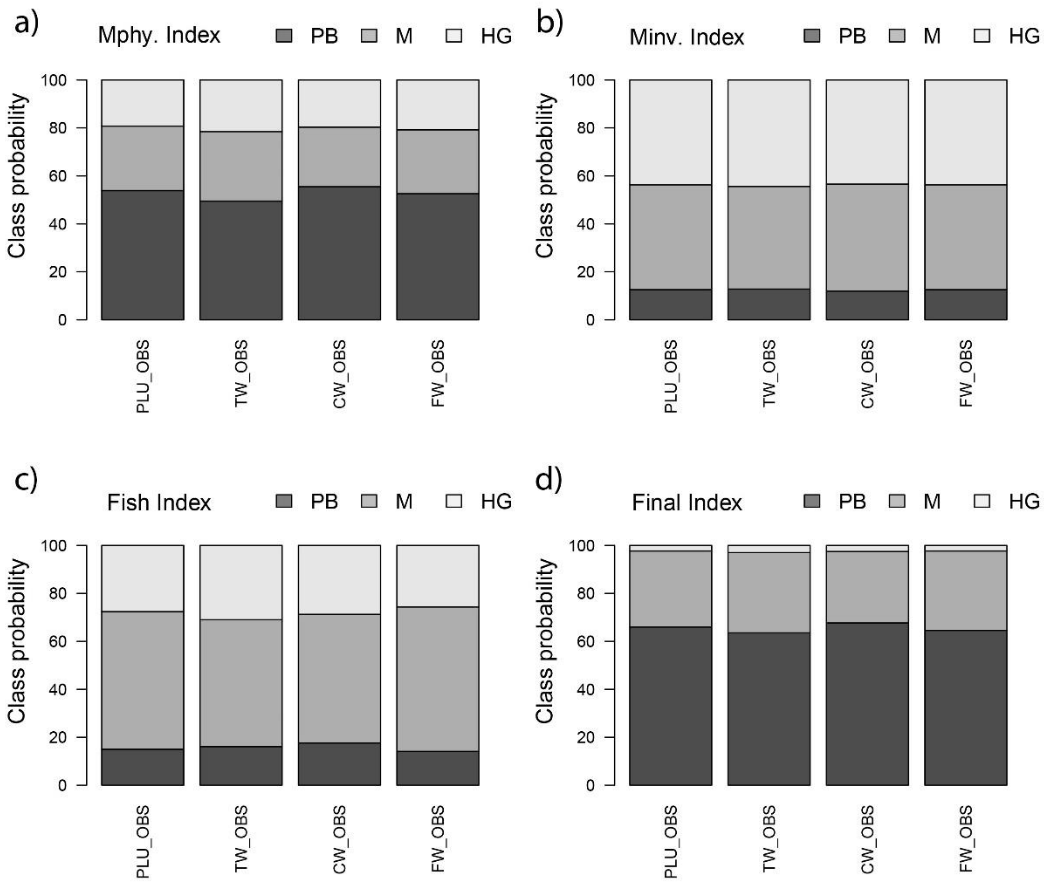

Fig. 5. Probability distributions (%) of biotic status classes (PB: Poor/Bad, M: Moderate, HG: High/Good) for the macrophytes (Mphy., a), macroinvertebrates (Minv., b), and fish (c) indices and of final ecological status classes (d) in the different land use change scenarios in the Odense Fjord basin under observed (OBS, 2001-2010) climate (PLU: Present Land Use, TW: Techno World, CW: Consensus World, FW: Fragmented World).

In the Sorraia basin, except for macrophytes, BBN projections showed an increase of Poor/Bad class probability and a decrease of High/Good status classes for the techno world LUC and the fragmented world LUC scenarios (Figs. 6a, 6c and 6d). In the case of macrophytes, a very slight decrease of Poor/Bad class probability and increase of the High/Good status classes for the techno world LUC and the fragmented world LUC scenarios was predicted (Fig. 6b). For all ecological quality indices, there was a slight decrease of the Poor/Bad and a slight increase of the High/Good status classes for the consensus world LUC scenario. The variation of the final ecologic status followed the same overall trend as most indices of each biotic quality element (Fig. 6e).

Regarding stressor predictions in the Sorraia basin, isolated LUC scenarios showed noticeable impacts on Total N and on the mean annual duration and number of extreme low flow events. Probabilities slightly shifted towards high class for the techno world LUC and the fragmented world LUC scenarios and markedly shifted towards low TN for the consensus world LUC scenario (Appendix A, Fig. S1-B). Marked increase of the intermediate probability class and decrease of mean annual duration of extreme low flow events were predicted for the techno world LUC and the fragmented world LUC scenarios. An increase of the low probability class of mean annual number of extreme low flow events was found for the three land use change scenarios, in an increasing order from the techno world LUC scenario to the fragmented world scenario (Appendix A, Fig. S1-B).

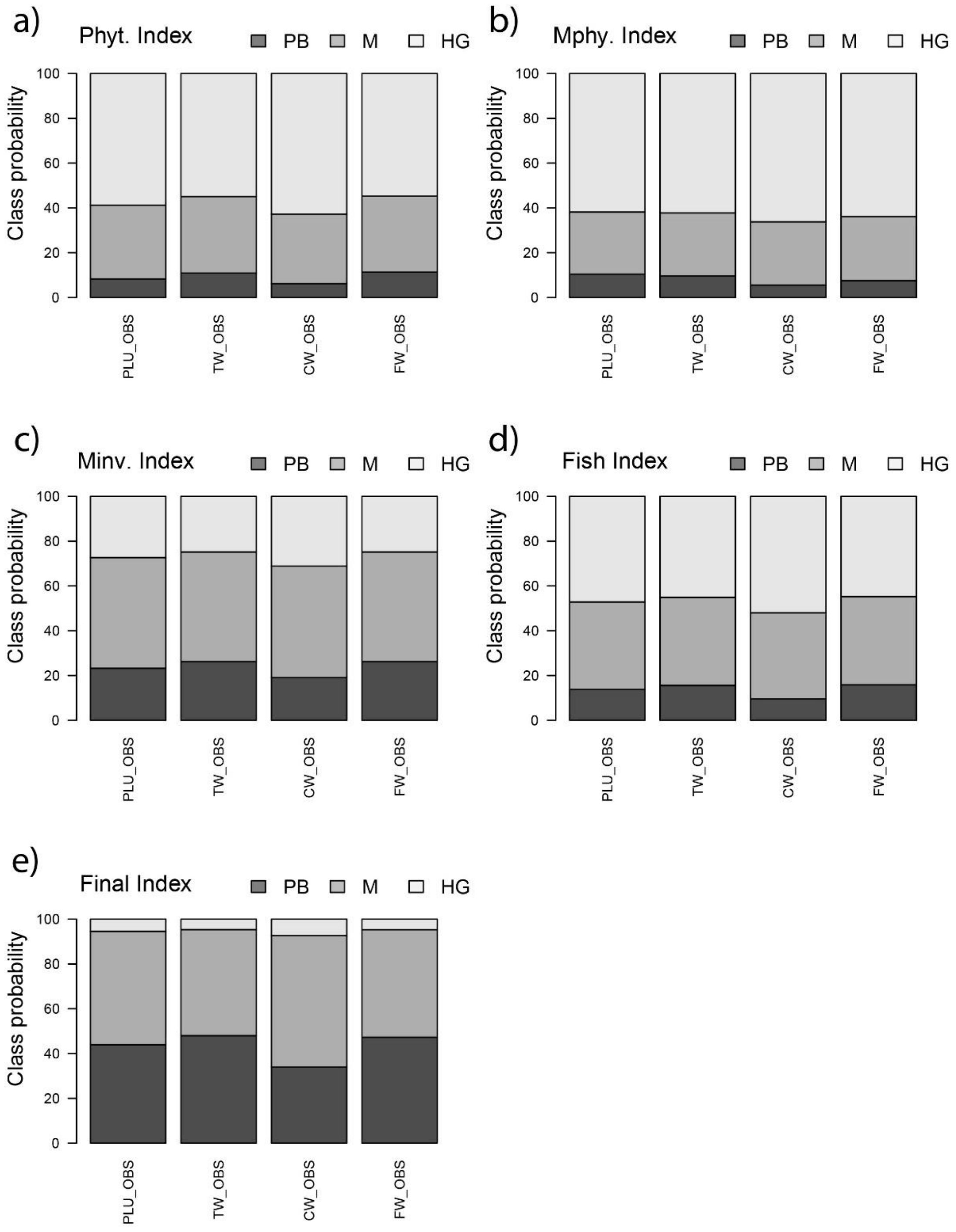

Fig. 6. Probability distributions (%) of biotic status classes (PB: Poor/Bad, M: Moderate, HG: High/Good) for the phytobentos (Phyt., a), macrophytes (Mphy., b), macroinvertebrate (Minv., c) and fish (d) indices and of

final ecological status classes (d) in the different land use change scenarios in the Sorraia basin under observed (OBS, 2001-2010) climate (PLU: Present Land Use, TW: Techno World, CW: Consensus World, FW: Fragmented World).

3.3 MARS storylines

Similarly to isolated LUC scenarios, the probability distributions of biotic status classes for the different scenarios remained quite stable across MARS storylines for most of the indices in both study areas. The most noticeable differences in class probabilities were observed in the macrophyte index for the Odense basin and in the fish and overall indices for the Sorraia basin (Figs. 7 and 8).

In the Odense Fjord basin, probability variations in the macrophyte index were especially relevant for the 2060 horizon (Fig. 7a). In techno world and fragmented world scenarios, High/Good status probability increased, while probabilities of Moderate and Poor/Bad status decreased, and vice-versa for consensus world (M remained stable). The effects of scenarios observed for the Danish macroinvertebrate index probabilities were neglectable (Fig. 7b), while the general trend for the fish index in the future storylines was an increase of probability of High/Good status and a decrease of Moderate status (Fig. 7c).

Probabilities of final ecological status classes (Fig. 7d) barely changed for the short term (2030). For the 2060 horizon, however, Poor/Bad status probability decreased for techno world and fragmented world (-6.1% and -4.3%, respectively), increasing slightly both Moderate and High/Good status probabilities. Conversely, for the consensus world scenario, Poor/Bad status probability increases (+8.2%), while Moderate probability decreases (-7.4%). Despite these slight variations, the BBN predicted that the ecological status of rivers in the Odense Fjord basin would remain mostly Poor/Bad in the future (% of Poor/Bad probability varies between 56.7% and 69.2%, Fig. 7d).

As for isolated LUC scenarios, TN was the process-modelling derived stressor showing greater variations in its probability distribution after BBN modelling, decreasing high TN probabilities in techno world and consensus world and increasing in fragmented world (Fig. S2-A of Appendix A).

