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A Multi-Scale Assessment of Land-Use Impacts on Hydrologic Ecosystem Services in the Vouga Basin, North-Central Portugal

A

DISSERTATION

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Daniel Robert Hawtree

MSc. Geography

born on March 9, 1979 in San Diego, United States of America

Supervisors: Prof. Dr. Karl-Heinz Feger (Technische Universität Dresden)
Prof. Davide Pettenella (Università degli Studi di Padova)

Reviewers/Examiners: Prof. Dr. Karl-Heinz Feger (Technische Universität Dresden)
Prof. Davide Pettenella (Università degli Studi di Padova)
Prof. Dr. Martin Volk (Helmholtz-Zentrum für Umweltforschung)

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Abstract

Sustainable water resource management requires understanding how hydrologic processes are impacted by environmental management and land-use decisions across multiple spatial and temporal scales. A key concept in this respect is hydrologic ecosystem services (HES), which are the water related 'goods' produced by the environment which are valuable to humans. This dissertation assesses a range of topics concerning HES in the Vouga basin (north-central Portugal), and their connection with land-cover and land-use practices. Specifically, the relationship between changes in forest and agricultural land-cover and management practices, and associated changes in HES were examined using a range of statistical and modeling approaches. To quantify the effects of different agricultural scenarios on both HES and potential stakeholders, the 'Soil and Water Assessment Tool' (SWAT) was utilized, in conjunction with economic assessment methods.

The first research section (Section 6) of the dissertation assesses the trends in streamflow quantity and yield in the Águeda watershed (a sub-basin of the Vouga) over a 75-yr period which coincided with large-scale afforestation of *Pinus pinaster* and (later) *Eucalyptus globulus*. Counter to the findings from meta-analysis studies of the effect of forest change on water availability, this study did not detect statistically significant trends in streamflow. By contrast, these findings support the view that there are prerequisite climatic, pedological, and eco-physiological watershed conditions that are necessary to observe hydrologic impacts at the watershed scale (which are not present in the Águeda watershed). By contrast, the significant changes which were detected are related to baseflow, which correspond with different periods of afforestation, and may be attributable to the promotion of soil water repellency under the mature pine and eucalypt stands.

In the second research section (Section 7), an assessment is carried out on the hydrologic and nitrate dynamics at the whole basin scale, using the SWAT model. This assessment indicated that there is a high degree of variability in nitrate export from the different parts of the basin, with the highest rates coming from the lower (agriculturally dominated portion) of the basin. The main flow pathways for nitrate export were found to be leaching from agricultural land-cover types, which consistently had the highest export for all land-use and pathways. These findings indicate that the water bodies at the highest risk of nitrate pollution in the Vouga basin are the groundwater aquifers.

The final research section (Section 8) utilizes the SWAT model to examine how reduced rates of fertilizer inputs would affect nitrate leaching, crop yields, and agricultural profitability in the lower Vouga basin. This research found that reduced rates of fertilization would reduce the amount of leached nitrate substantially, but that this would also lead to a large decrease in crop yield and profitability. A large

difference in the inefficiency (*i.e.* crop production vs. nitrate export) between different HRUs was found, which could provide a focus for potential management action. This research strongly indicates that such actions may be needed to reduce the negative impacts of this pollution on the value of the groundwater aquifers, and to avoid associated costs which are otherwise passed on to local water users (*e.g.* through higher water treatment costs).

The overall findings of the dissertation highlight the importance of the upper (forested) basin as a drinking water supply area, given the prevalence of nitrate pollution in the lower basin. However, the historic afforestation in the Vouga basin has resulted in a reduction in baseflow, which is negative from a drinking water supply perspective. Therefore, while the forested uplands are beneficial from water quality standpoint (compared to intensive agriculture), they also have altered flow patterns in a manner which will reduce available supply. The findings from the upper basin contrast sharply with the lower basin, where there are potentially large negative HES impacts due to current agricultural practices. These practices will primarily impact groundwater aquifers, and therefore the water quality within the lower basin receive little benefit from the relatively high-quality water from the upper basin. This highlights the importance of considering the interconnectivity of HES across spatial scales, which will depend on the specific site characteristics of the river basin.

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Abbreviations / Acronyms

AVIPE	Associação de Viticultores do Concelho de Palmela
BF	Baseflow Quantity
BFI	Baseflow Index
BMP	Agricultural Best-Management Practices
CMB	Conductivity Mass-Balance
CRU	Climatic Research Unit at the University of East Anglia
ES	Ecosystem Services
EU	European Union
FAO	Food and Agriculture Organization of the United Nations
GD	Groundwater Directive
HES	Hydrologic Ecosystem Services
HRU	Hydrologic Response Unit
IPMA	Instituto Portugues do Mar e Atmosfera
KGE	Kling–Gupta Efficiency
KS	Kolmogorov–Smirnov
NCDC	National Climatic Data Center
NSE	Nash-Sutcliffe Efficiency
PET	Potential Evapotranspiration
RMBPs	River Basin Management Plans
SDGs	Sustainable Development Goals
SNIRH	Sistema Nacional de Informação de Recursos Hídricos
SWR	Soil Water Repellency
SWAT	Soil and Water Assessment Tool
WFD	Water Framework Directive

1 Introduction

1.1 Background and Motivation

Freshwater is a limited resource that must meet many different demands, including food production, human consumption, sanitation, industrial processes, and habitat for aquatic species. If water of adequate quantity and quality is not available to meet all these different needs, then competition and conflict will occur, and some demand will go unmet. The fair use and allocation of water resources has many challenges, as water resources frequently cross administrative, regional, and national boundaries; and the actions of any individual stakeholder will affect the immediate environment but will also have far reaching impacts on downstream users. In many cases, available water resources will exceed the total quantity demanded, or quality needed; and without adequate management this can lead to negative environmental, economic, and societal consequences. This highlights the need for the sustainable management of water resources, and the recognition of the need to balance the often competing needs and demands of different stakeholders (Calder, 2005)

Achieving sustainable water resource management requires improving our understanding of how the hydrologic cycle is impacted by wider environmental management decisions across multiple spatial scales. A key concept in this respect is the role of water as an **ecosystem service**, meaning that it is an environmental 'good' produced by the environment which is has value to humans (Brauman *et al.*, 2007; TEEB, 2012). The concept of ecosystem services is based on the inherent link between the well-being of the natural environment and the well-being of people, by recognizing the critical role that the environment plays in underpinning economic and social activities (MEA, 2005). All land-management decisions have inevitable positive and/or negative impacts on the environment, which in turn affects the capacity of the environment to provide societies with ecosystem services. This production capacity can be quantified through the application of ecosystem service assessment and valuation methods, by which a monetary value can be placed onto the services provided (de Groot *et al.*, 2012).

The ecosystem services concept has become widely established in environmental sciences and is now a common framework from which to view the provision and management of natural resources. Despite this, many open questions remain regarding how to assess water resources within an ecosystem services context. Most traditional hydrologic assessment tools and methods were not designed with ecosystem services in mind, and considerable gaps remain between our ability to assess the impacts of environmental changes on water resources, and our ability to understand the final impacts on (multiple) ecosystem services at a scale relevant for human wellbeing. Improving this understanding requires ongoing development and improvement of the tools and strategies used to assess hydrologic ecosystem services in a way which are relevant and useful for environmental planning and decision making.

Within this context, this dissertation conducts a multi-scale assessment of land-use dependent hydrologic ecosystem services. This assessment is carried out in the Vouga river basin in north-central Portugal, which has several relevant land-use and water resource management issues to explore. Through this dissertation, the current status, developments, and future prospects of hydrologic ecosystem services assessment are examined in detail. Throughout this research, emphasis is given to the development and application of modeling methods which are designed to improve model assessments in a data scarce region with a high level of hydrogeochemical complexity.

1.2 Structure of the Dissertation

The dissertation consists of 9 sections; **Sections 1 through 3** provide the introduction, research background, and research topics and hypotheses; **Sections 4 and 5** provide a review of the research methods used in the study, and an overview of the study region; **Sections 6 through 8** present the three component studies which address the research topics; and **Section 9** provides a research summary and conclusion of findings. A brief description of the individual sections is as follows:

- **Section 1** introduces the dissertation, including the overall background and motivation for the research topic.
- **Section 2** provides context in which the research is conducted by detailing the specific themes addressed in the research; including a discussion of Hydrologic Ecosystem Services (HES), the role of land-use/management on HES provision, a review of the relevant methods for HES assessment, and the concepts and methods behind ecosystem service valuation.
- **Section 3** presents the research topics examined in the three research sections, and the specific hypotheses which are tested.
- **Section 4** gives a description of the research methods used in this study, broken down into the corresponding three research sections.
- **Section 5** describes the geographical, hydrological, and land-use characteristics of the study region; the Vouga Basin of north-central Portugal; and provides an overview of the current status of hydrologic ecosystem services and related water resource of concern in this basin.
- **Sections 6** is the first of the research sections, which presents the results of research conducted on a forest-dominated sub-basin of the Vouga basin (*i.e.* the Águeda watershed), where a statistical/trend-

testing approach was applied to examine the long-term impacts of afforestation on hydrologic processes. This section presents a re-examination of the findings from the publication “Time series analysis of the long-term hydrologic impacts of afforestation in the Águeda watershed of north-central Portugal” (Hawtree *et al.*, 2015), within the broader context of the overall dissertation.

- **Section 7** presents the research findings from a hydrologic assessment of the overall Vouga basin, using the eco-hydrological SWAT model to assess the impacts of current agricultural practices on water quality (specifically nitrate).
- **Section 8** builds upon Section 7 by focusing in greater detail on the agricultural-dominated lowland sub-basins of the Vouga basin. This section examines the potential for HES improvements from reduced fertilizer inputs, the impacts on agricultural production and profits, and a discussion of the economic impacts of changes in HES.
- **Section 9** provides a synthesis and the overall conclusions from the findings of the dissertation, and an outlook on recommendations for further research.

2 Research Background

The following section provides an overview of the context in which the research is conducted; including a discussion of the concept of 'Hydrologic Ecosystem Services' (HES); the connections between forests, agriculture, soils and HES provision; a discussion of landscape multi-functionality/scales and HES; and a brief overview of HES valuation.