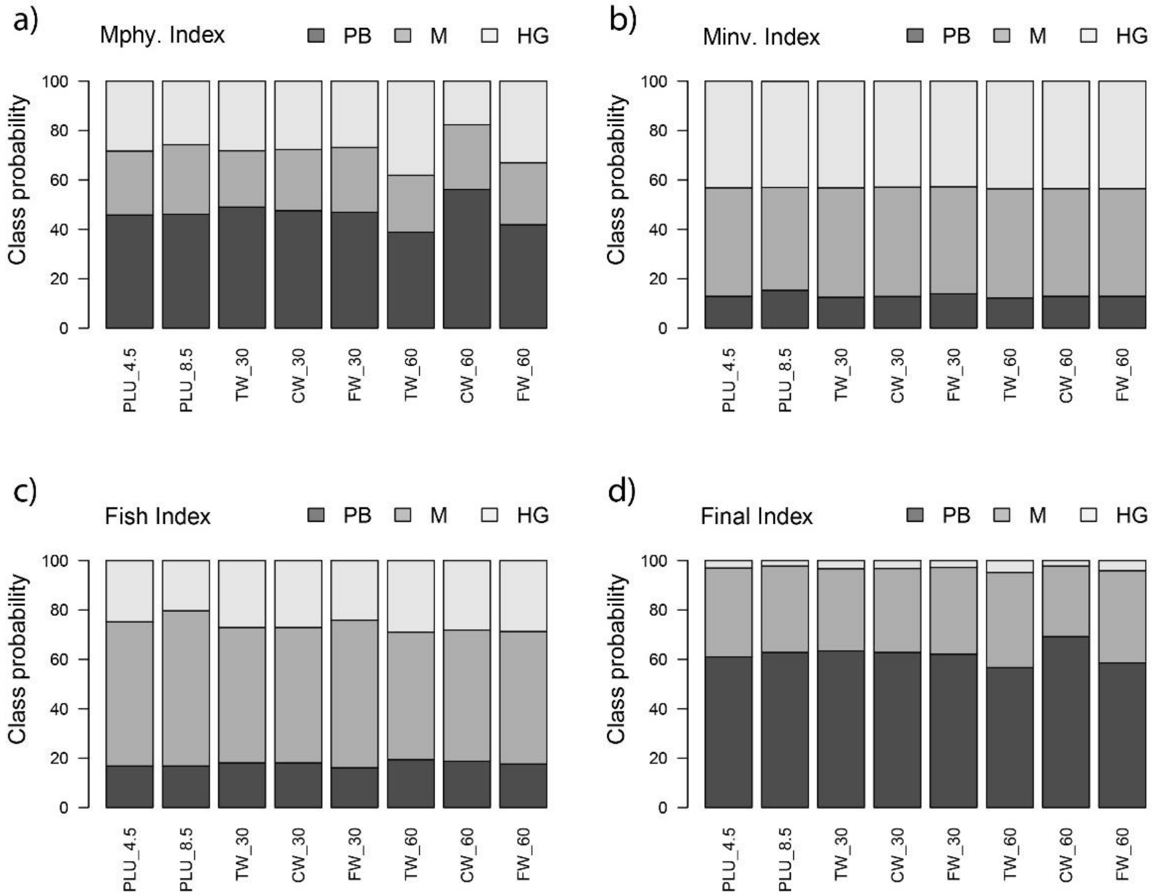

Fig. 7. Probability distributions (%) of biotic status classes (PB: Poor/Bad, M: Moderate, HG: High/Good) for the macrophytes (Mphy., a), macroinvertebrates (Minv., b) and fish (d) indices, and of the final ecological status classes (d) for the baselines (PLU_4.5, PLU_8.5) and the future storylines scenarios in the Odense Fjord basin (PLU: Present Land Use, TW: Techno World, CW: Consensus World, FW: Fragmented World, 30: 2030 time horizon, 60: 2060 time horizon, 4.5: Representative Concentration Pathway 4.5, 8.5: Representative Concentration Pathway 8.5).

In the Sorraia basin, the projections under scenarios for the 2030 and 2060 horizons also resulted in subtle, although consistent, trends of class probabilities among each BQE and the overall biotic status (Fig. 8). For the fish index, Poor/Bad class increased and Moderate and High/Good classes decreased in all the storylines. Fragmented world and techno world storylines, however, resulted in the highest increase and decrease of, respectively, Poor/Bad and High/Good status probability, and this trend was overall slightly more marked in the projection for the 2060 horizon. In the cases of phytobenthos and macroinvertebrates indices, a slight increase of High/Good and a decrease in Poor/Bad was projected for the consensus world in the future time horizons, in relation to the respective baseline (PLU_4.5). On the contrary, for the remaining BQE, an increase of Poor/Bad was projected for the consensus world in both future time horizons.

The class probabilities projections for the final ecologic status showed a clear increase and decrease of, respectively, Poor/Bad and Moderate status probability for all storylines. For the 2030 horizon, the Poor/Bad status probability increased 20.8% for techno world, 14.8% for consensus world and 23.3% for fragmented world; the Moderate status probability decreased 18.6% for techno world, 13.3% for consensus world and 21.0% for fragmented world. For the 2060 horizon, the Poor/Bad status probability increased 24.3% for techno world, 14.8% for consensus world and 25.2% for fragmented world; the Moderate status probability decreased 21.8% for techno world, 13.4% for consensus world and 22.6% for fragmented world.

Regarding stressors, TN and low flow duration were the most affected, increasing high probabilities of both in all the scenarios (Appendix A, Fig. S2-B).

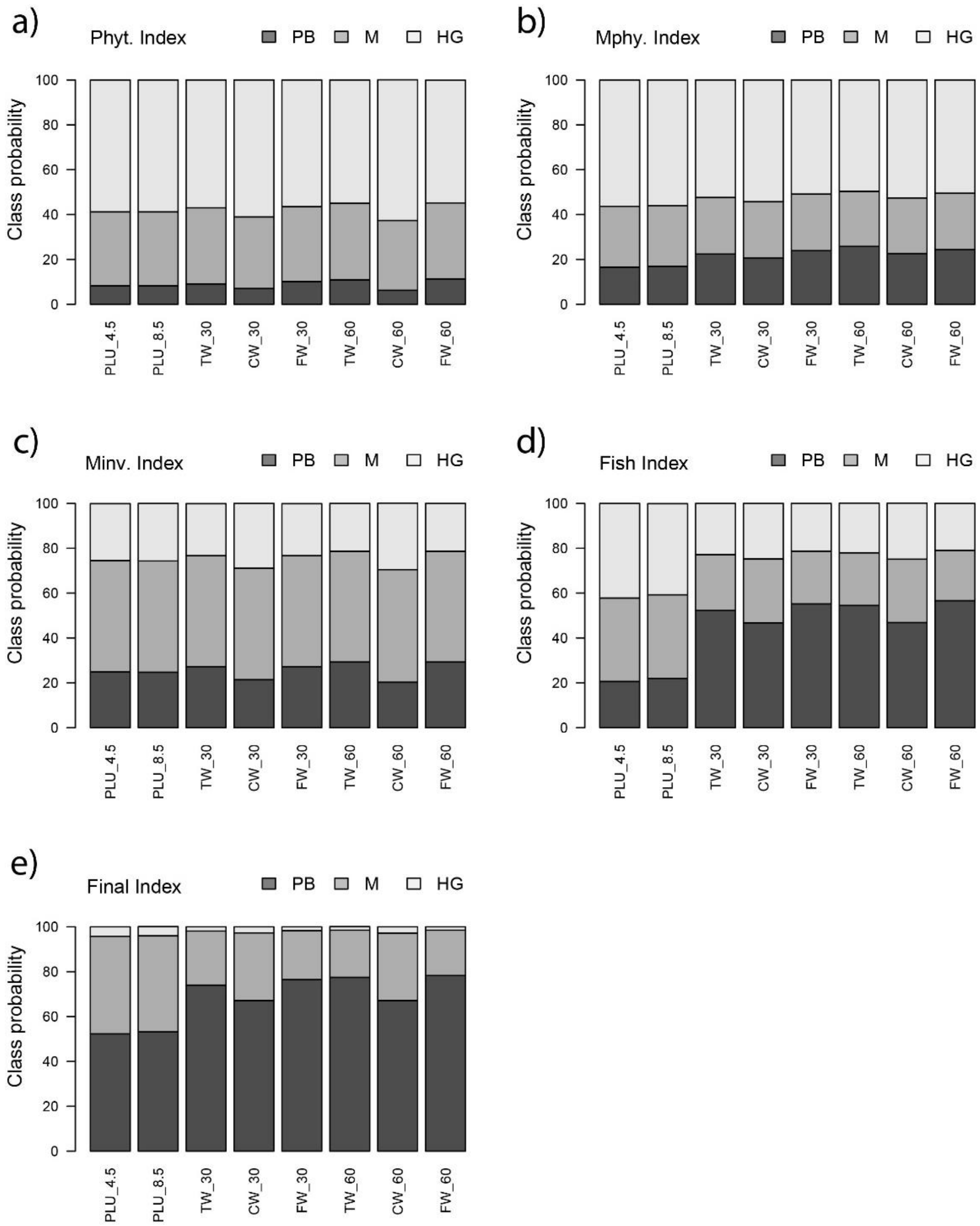

Fig. 8. Probability distributions (%) of biotic status classes (PB: Poor/Bad, M: Moderate, HG: High/Good) for the phytobenthos (Phyt., a), macrophytes (Mphy., b), macroinvertebrates (Minv., c) and fish (d) indices, and of the final ecological status classes (e) for the baselines (PLU_4.5, PLU_8.5) and the future storylines scenarios in the Sorraia basin (PLU: Present Land Use, TW: Techno World, CW: Consensus World, FW: Fragmented World, 30: 2030 time horizon, 60: 2060 time horizon, 4.5: Representative Concentration Pathway 4.5, 8.5: Representative Concentration Pathway 8.5).

4. DISCUSSION

4.1 BBNs validation

For some indices, there were obvious discrepancies between the biotic status classes probabilities derived from the BBN and those observed in both basins (Figs. 3 and 4). BBN predictions tend to be conservative by underestimating the High/Good class probability and overestimating the Poor/Bad status in many cases. In fact, poor validation is a known problem in BBN studies (McDonald et al., 2015), as it often incorporates non-testable information, e.g. based on expert judgement. The discrepancies found in our study can be partly explained by data limitation: in Odense, the availability of observed data for macrophytes and fish from the Basin Management Plans was scarce (Fig. 3). In Sorraia, not all the sites in the database have complete data regarding EQR values for each BQE index, so the 2011 data for validation represents only a subset of the biomonitoring dataset. Some authors have also emphasised the need to validate BBNs with independent data, but they also admit that it can be difficult when probability distributions are derived from data sources other than observed (Barton et al., 2008; Moe et al., 2016). In general terms, the average trend for most indices in both BBNs results and observed data were relatively similar. Moreover, CPTs calculations relied on already calibrated/verified models and therefore the BBN may already be considered partially validated from the beginning. The use of several BQEs also helps to offset problems from a less ideal validation.

4.2 BBN modelling: simulation of scenarios

4.2.1. Isolated Land Use Change (LUC) scenarios

The probability distributions of the biotic status classes showed minor variations across scenarios for all the indices in both basins, and also for the final ecological status, as a result of the combination of the three indices under the "one out, all out" principle (Van de Bund and Solimini, 2007).

Thus, isolated LUC scenarios might not affect much the ecological status of rivers in neither the Sorraia basin nor the Odense Fjord basin. Similar results were obtained by Barton et al. (2008) when using a BBN to evaluate eutrophication mitigation in a Norwegian lake, finding that agricultural measures were insufficient to reach a good ecological status.

4.2.2 MARS Storylines

Probability distributions of biotic status classes exhibited only small variations under MARS storylines for most indices in both study sites.

In the Odense Fjord basin, the probability changes observed for the macrophytes index for the 2060 time horizon in the Odense basin (Fig. 7a) were not consistent with the projections under LUC only scenarios, illustrating the consequence of the different climate inputs (RCP 4.5 in consensus world, RCP 8.5 in techno world and fragmented world), and actually a response to the variations in DUR3 (Appendix A, Figure S2-A). Other studies in the basin also showed that climate changes and different climate inputs within scenarios (and not LUC) were the main drivers of stream flow (Molina-Navarro et al., 2018), which is directly related to the main stressors affecting the macrophytes index in the BBN (Fig. 2). Dyer et al. (2014), using also a BBN approach to study the effects of climate change on ecologically-relevant flow regime attributes, also found the duration of high (and low) flows to be a relevant stressor for water quality modelling.

The trend observed for the fish index demonstrates an additional effect of climate over land use changes, and might be explained by higher probabilities for the high BFI class in all the scenarios (Appendix A, Figure S2-A. Nonetheless, a slight increase of the fish index Poor/Bad status was also predicted, balancing the probability distributions so that the average biotic status was not expected to change substantially.