2.1 Hydrologic Ecosystem Services

The hydrologic cycle is one of the fundamental biogeochemical cycles which underpins the Earth system, by recycling the water precipitated from the atmosphere through the terrestrial system (Dingman, 2015). The hydrologic cycle, as with the other biogeochemical cycles, provides services which are critical for the survival, health, and prosperity of human societies. These are known as **ecosystem services (ES),** which can be broadly categorized as falling into four categories: **(1) supporting services** are the fundamental services provided by ecosystems without which the other services could not function, **(2) provisioning services** are the products obtained from ecosystems, **(3) regulating services** are the benefits obtained from the regulation of ecosystem processes, and **(4) cultural services** are the non-material benefits obtained from ecosystems (MEA, 2005). From these four categories, those ES which are related to water resources are known as **hydrologic ecosystem services (HES)** (Brauman *et al.*, 2007). Table 1 provides an overview of the different ES categories, with general and hydrologic examples from each type.

The type, quantity, and quality of HES that an ecosystem produces are inseparably linked to both land-cover type and its environmental condition, which is closely linked to human activities (*i.e.* land management). Multiple different ES are frequently provided by the same or by interconnected ecosystems, and the relationship between the different ES may be synergistic, or may include trade-offs (Cord *et al.*, 2017). An example of a landscape which often provides synergistic ES is a mature forested landscape, which can provide the hydrologic ES of both flood protection and the climatic ES of carbon sequestration. By contrast, this same land-cover type may have an ES trade-off, in the form of reductions in water provision, due to higher consumption of water by forests when compared to alternative land-cover types (Brown *et al.*, 2005; Calder *et al.*, 2007). Given this inter-connectivity, understanding how different land-cover types and management options will affect ES is an important consideration for evaluating alternative land-use options and their potential synergies and/or trade-offs.

Table 1. Examples of ecosystem services (ES) and hydrologic ecosystem services (HES) from the different of ecosystem service categories.

CATEGORY	ECOSYSTEM SERVICE (ES)	HYDROLOGIC ECOSYSTEM SERVICE (HES)
SUPPORTING SERVICES	▪ Primary Production ▪ Nutrient Cycling ▪ Soil Formation	▪ Water and nutrients to support ecosystem functioning (*e.g.* aquatic habitats, plant transpiration/nutrition)
PROVISIONING SERVICES	▪ Raw Materials ▪ Food ▪ Genetic Material	▪ Water supply for municipal use, agricultural production, energy production, transportation, fisheries, *etc.*
REGULATING SERVICES	▪ Climate Regulation ▪ Disease Control ▪ Waste Decomposition	▪ Water quality protection, flood mitigation, protection from salinization/saltwater intrusion, erosion control
CULTURAL SERVICES	▪ Spiritual Value ▪ Recreational Value ▪ Science/Education	▪ Recreational/sporting use, conservation value, property value benefits of proximity to water bodies.

Two of the most critical land-cover types with respect to HES are **forests** and **agriculture**, both of which can have a major impact on the quantity and quality of available water resources. For both land-cover types, the characteristics and management of their **soil resources** is also inter-connected with HES provision. Additionally, while many landscapes are dominated by a single function (*e.g.* agriculture, urban areas), other landscape functions and services are often provided for as well, a concept which is known as **landscape multi-functionality** (Stürck and Verburg, 2017)**.** Increasing landscape multi-functionality has become a common goal as a means of improving the provision of ES, including HES (Mastrangelo *et al.*, 2014). It is also important to consider HES within the context of the value of their ecosystem services. **ES valuation** is the process of estimating how different environmental conditions will alter not only the production of ES, but the economic benefits and financial costs of these changes as well. This valuation process can help to make changes in ES more ‘concrete’ when being considered by decision makers, and lead to improved assessments of the anticipated benefits and trade-offs of management alternatives.

2.2 Forests and HES

Forests are the dominant land-cover types in large portions of the Vouga basin and can potentially have a major role effect on hydrologic ecosystem services (HES), both in terms of regulating service (*i.e.* flood retention, water quality) and provisioning services (*i.e.* water quantity). In terms of regulating services, forests typically provide beneficial processes for the production of good quality water. Forested land-cover provide a high degree of protection for soils, both by reducing erosion potential and by reducing sedimentation rates. Forests typically have low rates of runoff, and have characteristics which promote infiltration (*e.g.* low compaction and high porosity), leading to high rates of soil water recharge (Bruijnzeel, 2004). Through sub-surface soil-water processes, soils retain chemicals, minerals, and organic materials which are present in water, and thereby act as a physical filter on the water flowing through it. In addition to this natural filtration process, forests also normally have very low inputs of nutrients, biocides, or other contaminants, as compared to alternative land-cover types (*e.g.* agricultural lands, urban areas).

Given the benefits of forests on hydrologic processes, forests are an important landscape type with respect to protecting drinking water supplies (*i.e.* regulatory HES; Stolton, 2003). Forested upland areas are therefore a critical source of water for municipal use or other sectors requiring high quality water (*e.g.* high-tech industrial processes). Both in upland and in lowland areas, forests can be established to provide a "buffer zone" around reservoirs or riparian areas, and thereby reduce the input of pollutants which would otherwise enter water bodies. The water quality benefits of forests can also serve as a protection for human health by reducing biological contaminants, which will be of particular importance in rural areas and/or areas with low levels of built capital, where well-functioning forests can potentially reduce the incidence of disease (Herrera *et al.*, 2017).