In the Sorraia basin, the major projected variations of biotic status were found in the fish index, indicating that climate change might be the main responsible for the overall observed changes. However, contrary to the Odense basin, a deterioration of the biotic status, as expressed by a decreasing High/Good class and an increasing Poor/Bad class (Fig. 8d), can be expected to occur in Sorraia. This deterioration is mainly the result of a temperature increase in all storylines (Appendix A, Figure S2-B). Indeed, mean annual temperature was shown to have the strongest negative effect on fish biotic status, among a set of stressors of different nature (Segurado et al. 2018). Other stressors that may contribute to the projected deterioration of fish biotic status are the yearly mean duration of low flow events and TN (Segurado et al. 2018), both predicted to increase in future scenarios (Appendix A, Figure S2-B).

The macrophytes index was found to be responding mainly negatively to the frequency of low flow events and TN (Segurado et al. 2018). Nevertheless, the slight deterioration of the biotic status predicted by the BBN (Fig. 8b) might be mainly related to the projected marked increase of TN (especially in techno world and fragmented world storylines, Appendix A, Figure S2-B), since the frequency of low flow events was not predicted to show high variations.

Projections of phytobenthos and macroinvertebrates indices seem to indicate that future changes might be related to LUC and not to climate change. Indeed, empirical models showed a stronger effect of land use variables in biotic quality for both phytobenthos and macroinvertebrates, namely the percentage of agriculture in the upstream basin, in comparison to hydrological or nutrient stressors (Segurado et al. 2018).

As a result of applying the "one out, all out" principle (Van de Bund and Solimini, 2007), the probability of the Poor/Bad ecological status became higher than in the individual indices in all scenarios and in both basins (Figs. 7d and 8e). The more pessimistic product of this principle has already been reported by other authors using BBNs (e.g. Lehikoinen et al. 2014; Moe et al., 2016). Comparing the probabilities obtained for MARS storylines with those obtained with observed climate and present land use (Figs. 5 and 6), results suggested that climate change impacts on the rivers overall ecological status might be more relevant in the Sorraia basin than in the Odense Fjord basin. Mean annual temperature, a stressor only dependent on climate change, was found as one of the relevant stressors for predicting the fish index in Sorraia basin, spreading its influence to the overall status due to the "one out, all out" principle. However, for all the other indices in both basins, both climate and land use changes might not exert a large effect on the ecological status of the rivers.

To the best of our knowledge, this paper uses for the first time an ensemble of BQEs for assessing river and stream water quality at an international scale, predicting ecological effects of future scenarios (combining both climate and socio-economical changes). Thus, finding similar studies using BBNs is challenging. Dyer et al. (2014) also predicted small water quality changes in rivers due to climate change in contrast to significant projected hydrological changes. Moe et al. (2016) and Couture et al. (2018), assessing lake ecological status through BBNs, also revealed a minor influence of climate change on future lake status. However, contrasting with our study, both these studies found a significant impact of future land use management scenarios. Different basin characteristics and object of study (lake vs. rivers), together with different storyline downscaling methods, might explain these differences.

TN concentration might serve as a chemical water quality proxy. In the Odense case, small variations were found, e.g. a larger probability of high TN in the techno world scenario in 2030 than in the techno world LUC scenario under observed climate (despite same decrease in fertilization), or a lower probability of high TN in the fragmented world scenario in 2060 than in the fragmented world LUC scenario under observed climate. These changes might result from an additional effect of climate change: higher flows favour dilution, but also lead to higher organic N load (Molina-Navarro et al., 2018, Couture et al., 2018). Moe et al (2016) also found that the benefits of better land use management could be partly counteracted by future warming.

In the case of Sorraia, a much slighter increase of the higher class probabilities for TN was found under the isolated LUC scenarios for techno world and fragmented world storylines under observed climate compared with the scenarios that incorporated climate change, despite the use of the same fertilization scenarios. All simulated future scenarios showed a significant decrease in water flow due to the lower predicted precipitation according to GFDL climate models (Almeida et al., 2018), which might explain the higher increase of TN concentration. In the case of the consensus world LUC scenario under observed climate, an overall decrease of TN was projected, which is in line with the decrease on the use of fertilizers in this storyline. In the equivalent scenario that incorporates climate change, the effect of the decrease in precipitation overrode the decrease in fertilizer input, resulting in a slight increase of TN. The high solubility and leaching susceptibility of nitrate (Ramos et al., 2012) might explain the sensitivity of TN to variations in water quantity.

4.3 Consequences for management

BBN modelling predicted that most water bodies from both catchments would fail to achieve the ecological status criteria required in the EU Water Framework Directive ("Good" or "High" ecological status, (European Parliament and Council, 2000).

In the Odense Fjord basin, the changes simulated in the fragmented world storyline would not deteriorate the ecological status of the rivers, but those in the consensus world storylines would not improve it either. Actually, a small improvement is predicted in techno world and fragmented world in 2060, but because of a different climate input (see 4.2.2). Results show that the BQE most responsible for a non-desirable overall ecological status is the macrophytes index. Thus, water managers in the Odense Fjord basin should place particular emphasis on improving the macrophytes' status in the basin´s streams, thus counteracting the plausible effects of climate change on the macrophytes communities.

In the Sorraia basin, the percentage of rivers not fulfilling the WFD is worse in all the scenarios compared to the baseline (Fig. 8e). The main BQE governing the bad overall ecological status is the fish component (Fig. 8d). Fish biotic status is predicted to decrease under the three storylines due to higher temperatures. Thus, water managers in the Sorraia basin need to put into practice measures to counteract the effect of higher temperatures in the fish communities.

4.4 Strengths and weaknesses of the BBN approach

The main advantage of the use of BBNs is that it allowed to bridge into a single framework information of very different nature, including direct data-driven patterns, process-based models, empirical models, expert judgement and more arbitrary management rules (e.g. "one out all out" WFD rule). Predicted changes are expressed as probabilities, which directly show decision-makers the chances of achieving certain outcomes under alternative socio-economic scenarios.

Despite obvious strengths, BBNs are not without drawbacks. In this study we tried to circumvent most of the BBNs known shortcomings (Barton et al., 2008; Borsuk et al., 2004; Borsuk et al., 2012; Forio et al., 2015; McDonald et al., 2015; Qian and Miltner 2015). First, the acyclical structure of BBNs that, by not allowing feedback effects, restrict relationships to be based on steady-state conditions (Borsuk et al., 2004; McCann et al., 2006). Given the objectives proposed in our case-studies, this does not constitute a problem because we define fixed time windows to which we assume fixed socio-economic storylines and climate scenarios that do not have dependencies on the outcomes.

A second issue is the tendency to define over-complex network structures in relation to the scale of the management problem (Barton et al., 2008). We made an effort to use network designs as parsimonious as possible, by restricting variables to those that could be measured or modelled at least at the sub-basin scale, i.e. the portion of basin draining into each of the modelled rivers, which are the WFD management units (water bodies). In this way, we also coped with the ongoing challenge in aquatic ecology of minimizing model structures to present the simplest form (Marcot, 2012; McDonald et al., 2015), because a large number of model nodes does not necessarily warrantee a lower uncertainty (Barton et al., 2008). Furthermore, to ensure management applicability, the BBN models focused on two stressor types - flow and water quality (nutrient loads) - which are key targets of river management (Dyer et al., 2014).

A third issue is related with the sensitivity of BBNs outcomes to discretisation of probability distributions (Aguilera et al., 2010; Uusitalo, 2007). To deflect this problem we followed the general recommendations to define both the breakpoints and the number of intervals (Uusitalo, 2007), taking into account limitations in our data, in particular ensuring that each interval had a reasonable amount of observations. For biotic status variables and final biotic status, discretization had a management significance since we used the quality boundaries of biotic quality indices that are officially used as criteria for management actions, namely the border between moderate and good condition.

5. Conclusions

BBNs have been developed to simulate the ecological status of streams and rivers in two European river basins (Odense Fjord and Sorraia) as the result of different climate change scenarios and their potential consequent socio-economic storylines (i.e. land use and agricultural management changes). The outputs of BBN modelling suggest little changes in the biotic status of rivers in the majority of the BQEs analysed. As a result, both in the Odense Fjord and in the Sorraia basin, a large percentage of the rivers would not cope with the WFD criteria of good or better ecological status, similar to the present situation in Odense, and slightly worse than in Sorraia. In Odense, the macrophytes BQE was the main responsible for this and in Sorraia it was the fish BQE; managers should allocate their efforts into reducing the effects of stressors into these BQEs respectively for each basin. Despite all potential limitations, the BBN projections may represent the best possible outcomes taking into account the typical limitations of bioassessment data availability from environment agencies and may provide useful qualitative insights to decision-making on water management under future climate change.

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APPENDIX 3 - SCORE—A SIMPLE APPROACH TO SELECT AWATER QUALITY MODEL

water

MDPI

Article

ScoRE—A Simple Approach to Select a Water Quality Model

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Abstract: Over the past decades, water quality models have become unique tools in the management of aquatic resources. A consequence of their widespread application is the significant number of models now available. Available methodologies to compare models provide limited support for their choice in the first place, especially to end-users or modelers with limited experience. Here we propose a method to assist in the selection of a particular model from a set of apparently similar models. The method is termed ScoRE, as it grades models according to three main aspects: Scope (aim, simulated processes, constituents, etc.), Record (reference to the model in publications, its range of applications, etc.), and the Experience of using the model from the user perspective (support material, graphical user interface, etc.). End-users define the criteria to be evaluated and their relative importance, as well as the conditions for model exclusion. The evaluation of models is still performed by the modelers, in open discussion with end-users. ScoRE is a complete approach, as it provides guidance not only to exclude models but also to select the most appropriate model for a particular situation. An application of this method is provided to illustrate its use in the choice of a model. The application resulted in the definition of 18 criteria, where 6 of these were defined exclusively by the end-users. Based on these and the relative importance of each criterion, ScoRE produced a ranking of models, facilitating model selection. The results illustrate how the contributions from modelers and end-users are integrated to select a model for a particular task.

Keywords: water-quality modeling; model choice; CE-QUAL-W2; MIKE HYDRO River; MOHID Water; SIMCAT; SisBaHIA; TOMCAT; QUAL2Kw; WASP7

1. Introduction

The widespread use of water quality models over the past decades has increased the capacity to manage water quality in both marine and freshwater systems. Water quality models have become important, if not irreplaceable, tools in management, planning and pollution control for government agencies, local authorities and many other entities supervising water resources [1–3]. This is evident in the significant number of water quality models produced over the years [4–6]. Now, the question is no longer whether to use models in water management but, instead, which models to use. In the current paradigm, the selection of a model is a determinant step in the study for understanding and managing a particular aquatic system or water body [7]. However, the selection process can be a challenge, especially to end-users lacking the modelling, computational or mathematical skills to undertake a thorough evaluation of the models.

Given the implications that model results can have in the selection of management practices, both the model and its selection process must be robust and valid. Transparency and accountability are critical for robustness and essential for validating the method. This is particularly relevant, as most likely stakeholders will be involved at later stages of the water management process, whether in the modelling stages, in the development or evaluation of courses of action, or the implementation processes, and therefore, stakeholders will need to understand which management options are being proposed and why. While the literature is prolific in testing and evaluating models [8–14], it is quite omissive regarding approaches to assist end-users in the choice of models.

In the present paper, we address the model selection stage. Model selection is usually a small part of the whole decision-making process. Consequently, the same effort put into the entire process of modelling and water management, concerning time, resources and stakeholder involvement, cannot be expected to be reflected in model selection. A simple procedure is required, with a compromise between the degree of participation of stakeholders (and modelers) vs. practicality of this step. The use of participatory approaches in the context of environmental resources decision making and modelling shows an increasing trend [15–17]. However, the degree of involvement of end-users and modelers (technical team) at the model selection stage, i.e., whether end-users should be involved in the evaluation of the models and to which degree, is still subject of a debate within the literature (e.g., Solaranta et al. [18] vs. Boorman et al. [19]).