In the United States, a prominent example of a forested watershed protection area is the upland region of New York State (*i.e.* the Catskill Mountains), which provides drinking water for New York City and surrounding metropolis. The environmental protections established in this area have secured the provision of high-quality water with minimal additional treatment requirements, which avoided the need for the establishment of an extensive water filtration system. By establishing this watershed protection region, an estimated cost of $4-6 billion for construction of a new filtration plant, plus $250 million per year in operating costs were avoided (Grolleau and McCann, 2012).

The role of forests in maintaining regulatory hydrologic ecosystem services has been well-established in the framework of the '2030 Development Agenda' and the 17 'Sustainable Development Goals' (SDGs) adopted by the UN General Assembly in 2015. Two of the stated SDG goals (#6 and #15) directly recognize the importance of the relationship between forests and water; as Target 6.1 establishes the goal of "*by 2020, protect and restore water-related ecosystems, including mountains, forests, wetlands, rivers, aquifers and lakes*"; while Target 15.1 establishes the goal of "*by 2020, ensure the conservation, restoration and sustainable use of terrestrial and inland freshwater ecosystems and their services, in particular forests, wetlands, mountains and drylands, in line with obligations under international agreements*" (UN, 2015). While progress towards these goals to-date have been mixed, this prominent recognition of forests for the protection of hydrologic ecosystem services within this international framework is an important step in the establishment of their importance in achieving a sustainable water resources future.

In terms of provisioning hydrologic ecosystem services (*i.e.* water quantity), the relationship between forests and HES is more mixed. Changes in water availability due to afforestation/deforestation are driven by several factors controlling the water consumption of different vegetation species, in particular canopy interception and evapotranspiration rates, which are typically higher in tree species than in shrub and herbaceous species (Calder, 1998). Meta-analyses of paired catchments studies have found that afforestation typically results in decreased streamflow while deforestation typically leads to increased streamflow (*e.g.* Bosch and Hewlett, 1982; Brown *et al.*, 2005).

However, the hydrologic response to deforestation is in general more consistent than the response to afforestation. This difference may be due to higher variability in land cover following afforestation compared to deforestation, and the effects of different transitional species and/or changes in forest physiology (Andréassian, 2004). In a global synthesis of afforestation studies, Farley *et al.* (2005) found that afforestation of grasslands or shrublands will lead, on average, to reductions of one-third to two-thirds of streamflow, with these reductions occurring rapidly after planting (*i.e.* within the first 5 years) and reaching their maximum reduction 15 to 20 years following planting. Given this higher water consumption in comparison to alternative land-cover types, forests have the potential to significantly reduce local water yields (Andréassian, 2004; Farley *et al.*, 2005). A prominent example of this effect is in South Africa, where the introduction and rapid spread of invasive alien tree species led to a significant reduction in water availability throughout much of the 20th century (Dye and Versfeld, 2007).

While there is strong evidence for local scale reductions in water availability due to forest conversion, provisioning HES may also be impacted by the improvements in soil characteristics which are induced by forests. Forest land cover tends to increase the infiltration, storage capacity, redistribution, percolation, and drainage of soil water; and these factors can enhance baseflow and increased groundwater recharge, which can help maintain water availability during dry seasons and/or drought (Scott and Lesch, 1997). This can be a particularly important consideration in regions with highly seasonal precipitation patterns, where there is an excess of water in the wet season and a deficit in the dry season, which an increase in baseflow can help offset. The increased infiltration capacity of forested areas may also help mitigate storm-driven peak flows, and therefore reduce potential flood damage; however, this effect may be subordinate to other watershed characteristics, particularly during severe flooding events (Wahren *et al.*, 2009).

In addition, while forests will typically reduce water availability at the local scale, they may play an important role in precipitation recycling at regional and continental scales, and many be particularly important source of moisture for inland areas far removed from large water bodies (Ellison *et al.*, 2017). Forests can also increase HES provision in areas where they generate fog and cloud water capture, which can occur particularly at higher elevations, thereby functioning as 'water towers' for downstream areas (Bruijnzeel *et al.*, 2011).

While the hydrologic impacts of forests at the plot and watershed scales are generally well understood, there are many local factors which will modify this relationship for any given site. Therefore, when attempting to evaluate the effects of a forest land-cover change for a specific watershed, a consideration of both the physical site conditions and vegetation types involved must be made. In this respect, Andréassian (2004) posits that there are several prerequisite conditions that need to be met in order to observe hydrologic impacts at the watershed scale. These include climatic conditions (*i.e.* periods of hydrologic surplus/deficit), pedological conditions (*i.e.* soil depth) and eco-physiological conditions (*i.e.* forest age-dependence). If these conditions are not met, then the typical 'forest-water relationship' identified from meta-analyses may not hold true.

Section 6 further examines the connection between afforestation and HES provisioning (*i.e.* water quantity) in the north-central region of Portugal, and considers a case study where the prerequisite conditions posited by Andréassian (2004) are examined.

2.3 Agriculture and Hydrologic Ecosystem Services

Large portions of the Vouga basin are dominated by agricultural land-cover, particularly the agriculturally intensive production areas of the lower basin. Agricultural activities are interconnected with hydrologic ecosystem services (HES) in a tightly coupled relationship, and often have large impacts on HES both in terms of water quantity and quality. Agriculture is the largest global consumer of water for human uses, accounting for 69% of all withdrawals, and current levels of water usage are already at, or exceeding, levels of available supply in many regions (Vörösmarty *et al.*, 2000). Groundwater extraction for both municipal use and agricultural production has greatly increased since the mid-20th century (Konikow and Kendy, 2005), and many agricultural areas worldwide are currently pumping underground aquifers at rates which far exceed their replenishment rate (*e.g.* the Central Valley of California, the Indo-Gangetic Plain of India). This overdraft can lead to a number of detrimental landscape and HES impacts, including soil subsidence and aquifer salinization (Konikow and Kendy, 2005).

Agriculture also has a major impact on HES with respects to water quality, due to pollution from the export of fertilizers, biocides (*e.g.* herbicides, pesticides, fungicides), and sediments from agricultural areas. Fertilizes and biocides can lead to significant alterations in the water chemistry of aquatic ecosystems, and high fertilizer concentrations can result in the eutrophication of water bodies, leading to severe damage to aquatic habitats and reducing the value of the associated water bodies (*e.g.* reduced drinking water quality/intake, damaged fisheries, reduced recreational value). Suspended loads from soil erosion leads to sedimentation of lakes and reservoirs, reducing both water holding capacity and hydropower generation potential, and are also damaging to aquatic species reliant on non-turbid water. Furthermore, suspended materials are also carriers of nutrients (*i.e.* nitrogen, phosphorus) or contaminants (*e.g.* heavy metals, pesticides) that are carried within or adsorbed to the particles.

The expansion in agricultural production seen in 20th century (*i.e.* the 'Green Revolution') was largely enabled by a reduction in cost and increased usage of manufactured agricultural products, such as synthetic fertilizers and various biocides (Lassaletta *et al.*, 2014; Tilman *et al.*, 2011). While this intensification in agricultural inputs led to large increases in agricultural yields, it also greatly increased the generation and export of contaminated farm runoff, much of which historically was unmanaged and entered water bodies without regulation or controls. Despite recent considerable efforts made to improve management approaches, agriculture is still a major source of water pollution, and controlling **non-point source pollution** has remained a persistent problem worldwide (Ongley, 1996).

The issue of agricultural impacts on HES is expected to persist for the foreseeable future, as population estimates predict that the global population will reach 9 to 10 billion by the second half of the 21st

century, while demographic factors are expected to increase food demand at an even higher rate than population growth (Godfray, 2014; Tilman *et al.*, 2011). This implies the need for a large increase in food production to meet growing demand, while at the same time there is an urgent need to avoid the negative environmental and health impacts which have historically characterized intensification in agricultural production. The challenge of simultaneously addressing the need for both increases in food production and decreased agricultural impacts has been dubbed "sustainable intensification", and is considered to be one of the major developmental and environmental challenges of the coming decades (Garnett *et al.*, 2013; Godfray, 2014).

In the research sections of the dissertation, the relationship between agricultural production and regulatory HES (*i.e.* water quality) is examined in **Sections 7 and 8**, specifically with respect to nitrogen fertilizer inputs, non-point source pollution, and nitrate leaching to groundwater.

2.4 Soils and Hydrologic Ecosystem Services

The maintenance of healthy and well-functioning soils is a critical component for the production of many ecosystem services. The critical ecologic services supported by soils include: carbon sequestration; habitat for plants, animals, and microbial life; a reservoir for genetic materials; and for a wide range of HES related to the intake, storage, transmission, and filtration of water (FAO, 2015). Soil is the primary medium in which water is held that supports biomass and agricultural production, as well as preventing excess surface runoff, and therefore mitigating both erosion and flooding. Water is redistributed through soils *via* vertical and lateral flow pathways, which both recharges aquifers and provides baseflow to streams. In the process of moving through the soil, water comes into contact with soil particles and biota, through which contaminants are removed, improving water quality over time (Brady and Weil, 2008).

The ability of soils to perform these hydrologic functions is controlled by their physical, chemical, and biological properties, with the amount and quality of organic carbon being a particularly important factor. The amount and quality of organic carbon in soils is largely dependent upon the type of land-cover and management practices applied at a location (Feger and Hawtree, 2013). Agricultural practices such as conservation tillage, mulching, and agroforestry will tend to promote increases in the level of soil organic carbon; while factors such as conventional tillage, erosion, and high-intensity fires will tend to deplete levels. The use of improved land-management approaches for increasing soil organic carbon, and therefore the production of HES, represents a valuable tool for water resource management. This is particularly important given that many soil properties that control hydrologic functioning are difficult (or impossible) to modify on a short time scale (*i.e.* texture and mineral composition) and are therefore relatively fixed characteristics from a management perspective. By contrast, amount and quality of soil organic carbon, together with the (inter-)related soil structure, can be changed fairly quickly through management practices. Consequently, adapted soil management can present a good method for improving HES from agricultural lands.

Both the positive and negative effects of different land-cover types on hydrologic processes are interconnected with soil processes and characteristics, in particular for forest and agricultural land-cover types. In this respect, soils are a cross-cutting element in HES production, and soil resource management should be a central consideration in environmental planning.