This paper contains a review of the main approaches found in the literature for water quality model selection. This review is discussed from a multicriteria decision analysis perspective. Building on the results from this literature review, we propose an approach for model selection providing more detailed guidance on how to select a model, producing a more flexible process and promoting the dialog between end-users and technical teams. The proposed approach applies only to model selection, and it excludes the socioeconomic and institutional spheres of water management.

Throughout this paper, we refer to the terms model end-user and modelers. By model end-user, we refer to those that will use the model results, such as water managers and other stakeholders. By modeler, technical team or expert, we mean the person who has the knowledge to understand the processes behind the model and knows the modelling approaches.

2. Procedures for Selecting Water Quality Models

One of the earliest guidelines to select water quality models for lakes, rivers or estuaries dates back to a 1976 guidebook developed for governmental use by the US Environmental Protection Agency (EPA) [20]. The volume described a selection process with four levels of criteria. The first two phases allow the elimination of models and the latter two stages rank the remaining models. In brief, the phases are:

- Phase I: eliminatory phase, based on: appropriateness of the model to the problem at hand (type of water body, time variability, discretization, constituents modelled, model input data, driving forces and boundary factors);
- Phase II: eliminatory phase, based on: cost (model acquisition requirements, equipment requirements, data acquisition costs, machine costs, manpower costs);
- Phase III: ranking models, based on: weights attributed to the criteria from phases I and II;
- Phase IV: further ranking of models based on: relevant processes included, accuracy (model representation, numerical stability, dispersion), sufficiency of available documentation, output form and content, data deck design, ease of modification.

Only in the last 15 years have new complete frameworks for water quality model selection started to appear, guiding the whole process of model selection, including the definition of which characteristics of the models are being compared (i.e., defining the criteria of comparison) and how to compare these [18,19,21,22]. Some approaches [18] identify a set of questions to guide the definition of criteria to be used as a means of comparison between models. Some examples are "How well does the model's output relate to the management task", "How well is the model suited for sensitivity and uncertainty analyses and how well have these analyses been performed and documented?" or "How are the model's user manual and tutorial?" In another study [19], authors defined the evaluation criteria itself for model selection, along with some guiding questions for the water manager to help to determine further criteria to be used for model comparison. In this particular study, modelers then evaluated the different models under those criteria. In a more recent protocol for model selection [21], the main aim was to provide a framework to assist inexperienced model users, as well as to provide an auditable process. Although not explicitly identified, this protocol is based on a Multi-Criteria Decision Analysis (MCDA) process. The main distinction of this protocol with the previous work referred to Boorman et al. [19] is that this latter work does not require the involvement of modelers in evaluating the models, just end-users. While modelers make the questions that guide the protocol, it is up to end-users to evaluate criteria through a literature review.

In our review of the literature, we considered the following concepts: (i) criteria: the attributes used to compare the different models; (ii) valuation or scoring: stage in which all models are compared under each criterion, resulting in a model rank for each criterion; (iii) aggregation procedure: process of aggregating the results from the different criteria (i.e., converting all ranks to the same scale in order to be compared), usually by attributing weights to the criteria, which represent the "conversion factors" between them.

2.1. Valuation of Models

There is intense debate in the literature about which stages model users should be involved in. A particular point of disagreement relates to the valuation of models or scoring, a term used in MCDA to refer to the evaluation of the models in each criterion. Some authors [18,20–22] claim that the scoring (and the whole model selection process, including choice of criteria and which models to evaluate) should be carried out exclusively by end-users, for transparency reasons and to reduce time and costs of the model selection stage. Chinyama et al. [21], for instance, suggested that model users can score the models on the criteria based on a literature review on the models. Interestingly, in the case study proposed here, authors (modelers), not the end-users, score the criteria. However, no test has been made to evaluate if end-users can access the literature and understand it to be able to score all criteria regarding the models or have the time for such a process. Grimsrud et al. [20], on the other hand, considered that external consultants might be used and, in this case, give planners (end-users) the tools to know what to ask for and what to expect.

Other authors (e.g., Boorman et al. [19]) claimed that end-users might not process all the knowledge necessary to adequately evaluate the models under the criteria defined and, therefore, argued that modelers should conduct the process of assessing models within each criterion. In this particular case ([16]), although the valuation of models is left to the modelers, criteria are still defined by end-users.

It is the opinion of the authors of the present work that knowledge of end-users is essential to score the criteria, but some criteria might require knowledge that some end-users may lack.

2.2. Aggregation Procedures

The aggregation procedure corresponds to the phase where the scores of each model in all criteria are aggregated together to obtain a final value per model. The final result is a ranking of the models. The way the scores from models in each criterion are "converted" into a standard unit to be aggregated can vary. Within the literature on water quality model selection, there is a fair degree of similarity between the process of aggregating values from different criteria. Most methods consider eliminatory criteria, setting a minimum base level so that, if not satisfied, the model is excluded from the process [18–22]. No additional guidance is provided to select one model out of the remaining adequate models (Figure 1). With no further guidance, end-users end up with a reduced list of models to choose from. An additional process is required to assist end users to identify which of the remaining models should be selected. Very few studies provide guidance on this [20,22].

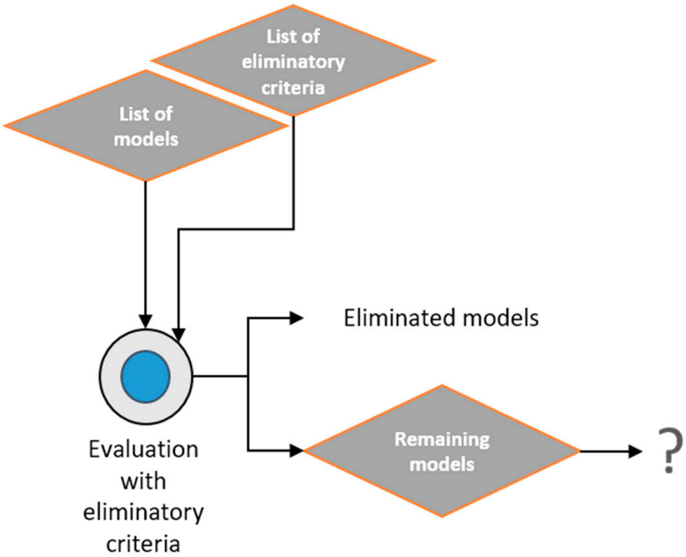

Figure 1. The use of eliminatory criteria on model selection for water quality.

The EPA Model Selection Process [20] considers eliminatory criteria (corresponding to Phases I and II from the process). However, they also present weighted criteria (corresponding to Phases III and IV from the process) where (ranges of) weights for the criteria are suggested by the authors for the remaining (not eliminated) models. The aggregation procedure used in this guidance manual is a linear additive process. In Tuo et al. [22], on the other hand, there are some eliminatory criteria, linked with the modelling objective but also to other features such as model complexity. For non-eliminatory criteria, the criteria are assumed to have equal weights, although authors recognize that different weights could be provided to the criteria if the method is compatible with that situation.

The use of eliminatory criteria, as mentioned before, makes the methods non-compensatory or partially compensatory. Compensatory methods are methods where weights are seen as trade-offs, i.e., where a model is selected by being good when judged against one criterion, even if it performs low against another criterion. Non-compensatory methods attribute weights or importance coefficients to criteria, expressing the relative importance of each criterion [23,24].

3. The ScoRE Method

ScoRE is a multicriteria-based method for water quality model selection, applying only to model selection, and excluding the socioeconomic and institutional spheres of water management. The main features of the method are that it provides detailed guidance on how to select a model, it is a more flexible process and promotes the dialog between end-users and technical teams. The method is grounded on a set of three broad clusters (as in Parsons et al. [25]), through which end-users and a technical team define a set of criteria for model evaluation and selection. Water quality models are then evaluated on each criterion by the technical team, which will then discuss the weights for the clusters with end-users. Weights are applied to the clusters to provide a final ranking of the water quality models. ScoRE engages model end-users by involving them in the definition of the criteria, in the selection of models to be evaluated, and in the weighing of the clusters. End-users have the opportunity to go through the whole process and debate the final results with the technical team. Figure 2 provides an overview of ScoRE, and the next sections provide a more detailed description of the process.

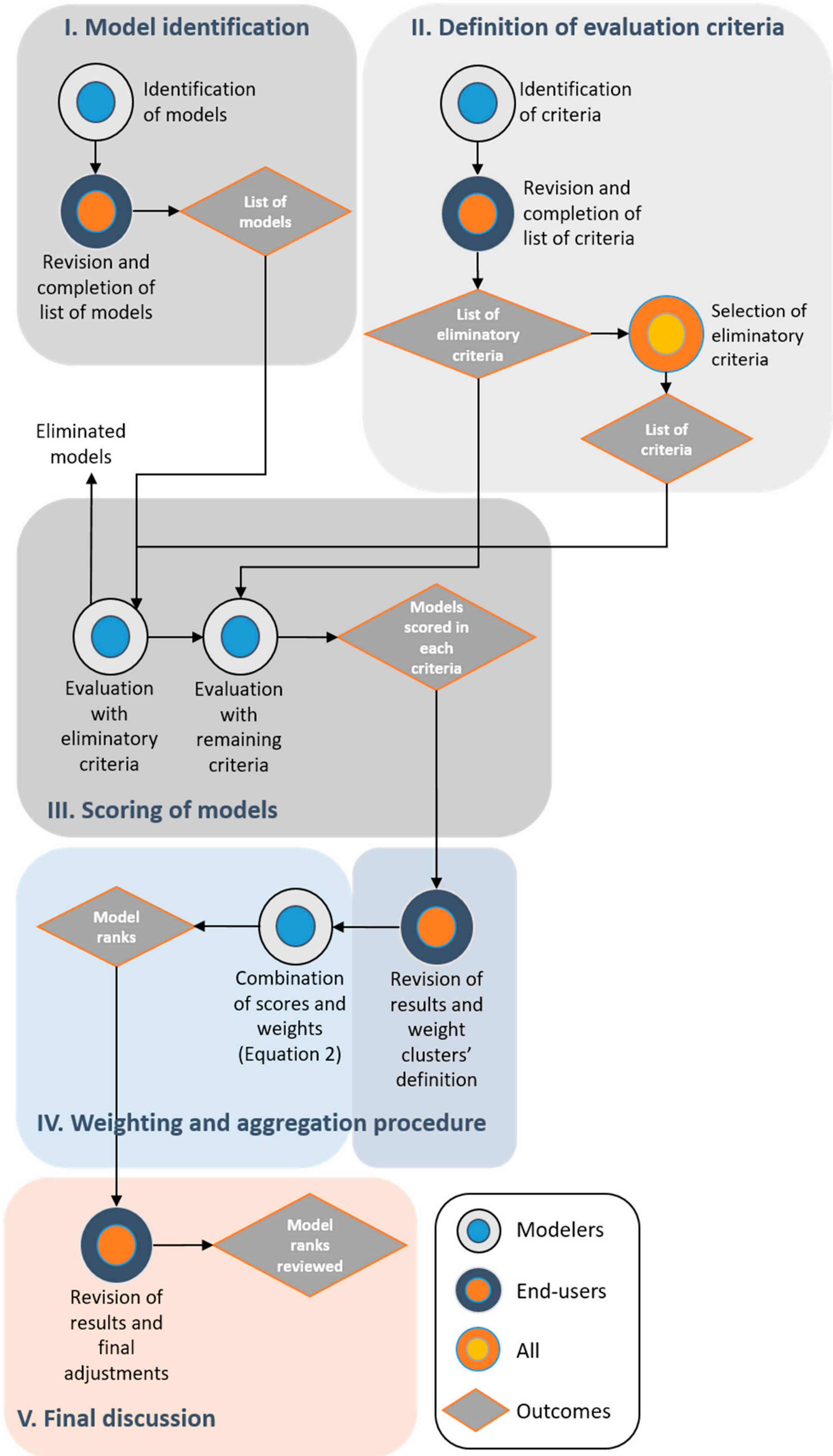

Figure 2. A schematic representation of the ScoRE process.