2.5 Landscape Multi-Functionality/Scales and Hydrologic Ecosystem Services

Similar to water resources, landscapes are multi-functional and multi-use in character. Although many landscapes are dominated by a single land-use and function (*e.g.* intensive agriculture, urban centers), all landscapes generate multiple functions beyond their primary use. This capacity of landscapes to provide multiple functions is termed multifunctionality, and increasing the capacity of landscapes functionality is a potential means of improving the provision of ecosystem services (Mastrangelo *et al.*, 2014; Stürck and Verburg, 2017). Hydrologic processes are inherently linked to landscape dynamics, and alterations in landscape multi-functionality will impact HES at multiple scales (Calder, 2005). HES which may be beneficial at one process-scale (*e.g.* local flood protection) may have a negative impact when translated to the regional scale. HES impacts will often also cross multiple economic scales, as individual stakeholders seeking to maximize their own HES utility may produce impacts on other stakeholders in a manner that can be difficult to reconcile. For example, land-cover change which may have financial benefits for a stakeholder at the local scale (*e.g.* conversion from natural land-cover types to agriculture) may impact wider stakeholders in a negative manner (*e.g.* increased water treatment costs). These impacts may be difficult quantify or control, given that they may cross multiple administrative scales and involve a potentially large number of stakeholders acting across different temporal scales.

Given the multiple relevant scales to consider for river basin management, their management and planning should be conducted at relatively large scales (*e.g.* the River Basin Management Plans of the EU Water Framework Directive). This process will inevitably require some trade-offs in ecosystem services to be made between stakeholders, as there will typically be more demands upon water resources than can be met by the available supply. Therefore, the objective of river-basin management is not to uniformly provide access to all hydrologic ecosystem services to all stakeholders, but rather to provide HES to stakeholders in a manner which is equitable to their individual and shared needs, and is sustainable long-term (Cord *et al.*, 2017; Seppelt *et al.*, 2013). Determining what is both equitable and sustainable is not a simple task, and requires working closely with stakeholders and planning authorities to develop long-term and strategic plans to meet multiple objectives, all of which should be considered within the context of wider landscape planning (from the regional to continental scale) to avoid adverse impacts across scales (Mwangi *et al.*, 2016; Wu, 2013).

2.6 Ecosystem Service Valuation

Basin-scale assessments of HES (*e.g.* through monitoring, eco-hydrologic modeling, etc.) are frequently undertaken to determine how different proposed management actions may affect the quantity and quality of HES for basin stakeholders (*e.g.* agricultural producers, municipal water managers). This sort of assessment is an important step in environmental planning and decision making, however, the information generated will not necessarily be sufficient for decision makers to determine appropriate management actions. While some environmental management decisions are primarily made based upon environmental factors (*e.g.* the protection of critically endangered species), most environmental management actions take wider social, economic, and financial factors into consideration. There are budget constraints in any decision-making processes, and not all options which are physically possible are also realistic to fund or would be acceptable to stakeholders. Based on these constraints, some economic prioritization must be undertaken and trade-offs between different options assessed, in order to allocate funds in an efficient and justifiable manner.

Given this, it is important that HES are not only considered with respect to physical changes in water quality/quantity, but also by considering the value of different HES within their local context (Guswa *et al.*, 2014). Within this context, a financial figure can be attributed to ecosystem services, by which their value can potentially be integrated into existing systems and methods used by decision makers to assess options (Duku *et al.*, 2015; La Notte *et al.*, 2017). Interconnected with the need for ecosystem service valuation is the need to consider what impact environmental management decisions will have on relevant stakeholders. Depending upon the proposed measures, the socio-economic impacts of different alternatives can be significant for some stakeholders, and this also needs to be taken into adequate consideration in planning. Measures to improve water quality, for example, will often require changes to be made at the farm scale, which will impact the financial interests of the affected farmers. If proposed measures are not perceived to be in a stakeholder's economic interest, then a process of negotiation can be used to find a balance between the provision of HES and the interests of the affected stakeholder. In this case, compensation mechanisms (*e.g.* monetary and fiscal incentives) can be an important tool in improving compliance from affected stakeholders, which may replace or compliment more "top-down" regulatory approaches.

To set the value of compensation at a rate which is equitable for both the individual stakeholders and for society, it is critical to have an adequate understanding of the balance between how a proposed action will affect the value of an ecosystem service on one hand, against the financial impacts/costs on the other hand. Inherent in this balance is the recognition that for society as a whole, many natural systems may be most valuable in an undisturbed state, yet some of this value has to be traded to meet the resource needs of human populations and the livelihood of individuals (Moss, 2008).

The **economic value of ecosystems** includes both 'use' and 'non-use' values (TEEB, 2012); different types of '**use values**' include: direct usage, including consumptive usage (*e.g.* drinking water) and non-consumptive usage (*e.g.* recreation use of water bodies); indirect usage (*e.g.* water quality benefits of forests); and option value (*e.g.* the protection of a water body for potential future use). Different types of '**non-use values**' include: existence value (*e.g.* the value of knowing a watershed is available); altruism (*e.g.* value of people's concern for the welfare of others); and bequest value (*e.g.* knowing that future generations will have water resource access). 'Use-values' are typically more straightforward to quantify, and therefore have been more commonly used in basin-scale assessments (*e.g.* eco-hydrologic models). It is important to consider that the full economic value of an ecosystem services includes both the 'use' and 'non-use' values. However, given constraints of time and expense, the full quantification of economic values are unrealistic, and in practice economic valuations typically focus on a single use type which is most relevant to the specific case.