3.1. Definition of the Evaluation Criteria

In ScoRE, criteria are defined by the technical team in dialog with end users. The scientific consistency of the criteria choice, a criterion identified as relevant by Loucks and Beek [26], is ensured by the technical team. Model end-users ensure that additional aspects are not left out of the analysis, either related to the particularities of the context being modelled, data availability or any sort of constraints from the user side (e.g., available funds or level of familiarity with modelling techniques). This procedure warrants results to better satisfy the needs of end-users.

The criteria are grouped in three clusters, defined a priori. These are "model Scope", its "publication/dissemination Record" and the "overall Experience to users", hence its designation: ScoRE (Scope—Record—Experience). Together, the three clusters aim at assessing the models for a variety of parameters, thus providing an overall evaluation. The cluster Scope addresses the nature of the model (stochastic, deterministic, process-oriented, etc.), its complexity and the range of constituents and processes the model simulates. The cluster Record provides a proxy for the dissemination and acceptance of the model amongst modelers, by quantifying the number of technical publications where a particular model features. The cluster Experience defines the experience of using the model, and how it can be defined as straightforward or difficult, based on the interface and material available to help the model user. A more detailed description of each cluster is offered in the next sections.

3.1.1. Model Scope

Considering that a model is a (simplified) representation of reality, the scope of a model is the purpose for which it was built in the first place. Water quality models, for instance, may be developed to simulate fresh-water systems, brackish environments or marine and coastal waters, focusing on pollutants, ecological processes, water chemistry, etc. Thus, the scope of a model defines its nature, methods, parameterization, processes simulated, and all other components that expresses its validity to simulate any particular system. These include the type of approach (conceptual, empirical, physically based), the nature of the model (deterministic or stochastic), the state (steady-state or dynamic simulations), and its spatial analysis (distributed, lumped), data requirements, dimensions (1D, 2D or 3D), and robustness, among other aspects [3,7].

3.1.2. Publication Record

Publication record is defined in ScoRE as the number of publications in science and engineering journals featuring a particular model. This can be seen as an alternative for the impact of a model, based on the assumption that a widely cited model implies wide acceptance by the scientific community and, consequently, a proxy to its consistency, validity and robustness.

Some examples of criteria within this cluster can be the number of papers featuring the name of the model in the title or in relevant fields such as the summary and keywords, or simply the number of times a given model is mentioned in the text body. The information for this indicator can be retrieved from web services such as *ScienceDirect* or *Web of Knowledge*. Also, the type of systems for which the model has been applied to, or its worldwide dissemination, can also be used to assess the model Record.

3.1.3. User Experience

Interface

The experience of using a particular model is strongly conditioned by the graphical user interface (GUI). The GUI aims to facilitate the input of data, running of the model and output visualization, and should provide a user-friendly environment, with graphical elements that allow the user to interact with the software. Most models come with a native GUI but some occasionally have alternative options created by third parties, frequently with additional features such as advanced pre- and post-processing tools, extra visualization options, etc. These alternative GUIs usually require payment for the software or a licensing fee of some kind.

Support Material

Support material is a basic requirement for any model and must be available either online or on paper. Numerical models, like any other software, should have a set of supporting documents containing information on the model structure, description of simulated processes, a list of the parameters, and additional relevant information on its functioning. Commercial models frequently have comprehensive guides while academic software and freeware usually rely on more concise manuals. Thus, user guides vary significantly in detail and quality among models and this difference can weigh on the choice of a model. The model can also have a published detailed model calibration, validation, and parameter assessment.

Technical Support

Technical support is a common service provided by commercial software developing companies, to help users overcome any difficulties or problems they may face when using a product. Since it requires having the staff to interact with the client (by phone, Skype, email, etc.), technical support is frequently a paid service or a service that is offered as part of a paid software package. Alternative ways to provide technical support to users may be less expensive or even cost-free, such as online forums, in which users and developers post technical questions and answers.

Cost

Numerical models, like any other software, are available to the user in many different ways, some of which may require payment of a licensing fee, implying that some models have a cost associated with their use and exploration. The implication of a payment can pose problems to some users, frequently depending on the price, so this criterion can have a significant influence on the selection.

3.2. Defining "Eliminatory Criteria"

"Eliminatory criteria" set the conditions that models need to satisfy in order to proceed to the next stage in the evaluation process. For example, type of water body could be an eliminatory criterion, defining that if a model does not apply to lakes, for example, the model would be excluded. Another example could be whether the model presents a vertical thermal structure of reservoirs, if essential for a particular case, and where models could be excluded from the analysis if they were not able to present such vertical thermal structure.

3.3. Valuation of Criteria

The first step in the valuation of criteria stage is to evaluate all models in the "eliminatory criteria" in order to weed out some of the models. The valuation of criteria is conducted by the technical team (and later discussed with the end-users). After the valuation according to the eliminatory criteria, the remaining models are evaluated in the criteria. All remaining models are compared in each criterion and ranked in a scale from 1 to n (n being the number of models), where 1 is the worst-performing model and n the best-performing model. If models are assumed to be equal for a particular criterion, then the same value can be assigned to both. This process is repeated for each criterion. The result is a rank of models in each criterion (i.e., if the number of criteria defined is nt, then there will be nt ranks).

3.4. The Aggregation Procedure of ScoRE

The aggregation procedure of ScoRE makes use of weights. First, criteria scores within each cluster are averaged:

$$\begin{aligned} S &= \left(\sum_{i=1}^{nt} S_i\right) \times {nt_S}^{-1}, \\ R &= \left(\sum_{i=1}^{nt} R_i\right) \times {nt_R}^{-1}, \\ E &= \left(\sum_{i=1}^{nt} E_i\right) \times {nt_E}^{-1}, \end{aligned} \tag{1}$$

where S, R and E are the average scores for each cluster, S_i, R_i and E_i are the scores of the criteria within each cluster, and nt_x is the total number of criteria per cluster. This means that the scores of criteria within the same cluster are seen as equally relevant. ScoRE values can range from 1 to n and so the result from Equation (1) will allow models to be ranked from the less suitable (lower ScoRE) to the more adequate (higher ScoRE), in each of the criteria.

Weights defined by end-users are attributed to each cluster. The aggregation procedure follows a linear additive model to provide a final ranking of models. This is expressed by (2):

$$\text{ScoRE} = (W_S \times S) + (W_R \times R) + (W_E \times E), \tag{2}$$

where W_S, W_R and W_E are the relative weights of each cluster, provided that $W_S + W_R + W_E = 1$.

A summary of the main characteristics of ScoRE and its comparison with other studies is presented in Table 1.

Table 1. ScoRE compared to other approaches.

Approaches	Criteria Definition	Who Conducts the Valuation of Models in Each Criterion	Aggregation Procedures
Saloranta et al. [18]	Predefined questions to guide criteria definition	End-users	Eliminatory criteria
Boorman et al. [19]	Predefined questions to guide criteria definition	Modelers	Eliminatory criteria
Grimsrud et al. [20]	Predefined	End-users with possibility of hiring modelers	Eliminatory criteria and detailed guidance for how to proceed for the non-eliminated models (weighting process)
Chinyama et al. [21]	Predefined questions to guide criteria definition	End-users	Eliminatory criteria
Tuo et al. [22]	Predefined	End-users	Eliminatory criteria. Some insights into how to proceed for non-excluded models
ScoRE	No pre-definitions. Criteria defined between modelers and end-users	Modelers. Results discussed with end-users	Eliminatory criteria. Detailed guidance for how to proceed for the non-eliminated models (weighting process)

4. Using ScoRE in a Real Case

4.1. Study Sites

The Ceará State in the northeast region of Brazil is characterized by semi-arid meteorological conditions, frequently leading to water scarcity. As such, a sound management of water resources is critical, requiring decisions from managers and regulators that balance water availability and quality for human and animal consumption. Most available water is stored in reservoirs scattered across the state, the majority of which are under significant pressures originating in the watershed, ranging from intense cultivation to human and industrial effluent discharge. Fundação Cearense de Meteorologia e Recursos Hídricos—FUNCEME (Ceará's Meteorological and Hydric Resources Foundation)—is the federal organization responsible for managing the water resources in the state, along with Companhia de Gestão dos Recursos Hídricos—COGERH (Water Resources Management Company). Over the past few years, FUNCEME and COGERH have explored new water management strategies, some of which require the use of numerical models. Both organizations were engaged in the choice of a water quality model to study three reservoirs located in the Ceará State, in the northeast region of Brazil: Acarape do Meio, Araras and Olho d'Água. The location of the reservoirs is depicted in Figure 3.

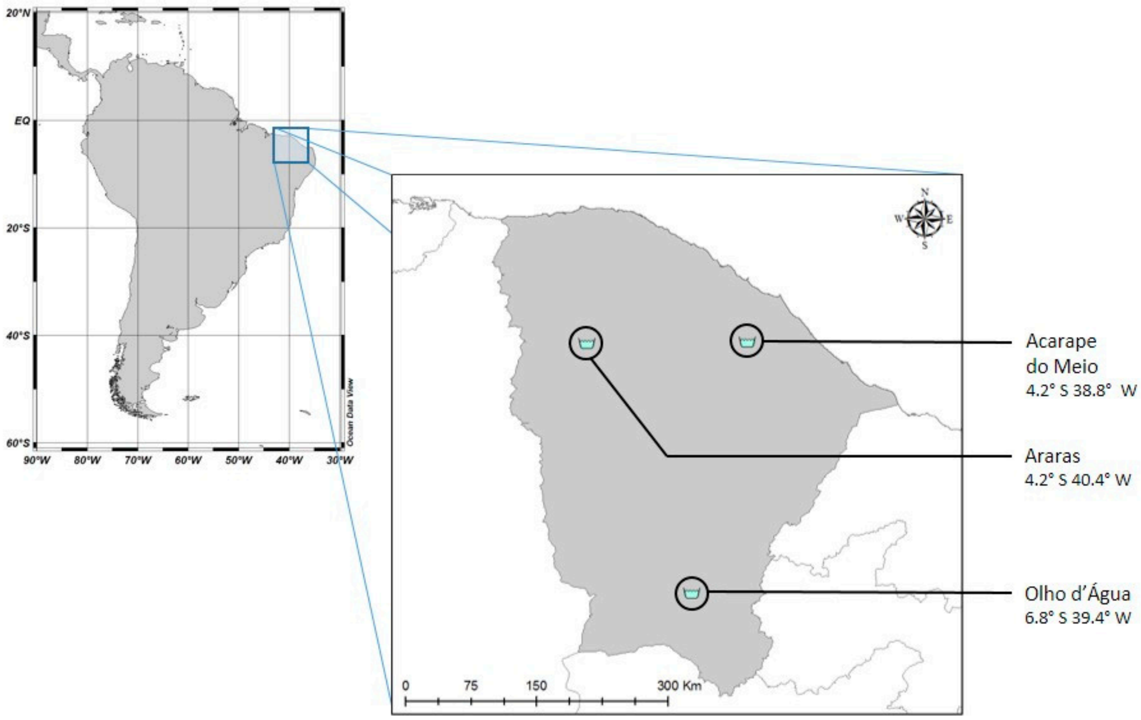

Figure 3. Location of the study sites in the Ceará State, Brazil.

These reservoirs differ in their characteristics, physical setting and pressures originated in the basin. They share, however, some basic features, such as a relatively low mean depth, high water temperatures all year around, the presence of a mild thermocline frequently disrupted by episodes of intense wind-induced mixing, strong vertical chemical stratification, and persistent oxygen-depleted bottom layers.

4.2. Application of ScoRE

The technical staff from FUNCEME and COGERH were the end-users and the modelers consisted of the authors of this paper. Modelers had a background in environmental modeling, ecology of aquatic environments and water quality. The application of ScoRE followed the process described in Section 3, schematized in Figure 2. The process is summarized below:

1. End-users were provided with a list of models identified by modelers. This list was defined by modelers taking into account existing validated models. The list was discussed with the end-users, who were given the possibility of including additional models if they had any they wanted to see included.
2. The criteria were defined by modelers, based on the conditions of the case study at hand. These criteria were defined taking into account three clusters of ScoRE. The list was discussed with the end-users, who added additional criteria to the list. End-users, together with the modelers, reviewed the criteria to select which of these should be eliminatory criteria.
3. Each model was evaluated within the eliminatory criteria first. This allowed the exclusion of some of the models. The remaining models were then evaluated in each of the criteria. The

valuation process was conducted by modelers. The result was a rank of the models for each criterion. The resulting scores were discussed with the end-users.

4. End-users attributed weights to the clusters of criteria. With the weights, it was then possible for modelers to average scores in each cluster (using Equation (1)) and apply the linear additive model (Equation (2)) to obtain the final rank of the models.
5. Final rankings were then discussed with end-users and, when necessary, final adjustments were made to the criteria, scores or weights in accordance.

The process was conducted over two meetings between end users and modelers. The first meeting included steps 1 and 2 and the second meeting included steps 4 and 5. Step three was conducted by the modelers alone and results were taken for discussion in the second meeting.

5. Results

5.1. Models Included in the Evaluation

Eight water quality models were selected by the technical team and reviewed by the end-users. These models were: CE-QUAL-W2, MIKE HYDRO River, MOHID Water, SIMCAT, SisBaHIA, TOMCAT, QUAL2Kw e WASP7 (Table 2). The models are process-based (or process-oriented), have been used worldwide to some extent, and encompass a wide range of complexity, both in parameterization and number of simulated processes. They are briefly described in their basic principles, simulation elements, limitations and intended use. While some have been used extensively in the past, others are less disseminated. A summary of their main features is presented in Table 3 and detailed descriptions can be found in the references provided.

Table 2. Models evaluated.

Model	Origin and model website
CE-QUAL-W2	US Army Corps of Engineers/Portland State University, Portland, USA http://www.ce.pdx.edu/w2/
MIKE HYDRO River	Danish Hydraulic Institute, Hørsholm, Denmark http://www.mikepoweredbydhi.com/products/mike-hydro-river
MOHID Water	Instituto Superior Técnico, Lisbon, Portugal http://www.mohid.com
QUAL2KW	Washington State Department of Ecology, Olympia, WA, USA http://www.ecy.wa.gov/programs/eap/models.html
SIMCAT	Environment Agency, Rotherham, UK
SisBaHIA	Fundação COPPETEC - COPPE/UFRJ, Rio de Janeiro, Brazil http://www.sisbahia.coppe.ufrj.br/
TOMCAT	Environment Agency, Rotherham , UK
WASP7	The United States Environmental Protection Agency, Washington, DC, USA http://www.epa.gov/athens/wwqtsc/html/wasp.html

5.1.1. CE-QUAL-W2

CE-QUAL-W2 (Table 2) is a public domain model that has been widely used in the study of stratified water systems, including lakes, reservoirs and estuarine environments [27–32]. CE-QUAL-W2 is a two-dimensional (longitudinal-vertical) hydrodynamic and water quality model. The model was originally developed by the U.S. Army Corps of Engineers [33,34], and a comprehensive description of CE-QUAL-W2 can be found in Cole and Wells [35]. The model is based on a finite-difference approximation to the laterally averaged equations of fluid motion and quantifies free surface elevation, pressure, density, vertical and horizontal velocities, and constituent concentration and transport. Explicit numerical schemes are employed to compute velocities, controlling the transport of energy and biochemical constituents. CE-QUAL-W2 simulations are rather fast and require low computational power, but need a significant amount of data. Also, the high number of parameters makes the calibration tasks difficult. Nonetheless, this model has been optimized for water quality in reservoirs and is one of the most used models in the study and management of these aquatic systems [36–41].

5.1.2. MIKE HYDRO River

The MIKE HYDRO River model (Table 2) is a one-dimensional modeling tool developed by the Danish Hydraulic Institute (DHI), for the detailed design, management and operation of river and channel systems with different levels of complexity [42]. This model has been widely used in the modeling of rivers and lakes [43,44]. The model is composed of several modules that can be either used together or as stand-alone simulators, including rain fall, hydrodynamic, advection-dispersion, sediment and water quality. The hydrodynamic module is one-dimensional and computes unsteady flow, discharge and water level based on Saint–Venant equations. This model has been optimized for operational modeling in flood forecasting, ecological assessment of water quality in rivers and wetlands, sediment transport and river morphodynamics. However, the MIKE HYDRO River model requires a large amount of data and a proper simulation of some constituents can be difficult to achieve if data are lacking [4]. The model is also highly dependent on bathymetric accuracy.

5.1.3. MOHID Water

MOHID Water (MOHIDw henceforth) is an open-source water modeling system (Table 2) designed for the effective simulation of 3D baroclinic circulation across river-to-ocean scales, using a finite volume approach that solves the primitive continuity and momentum equations for the surface elevation and 3D velocity field for incompressible flows. Temporal discretization is performed by a semi-implicit (ADI) algorithm with two time levels per iteration. MOHID Water couples the hydrodynamic model with two water quality/biogeochemical models with different levels of complexity: a simpler NPZ (nutrient-phytoplankton-zooplankton) model using the EPA formulation [45] and a complex multi-elements model for marine ecological processes [46]. The model was originally developed for marine systems but its modular code configuration allows its use in a variety of spatial and temporal scales to study processes occurring in reservoirs [47], estuaries and coastal lagoons [48–53], up to regional scales [54]. More recently the MOHID Land model has been developed for watershed and groundwater processes [55,56], aiming at a future full modeling of the land-to-ocean water continuum [57].

5.1.4. QUAL2KW

QUAL2Kw (Table 2) is the recent development of models in the QUAL 2 series [58–60], released by the EPA. QUAL2Kw is a 1D steady-state model for rivers, tributaries and well-mixed lakes. Unlike the previous versions, QUAL2Kw allows for unequal river reaches, and multiple water inputs and abstractions in each segment. The model solves both the advective and dispersion modes of transport in the mass balance of constituents. The model allows the simulation of several parameters: dissolved oxygen (DO), biochemical oxygen demand (BOD), temperature, pH, conductivity, suspended solids, alkalinity, total inorganic carbon, organic nitrogen, ammonia, nitrite, nitrate, organic phosphorus, inorganic phosphorus, algae (chlorophyll a), coliform bacteria, one arbitrary non-conservative constituent solute, and three conservative constituent solutes. QUAL2Kw is a well-documented freeware model and is specially designed for a system where macrophytes play an important role. It has been used to simulate lotic systems [61–63].

Table 3. Summary of the main characteristics of the selected water quality models (adapted from [7,61]).

Features	CE-QUAL-W2	MIKE HYDRO River	MOHID Water	QUAL2KW	SIMCAT	SisBaHIA	TOMCAT	WASP7
Dimensions/Types	2D, dynamic	1D, dynamic	3D, dynamic	1D, steady-flow	1D, steady-state (time-invariant), stochastic	3D, dynamic	1D, steady-state (time-invariant)	3D, dynamic
Modeling approach	ADE, unequal river reaches, river branches	ADE, unequal river reaches,	Regular grid, finite elements	ADE, unequal river reaches,	CSTR	Non-structured grid, finite differences	CSTR	ADE, dynamic compartmental
Element cycles	O, C, N, P, Si, Fe	O, N, P	O, N, P	O, C, N, P	O, N	O, N, P	O, N	O, N, P, Si
Constituents/processes	Temperature, pH, N (ON, NO_2, NO_3, NH_3), P (OP, PO_4), DO, CBOD, TIC, alkalinity, phytoplankton (4 groups), bottom-algae, SOD, detritus	User defined (ECO Lab module)	Temperature, N (ON, NO_2, NO_3, NH_3), P (OP, PO_4), DO, phytoplankton, detritus	Temperature, pH, N (ON, NO_2, NO_3, NH_3), P (OP, PO_4), DO, CBOD, TIC, alkalinity, phytoplankton, bottom-algae, SOD, detritus	DO, CBOD, ammonia, user defined conservative parameter	Temperature, pH, N (ON, NO_2, NO_3, NH_3), P (OP, PO_4), DO, phytoplankton, detritus	DO, CBOD, ammonia, chloride, user defined parameter	Temperature, pH, N (ON, NO_2, NO_3, NH_3), P (OP, PO_4), DO, CBOD, TIC, alkalinity, salinity, phytoplankton, bottom-algae, SOD, detritus, OCHEM
Open	Yes	No	Yes	Yes	-	No	-	Yes
Strength	Optimized for reservoir modeling; detailed parameterization of sediment diagenesis	Extensive support material	Full hydrodynamic simulation	Auto-calibration	Simulations requiring low computational time with limited data, auto-calibration	Grid adaptation to complex domain geometries	Simulations requiring low computational time with limited data, auto-calibration	Organic and heavy metal pollution
Weakness	Requires extensive data	Requires extensive data	Computational demand	Does not simulates branches	Over-simplistic	Limited number of users	Over-simplistic	Requires extensive data

Note: ADE: advection dispersion equation, CSTR: continually stirred tank reactor in series, DO: dissolved oxygen, CBOD: carbonaceous biochemical oxygen demand, OCHEM: organic chemicals, ON: organic nitrogen, OP: organic phosphorus, SOD: sediment oxygen demand, TIC: total inorganic carbon.

5.1.5. SIMCAT

SIMCAT (Simulation of Catchments, Table 2), originally developed by the Anglian Water Group, UK, is a one-dimensional, time-invariant (steady-state) model to simulate the fate and transport of solutes in a river [6,64]. SIMCAT is a stochastic model relying on Monte Carlo analysis techniques. The model includes the inputs from point-source effluent discharges including DO, non-conservative substances such as BOD with a decay rate, and conservative substances which are assumed not to decay. The model splits the river into user defined reaches, and in each run, the model randomly selects values for quality and flow from the given distributions for all the inputs. This model excludes processes such as photosynthesis and oxygen consumption in the sediments, thus becoming limited to model the reservoir dynamics. However, it is suited for modeling constituents in freshwater that do not rely on sediment interactions. SIMCAT is easy to use, allows fast runs and requires a relatively small amount of data to operate. The model can easily be applied at the basin scale and used as an evaluation and management tool by trained technicians [65].

5.1.6. SisBaHIA

SisBaHIA® (Sistema Base de Hidrodinâmica Ambiental) (Table 2) was originally developed to simulate coastal and in-land water bodies [66,67], and is composed of a 3D hydrodynamic model coupled to a water quality model. The advection–diffusion equation is solved individually for each constituent, taking into consideration the advective and diffusion terms, together with the transformation terms [68]. The model relies on finite elements and the finite difference approach in the spatial and time discretization, respectively. Turbulent stress is parameterized according to filtering techniques derived from the approaches known as large eddy simulation. The water quality model uses the same basic transformation equations presented in the WASP (Water Quality Analysis Simulation Program) model, and also uses the same spatial grid as the hydrodynamics model. SisBaHIA can have non-restricted used for non-profit applications such as research purposes. However, its use in a commercial activity (e.g., for consultancy purposes) can only be done under the payment of a fee defined by direct agreement with COPPE/UFRJ.

5.1.7. TOMCAT

The TOMCAT (Temporal Overall Model for Catchments) (Table 2) model was advanced in the 1980s by Thames Water, a UK water utility company, to assist in studying and improving effluent quality at all Thames water sites [69,70]. While TOMCAT follows a similar approach to SIMCAT, by assuming a continuous stirred-tank reactor (CSTR) method and Monte Carlo stochastics, it differs by allowing more complex temporal correlations. The model allows for setting the number of parameters by river segment, as well as the length, mean area, cross-section, and depth for each river reach. Equations relating the processes that control the concentration of solutes are identical to SIMCAT, except for temperature and DO. The simpler approach of TOMCAT requires a rather limited amount of data when compared to other models. However, its simpler approach also comes with some limitations, like the number of simulated processes, some of which are relevant for aquatic systems, such as photosynthesis, respiration, and sediment dynamics.