Ecosystem service valuation can be made at a wide range of spatial scales, ranging from the local scale (*e.g.* the value of improved water quality in a drinking water catchment), up to the regional, continental, or even global scale. A prominent example of a global assessment was made by Costanza *et al.* (2014), who estimated that ecosystem services contribute more than twice as much to human well-being as the entirety of global GDP. Additionally, they estimate that changes in global land-use between 1997 and 2011 resulted in a loss of ES between \$4.3 and \$20.2 trillion/yr (Costanza *et al.*, 2014).

The methods used for ecosystem service valuation can be broadly classified as being based on an analysis of **market values**, and those based on a **demand curve** (King and Mazzotta, 2018). Market value-based methods consist of using either benefits or costs as a proxy for the value of the ecosystem service, while demand curve-based methods estimate values based on the revealed or stated preferences of stakeholders. Table 2 provides a summary of different valuation methods, including a brief description of the methods and an HES relevant example (King and Mazzotta, 2018; UNECE, 2018).

Table 2. Summary of ecosystem valuation methods, with hydrologic examples (modified from UNECE, 2018)

A) ANALYSIS OF MARKET VALUE METHODS

A1) Benefits as Proxy

Method	*Brief Description*	*Hydrologic Example*
Opportunity Costs	Non-market benefit from water use derived from giving up the best alternative.	Value of water for irrigation which his instead used for biodiversity protection.
Production Function	Changes in value of output with changes in inputs.	Changed value in agricultural output with reduced water availability.

A2) Costs as Proxy

Method	*Brief Description*	*Hydrologic Example*
Direct Market Price	Based on the minimum amount that a buyer is willing to pay.	The price for water paid by water utility consumers.
Preventative Costs	The lowest cost alternative which could provide the same service.	Costs of a water treatment plant to provide the same water quality benefits as a forest ecosystem.

B) DEMAND CURVE BASED METHODS

B1) Revealed Preference Method

Method	*Brief Description*	*Hydrologic Example*
Travel Cost	Based on observed consumer travel behavior.	The time and money visitors are willing to pay to visit a water feature (*e.g.* lake or beach).
Hedonic Pricing	Effect of changes in ES on property values.	The difference is housing prices which have nearby access to water bodies.

B2) Stated Preference Method

Method	*Brief Description*	*Hydrologic Example*
Contingent Valuation	How much consumers would be willing to pay for an improvement in an ES.	The willingness of fishermen to pay for an improvement in water quality/fish habitat.
Choice Modeling	Estimating beneficiary preferences based on choices between alternative options.	Stakeholders selecting preferences from a list of options for watershed management.

From these different valuation methods, those based on the analysis of market values are typically better suited for model-based ecosystem service assessment, given that they can be more directly estimated from biophysical model outputs (Bagstad *et al.*, 2013; Francesconi *et al.*, 2016). Still, the demand curve-based methods are important tools for cases where the ecosystem service value is primarily a function of the preferences of beneficiaries, rather than strictly due to a change in an ecosystems capacity to provide services. For example, beneficiaries may indicate a willingness to pay for improvements to cultural ecosystem services, such as recreational services (*e.g.* swimming, fishing, boating) as well as other services (*e.g.* improved aesthetics, odor, biodiversity; Hynes *et al.*, 2013; Roebeling *et al.*, 2016).

Regardless of the specific valuation method used, this type of analysis has become more common in planning and management applications, along with the mainstreaming of the ecosystem services concept. An example of such an approach is the use of a modeling framework to assess the potential for applying improved land management methods and 'green infrastructures' as measures to protect both water resources and socio-economic well-being. These types of watershed protection programs are expanding worldwide, with the value of watershed investments in Europe currently estimated at €5.7 billion, covering over 13.4 million hectares, primarily in the form of public subsidies for watershed protection (Leonardi *et al.*, 2017).

A number of these types of investment projects have been established in Latin America and in Asia, and recently the first such project was established in Africa with the Upper Tana-Nairobi water fund (Vogl *et al.*, 2017). In this case, an eco-hydrologic model was utilized in combination with economic valuation tools to assess the potential benefits of a water fund to protect the watershed supplying the city of Nairobi, which estimated that a $10.0 million investment would return $21.5 in economic benefits over a 30-year period (Vogl *et al.*, 2017). This project highlights the potential for assessment methods using eco-hydrological models in combination with economic valuation methods to improve the management of HES.

Section 8 explores the topic of hydrologic ecosystem service valuation, by considering the output from an eco-hydrological model (SWAT) within an HES valuation framework at key points within the Vouga basin.

3 Research Topics & Hypotheses

3.1 Research Topic #1 (Section 6)

The first research topic considers how HES have been impacted by the long-term afforestation which has occurred in the Vouga basin. This topic is examined by applying statistical trend testing to the long-term data sets which are available within the Águeda watershed, a sub-basin located in the Vouga basin which underwent extensive afforestation over the 20th century. The watershed provides a representative example of the land-cover changes which occurred in the upper/middle portions of the basin. To this end, the following hypotheses are tested:

> **Hypothesis 1a:** The large-scale afforestation with pine and eucalyptus species which occurred in the 20th century in the Águeda watershed has led to a statistically significant reduction in in-stream water availability.
>
> **Hypothesis 1b:** The Águeda watershed meets the "prerequisite conditions" proposed by Andréassian (2004) needed to see a significant change in water availability due to changes in forest cover.