5.1.8. WASP7

The WASP model (Water Quality Analysis Simulation Program) (Table 2) is a freeware model developed by the EPA for surface water quality processes [71]. WASP7 can be coupled to hydrodynamic and sediment transport models that provide flow, depths, current velocities, temperature, salinity and sediment fluxes. As such, the WASP7 model can become a full 3D dynamic model, but linking the model to multi-dimensional hydrodynamic models is not a straightforward task. The model relies on the finite difference method to calculate the temporal and spatial evolution of these constituents in each segment of the computational geometry. WASP models have been applied to address several water quality problems in a variety of aquatic systems, such as ponds, lakes, rivers, reservoirs, estuaries and coastal waters [72–74]. WASP7 addresses processes that take place both in the water columns and sediment and is particularly useful to simulate organic chemicals. However, the model does not simulate mixing zones and near-field effects and does not handle the sinking and flotation behavior of some constituents.

5.2. Evaluation Criteria for the Case Study

A list of 16 criteria was defined (Table 4), with two identified as eliminatory criteria: criterion S9 (modelling approach) and criterion E6 (cost). If the modelling approach was CSTR (see Table 3) on criterion S9, then the model was excluded from the evaluation process, since this approach fails to reproduce the vertical thermal structure of the reservoirs, a relevant process for the present case study. The criterion for exclusion, E6, was based on the model not being freeware or open source. This exclusion factor was applied as long as there were enough open source or freeware models suitable for the case study in the evaluation process.

Table 4. Set of criteria defined for each cluster used in the evaluation of the models. Criteria defined by the technical team (^{T}) and/or the end-users (^{E}).

Clusters	Criteria
Scope	S_1: model outputs for chlorophyll (besides biomass) for a direct validation with field data ^{T,E} S_2: explicit simulation of different functional groups of primary producers, including cyanobacteria ^{T,E} S_3: inclusion of iron, given its role in the quality of water for human consumption ^{E} S_4: simulation of pH, for its relevance on fresh water chemical reactions ^{T,E} S_5: O, N and P cycles ^{T} S_6: carbon dynamics ^{T} S_7: sediment-water fluxes, with detailed parameterization of processes occurring in the sediment ^{T,E} S_8: adequate spatial description and hydrodynamics processes to simulate thermal stratification and related water movement ^{T} S_9: modelling approach ^{T}
Record	R_1: number of publications ^{T} R_2: model dissemination (local vs. global applications) ^{T,E} R_3: type of water systems (higher to lower score: reservoirs, rivers, estuaries/coastal lagoons) ^{T}
Experience	E_1: quality of the Graphical User Interface ^{E} E_2: availability and quality of support manuals ^{E} E_3: examples of running applications ^{T,E} E_4: user forums ^{E} E_5: technical support by the developing team ^{E} E_6: costs ^{E}

5.3. Valuation of Criteria for the Case Study

Three models were excluded from the evaluation process based on the eliminatory criteria. These were MYKE HYDRO River (criterion E6), SIMCAT (criterion S9) and TOMCAT (criterion S9).

For the remaining models (CE-QUAL-W2, MOHIDw, SisBaHIA, QUAL2KW and WASP7) the results for each cluster are shown in Figure 4 and the values for the ranking of models for each criterion are presented in Table 5. The results show that CE-QUAL-W2 had higher values for all clusters, with a clear gap to the remaining models. The WASP model showed the second-highest mark for all clusters, followed by MOHIDw and SisBaHIA in Scope, MOHIDw in Record and QUAL2Kw in Experience. A brief analysis is presented in the next sections for each cluster.

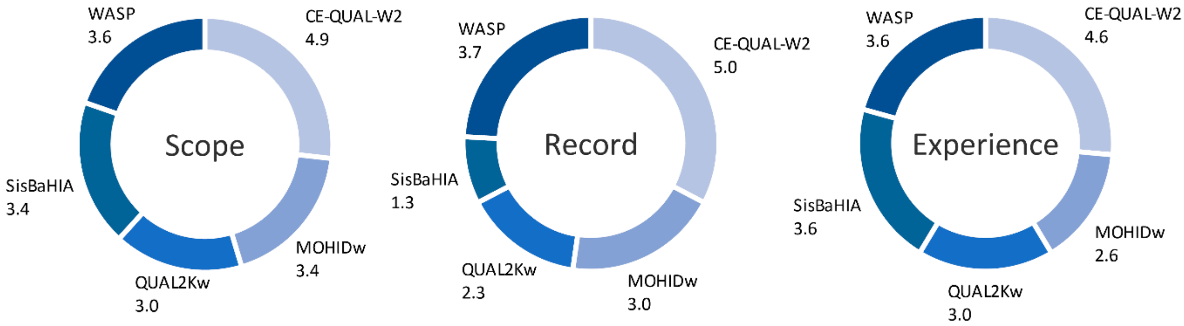

Figure 4. Scoring of models within each cluster, according to Equation (1) applied to their defining criteria (see text for details).

Table 5. ScoRE impact matrix. The scale represents the number of models under evaluation and, consequently, ranges from 1 (inferior) to 5 (better). Overall results for Scope, Record, and Experience are calculated according to Equation (1).

Criteria/Item	CE-QUAL-W2	MOHIDw	QUAL2Kw	SisBaHIA	WASP
S_1: chlorophyll	5	3	3	3	4
S_2: cyanobacteria	5	3	3	3	4
S_3: iron	5	4	4	4	4
S_4: pH	5	3	3	4	3
S_5: O, N and P cycles	5	3	4	3	4
S_6: carbon dynamics	5	3	4	3	3
S_7: sediment-water fluxes	5	3	1	2	4
S_8: hydrodynamic processes	4	5	2	5	3
Scope	**4.9**	**3.4**	**3.0**	**3.4**	**3.6**
R_1: publications	5	4	2	1	3
R_2: model dissemination	5	3	2	1	4
R_3: type of water systems	5	2	3	2	4
Record	**5.0**	**3.0**	**2.3**	**1.3**	**3.7**
E_1: GUI	4	1	2	5	3
E_2: support manuals	5	2	4	3	5
E_3: examples	5	4	5	4	5
E_4: user forums	5	4	3	1	2
E_5: technical support	4	2	1	5	3
Experience	**4.6**	**2.6**	**3.0**	**3.6**	**3.6**

5.3.1. Evaluation of Model Scope

Considering the criteria in model Scope, CE-QUAL-W2 had the highest score, denoting a better capacity to address all the characteristics of the studied systems under consideration. The WASP model followed in the ranking for Scope, since it also addresses most of the items. Like CE-QUAL-W2, the WASP model was developed for fresh water systems, having a detailed parameterization of chemical reaction characteristics of such water bodies, including sediment processes and water-sediment mass fluxes. MOHIDw and SisBaHIA both have an advantage with their 3D setup, allowing a more realistic simulation of hydrodynamic processes in larger reservoirs. WASP7 also enables the user to work on 3D systems, when coupled with a 3D hydrodynamic model. CE-QUAL-W2, on the other hand, only allows for a 2D setting, relying on the assumption that this approach is suited for most reservoirs. However, MOHIDw and SisBaHIA miss some relevant processes/constituents in fresh water systems.

5.3.2. Evaluation of Model Record

Models were searched for hits in *ScienceDirect* (SD), in both the combination of 'Title, abstract and keywords', and 'all fields', and *Web of Knowledge* (Wok), for both 'Title' and 'Topic'. The results are depicted in Figure 5. According to both portals, CE-QUAL-W2 stands as the model with the highest number of hits, except for 'Title' in SD where MOHIDw had the highest score. SisBaHIA was the model with fewer hits on both SD and WoK. Browsing available studies of each model reveals that CE-QUAL-W2 is the most disseminated model, having numerous applications worldwide, followed by WASP and MOHIDw models also with a global reach, but with lesser applications, and finally by SisBaHIA, almost confined to Brazil. CE-QUAL-W2 also ranks higher in the type of water systems, since it has been purposely developed for rivers and reservoirs, unlike other models that were mostly developed for coastal and transitional waters (e.g., MOHIDw and SisBaHIA).

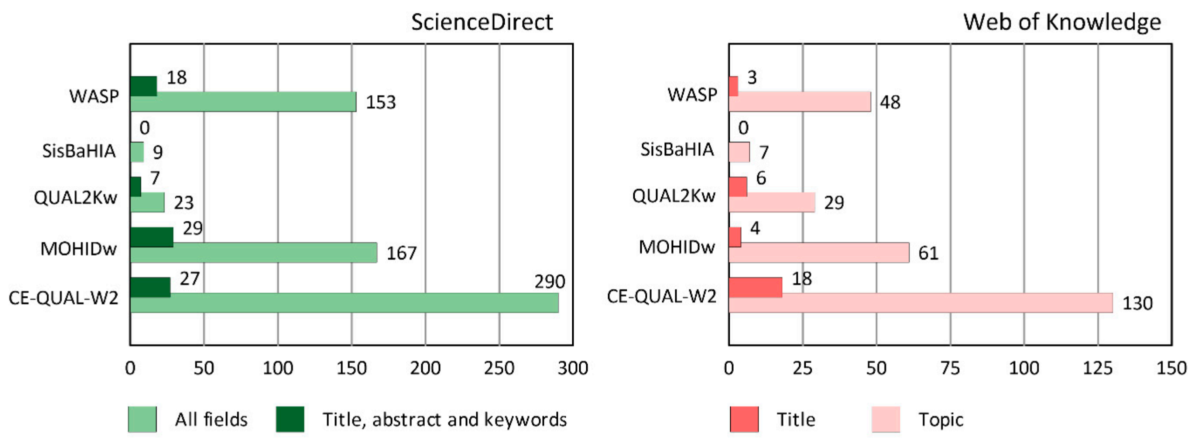

Figure 5. Number of hits obtained for each model in *ScienceDirect* and *Web of Knowledge* by 20 December 2016. Conditions for search: all journals and books available in *ScienceDirect* (SD) and available papers in *Web of Knowledge* (WoK); WASP model versions from 4 to 7 were considered.

5.3.3. Evaluation of Model Experience

All models provide a GUI interface, support material and running examples, and have user forums where users and developers can post comments and exchange information. These, however, vary in sophistication and completeness between models. CE-QUAL-W2 is the model that offers the more comprehensive user manual, detailed examples of running applications and a dedicated user forum. MOHIDw, for example, is a community model in continuous development by a number of users worldwide and, although a highly complex and comprehensive modeling platform, the support documents are dispersed over several sources and not centralized and updated in the form of a user manual. SisBaHIA has the most intuitive native GUI, followed by CE-QUAL-W2 with a software developed by the community of users. All other models have a suitable GUI, and MOHIDw even provides the use of an advanced GUI, in the form of the commercially licensed software MOHID Studio (Action Modulers: Mafra, Portugal). This software integrates model simulations with the management of field data, among many other modeling support tools. Likewise, CE-QUAL-W2 also has the option of using a GUI with additional options when compared to the native version. SisBaHIA is the only model that offers technical support in the form of a service, the terms of which are decided on a case-by-case basis. Other models offer interspersed support in the form of help to users provided by authors (e.g., CE-QUAL-W2), the institution responsible for the model (e.g., WASP7) or the team of developers (e.g., MOHIDw).

5.4. Model Ranks

Model ranks were obtained using Equation (2), and by assigning the relative weight of 50% to Scope (W_S), 25% to Record (W_R) and 25% to Experience (W_E), according to the end-users.

The ScoRE ranking, determined according to Equation (2) with the calculated values for each cluster (Table 5), showed that CE-QUAL-W2 was the most suited model (ScoRE = 4.8), followed by WASP (ScoRE = 3.6), MOHIDw (ScoRE = 3.1), SisBaHIA (ScoRE = 2.9) and QUAL2Kw (ScoRE = 2.8). In fact, not only did CE-QUAL-W2 perform better overall, it performed better in terms of the three clusters, being the best model in terms of Scope, Record and Experience for this particular case study. The results are graphically illustrated in Figure 6.

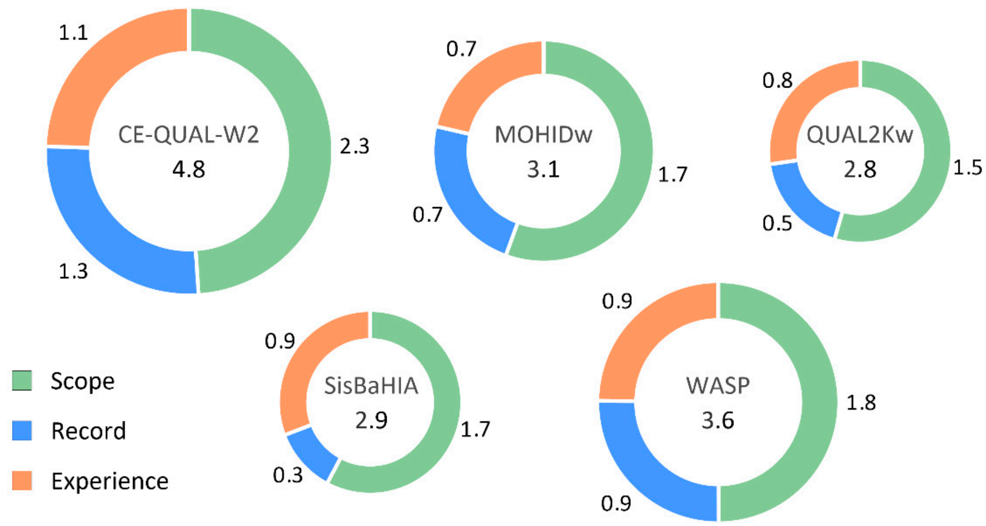

Figure 6. The ScoRE results for the evaluated models. Scope, Record and Experience values are calculated in Table 5. ScoRE was determined using Equation (2), with the following relative weights: W_S = 50%, W_R = 25% and W_E = 25%.

6. Discussion

6.1. Criteria Defined in ScoRE

The ScoRE approach starts with only three broad clusters of criteria and a blank list of criteria. Consequently, it imposes less framing regarding criteria definition than other methods found in the literature [18–20]. Reducing framing means the list is more flexible and allows new criteria to emerge, but it can also mean relevant criteria might not be identified and used in the analysis. This is the reason why authors propose the involvement of both the technical team and end-users in the criteria definition process; while the technical team has a better understanding of the processes being modelled, end-users have a better grasp of the relevant social, political, institutional and economic context and constraints. However, in the present case, end-users have only defined financial criteria.

A total of 18 criteria were defined. This is a higher number than other studies, which presented on average of 10 criteria [18,19,21,22], with the exception of Grimsrud et al. [20] which offered a total of 24 criteria (Table 6). From Table 4, we can see that half of the criteria were generated from the technical team and half generated from the end-users. Both defined six of the criteria. The criteria outlined by end-users were mostly related with the Experience cluster. This shows that both model users and modelers can contribute meaningfully to the definition of criteria.

Table 6. Number of criteria identified in ScoRE and in other approaches (approximate numbers).

Number of Criteria Related with	Saloranta et al. [18]	Boorman et al. [19]	Grimsrud et al. [20]	Chinyama et al. [21]	Tuo et al. [22]	ScoRE
Scope	5	8	13	5+(a)	3	9
Record	1	1	0	0	0	3
Experience	8	3	11	4	1	6
Total	14	12	24	9+	4	18

(a) the guiding questions proposed can give origin to more than five criteria.

The criteria defined in the case study are within the range of criteria found in the literature. Despite the freedom in criteria definition for ScoRE, novel criteria did not emerge from this particular case study. In this sense, ScoRE lead to similar results to those expected if other methods were used for criteria definition. From the literature analyzed, ScoRE was the only approach where the list of criteria is empty at the beginning of the process and where both modelers and end-user define the criteria for the evaluation process. The results obtained show that model users can define criteria for the evaluation, complemented with additional criteria suggested by the modelers. This means that criteria definition can be opened up for discussion between modelers and end users, in addition to the valuation stage.

The range of criteria defined for this particular case did not include, for example, criteria linked with the accuracy of the data and model, if the models include uncertainty or sensitivity analyses to the results, or even on the availability of data [18,20,25]. Such criteria, however, should be part of the criteria list in further studies, given their implications on the use of the model and validity of its results.

6.2. Valuation of Criteria in ScoRE

In ScoRE, the technical team performs the valuation of criteria, not the end-users. The particularity of ScoRE is that values for models in the criteria are discussed with the end-users, in particular, those referring to criteria within the cluster "Experience". The advantages of having the technical team performing the scoring are that the end-users might not process all the knowledge necessary to adequately evaluate the models under the criteria [19], in particular, the criteria falling under the cluster "Scope".

The disadvantages of such an approach are that the process can become less transparent (and less accountable), costlier (due to the costs of hiring a technical team) and lengthier [18,20–22]. The fact that ScoRE allows the discussion of the scorings with the end-users helps to restore transparency in the model selection process. Furthermore, for this particular project, the decision to use a technical team to model water quality has been made before the decision of whether to involve the technical team on model selection. Therefore, in this particular case, asking the technical team to select the appropriate model for the case study was just an additional small cost to the overall budget.

Another particularity of ScoRE was the use of eliminatory criteria that had two values linked with acceptable and not acceptable scores. Being scored unacceptable in any of these eliminatory criteria meant the elimination of the model from the process. In this case study, two eliminatory criteria were defined which resulted in the elimination of three models from the evaluation. In this regard, the main difference between ScoRE and Tuo et al. [22] is that, for the remaining models, ScoRE presents clear guidance for weight definition.

6.3. The ScoRE Aggregation Procedure

The results show that CE-QUAL-W2 performed better than the remaining four models analyzed (Figure 6). It is important to stress that results are specific for this particular case study, as the choice of criteria and the weights attributed to the clusters can vary from application to application, resulting in different rankings. The outcome of this method reflects the importance that the technical team and the end-users assign to different criteria. Even for a reservoir, for example, SisBaHIA or MOHIDw could have a higher ScoRE than other models, if the focus of the study relied heavily on hydrodynamics, since both achieved better spatial simulation of transport processes [38,75]. Likewise, if an integrated watershed–river–reservoir modelling approach was favored, MOHIDw would be a better option, reaching a higher ScoRE, as it can be coupled with MOHID Land, which describes the transport of water in the watershed [57,76].

In this case study, end-users attributed higher weight to the cluster "Scope," and equal weights to the clusters "Record" and "Experience" (Section 5.4). These results are not surprising and in line with other works on model selection, in which most of the criteria are related with the cluster "Scope" [19–21,25,77], as shown in Table 6. The only literature case analyzed that provided a higher number of criteria to another category rather than "Scope" was Saloranta et al. [18], which defined five criteria for scope, but eight for Experience (and one for record).

Although the clusters Record and Experience had equal weights (25% each, Section 5.4), the cluster Experience scores were higher or similar to the scores from the cluster Record (Figure 6), with a small exception for the model CE-QUAL-W2, where Record value was 0.1 points higher than the value for Experience. Interestingly, the literature shows more criteria related to the cluster Experience, than with the cluster Record [18–20,25,77]. Therefore, results obtained here seem to agree with the observed patterns in the literature concerning criteria relevance (Table 6).

The aggregation procedure used in ScoRE to obtain ranking is a procedure which includes a mixture of approaches: from eliminatory criteria [18–21], averaging scores of criteria (within the same cluster), and consulting with end-users to define weights to the clusters which are then added using a linear additive model (a compensatory aggregation procedure).

The proposed approach requires communication between modelers and end-users, thus promoting the pivotal exchange of information [78]. This, in turn, leads to rational reflection, and potentially, some learning from both sides. Additionally, by making use of a linear additive model for aggregating results, the outcome is more straightforward to understand by end-users, improving the transparency of the method. However, the linear additive procedure is a compensatory method in which weights are recognized as trade-offs. This is an essential issue for sustainability, as certain voices and some ecosystem services should not be traded off [23,79,80]. For models, it can mean that a combination of a high score in the interface with a low score regarding a specific relevant modeled parameter, can exceed a higher score in the referred parameter combined with a lower score on the interface. By using the eliminatory criteria, ScoRE allows reducing some of this compensatory nature, being a partially compensatory approach. However, criteria within each cluster are still averaged. By doing so, one is assuming that all criteria not classified as an eliminatory criterion within the same cluster are equally relevant, which might not always be the case.

In this case study, as in all the approaches reviewed in this paper, end-users are clearly defined and limited in the number of individuals, and it's not infrequent to have only one decision-maker. Under more complex decisions, with more decision-makers, a discussion on whether weights should or not be used needs to take place to avoid social traps, ensure all relevant voices are included, and ensure that value disparities and conflicts are recognized and managed correctly [16].

6.4. A Word on Robustness, Sensitivy and Transparency of the Process and Results Obtained

Finally, results from ScoRE are discussed with the end-user who can go through the whole process and change it. This way, results are exposed to validation by the end user. Furthermore, ScoRE starts with a clean sheet regarding the criteria to be used for the evaluation (and the relative importance of each criterion—the weights), which allows different end-users (and modelers) to participate in the identification of which criteria to include in the evaluation, potentially accommodating different perspectives in the process. The two factors mentioned help ScoRE to reduce ambiguity in its results and to be seen as potentially more robust than other approaches. This step also entails a sensitivity analysis in which some of the assumptions or parameters included in the model are given a different value, to test whether the final ranking of alternatives changes. This methodology is more in line with the post-normal approach to science (with the use of a peer-review community [81]). It is also in line with other approaches dealing with uncertainty (e.g., Stirling [82]), where the focus is not on accepting scientific inputs uncritically, i.e., without articulating the degree of risk associated with the results or the values that inevitably enter in the presence of uncertainty.

7. Conclusions

For many years, decision-makers have managed water quality in rivers and reservoirs empirically, relying to some extent on scientific tools and input, but frequently based on political motivations. The need for sound decisions, however, has pushed the development of numerical models to address specific environmental and socioeconomic setting. Eventually, this effort resulted in the myriad models that are now available, raising the problem of their choice by users. A model will hardly possess all the required functionalities for a specific application and, consequently, the choice of a model depends upon many conditions and requirements.

Given the significant number of available modeling tools for such tasks, water managers wanting to use numerical tools must, at some point, choose among the myriad options, frequently without any specific criteria or methodology. The debate on how to select water quality models is relatively recent, and only a few approaches to model choice have been proposed. While not being a method to compare models in their essence, ScoRE may be useful for that purpose.

The main advantages of ScoRE are:

- Criteria to compare models are defined in a dialog between the modelers and end-users. Introducing both perspectives into criteria definition can lead to a more comprehensive list.
- ScoRE is a transparent method, as end-users are invited to go through the whole process and to discuss final results with the technical team.
- The guidance on how to select a model when models are not excluded by eliminatory criteria (in contrast with most of the literature found, with some exceptions [22]).
- The final discussion of results with end users, allowing for the refinement of results, and producing a more robust outcome.

ScoRE is not free from limitations, nonetheless. In ScoRE, end-users have little say in the scoring stage, making the process more resource-consuming (concerning time and costs), as a technical team is required for the scoring stage. ScoRE's weighting procedure is still a complex procedure involving averaging scores within clusters and attributing weights to clusters. This could be further simplified. Finally, more emphasis can be put into eliminatory criteria (higher number of criteria classified as eliminatory). These will be the target of improvement in further stages of this research.

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