3.2 Research Topic #2 (Section 7)

The second research topic moves from a focus on the forest dominated upper/middle basin, to the agriculturally dominated lower basin, to assess how current agricultural practices in the Vouga basin impact water quality (specifically nitrate) at the basin scale. This assessment is made using the SWAT eco-hydrologic model, which was set-up, calibrated, and applied to the Vouga basin using a number of advanced modeling methods, intended to improve the hydrologic simulations at this study site. The first objective is to examine how nitrate export varies between different parts of the basin, to determine the main nitrate export regions and flow pathways. The second part of this topic assesses nitrate export at the scale of hydrologic response units (*i.e.* a distinct combination of land-cover/land-use, hydrologic soil class, and slope class), to determine what water bodies are at the greatest risk from nitrate pollution. To address these questions, the following two hypotheses are considered:

> **Hypothesis 2a:** The highest rates of nitrate export will occur in the agricultural lowlands, and the primary flow pathway will be *via* surface flows.

Hypothesis 2b: The water body in the Vouga basin at the highest risk of diffuse nitrate pollution is the Pateira de Fermentelos (an inland lake), followed by the groundwater aquifers, and lastly the Ria de Aveiro (a coastal lagoon).

3.3 Research Topic #3 (Section 8)

The third research topic builds upon the base SWAT model of the Vouga basin established in topic #2 and focuses on examining alternate fertilization scenarios in the agricultural lowland portion of the basin. This topic examines how reducing the amount of fertilizer applied affect the amount of nitrate leaching, crop yields, and estimated profits; and determine if there is any inefficiency in the rates of fertilizer being currently applied. Additionally, the HRU-scale output is examined in terms of the efficiency of different HRU types (*i.e.* crop production *versus* nitrate export). Finally, this section considers the potential economic costs of nitrate pollution, in terms of reduced water quality, and the need for additional treatment costs or other measures to offset this. To address these points, the following hypotheses are tested:

Hypothesis 3a: Fertilizer inputs could be reduced below current levels without substantially reducing crop yields and agricultural profits.

Hypothesis 3b: There are differences in the agricultural efficiency of the different HRUs in terms of crop yield vs. nitrate export, which could be used to assist in identifying further management options.

4 Research Methods

The following section provides an overview of the research methods used to address the topics presented in **Section 3**. **Section 4.1** deals with the statistical methods used to examine the long-term data records in the Águeda basin. **Section 4.2** provides background on the methods used for the eco-hydrological assessment conducted with the SWAT model, including a “best practices” guide based on challenges encountered in this study. Lastly, **Section 4.3** details the scenario-testing approach applied in this study and the methods of assessing the financial and economic impacts of the scenarios.

4.1 Statistical Trend Testing

Statistical trend tests are used to investigate trends in time-series data, typically *via* the explanatory variable of time with a null hypothesis (H_0) that there is no trend in the observed data. Trend tests can be classified as being either parametric, non-parametric, or mixed. In cases where a regression equation is known to be correct and the residuals are normal, then a parametric test is the optimal approach. However, these conditions are often not the case with real-world data sets, particularly with hydrological or climatic data, which tend to have irregular and/or non-normally distributed data. In these cases, a **non-parametric test** (*i.e.* Mann-Kendall), will perform as well or better than a parametric test (Helsel, 1993). Given this, non-parametric trend tests are the most widely used statistical tool for detecting trends in environmental data sets (Yue *et al.*, 2002).

4.1.1 Thiel–Sen/Mann–Kendall Trend-Testing

In research topic #1, a non-parametric trend-testing approach is used to examine a number of hydrometeorological variables from long-term data sets in the Águeda watershed. The methodology utilizes a combined Thiel–Sen/Mann–Kendall trend-testing approach, which considers the magnitude and significance of patterns in observed data sets. Based on this foundation, a multi-step trend-testing procedure was developed, following the general approach presented in (Yue *et al.*, 2002). An outline of these steps is presented below, which is then followed by a more detailed description:

Step 1) Thiel-Sen Slope Estimator

Step 2) Trend Free Pre-Whitening Procedure

Step 3) Mann-Kendall Test

Step 4) Benjamini–Hochberg–Yekutieli Procedure

Step 1 first determines the magnitude (*i.e.* slope) of any potential trend in the data using the non-parametric Thiel-Sen slope estimator (Sen, 1968). This value is determined by calculating the median slope among the set generated between all sample points. This method also estimates the 95% confidence intervals of the true slope, based on the set of slopes from the sample points, which provides a measure of uncertainty of the median Thiel-Sen value. In **step 2**, if a potential trend is detected by the Thiel-Sen test (*i.e.* a non-zero slope), then the data is processed using the 'Trend Free Pre-whitening' procedure of Yue *et al.* (2002). This step reduces the over-estimation of significance which can occur in time-series data that exhibits positive serial correlation, as is typically the case for streamflow time-series data.

After the 'Trend Free Pre-whitening' procedure, in **step 3** a Mann-Kendall test was applied to assess the statistical significance of any non-zero slope identified by the Thiel-Sen test. The Mann-Kendall test is a widely used, rank-based significance test, where the null hypothesis is that there is no trend in the observed data (Helsel, 1993). For this study, statistical significance was determined using an α value of 0.05.

When conducting multiple simultaneous hypothesis tests, it is also necessary to correct for the false discovery rate (FDR). FDR corresponds to the expected proportion of incorrectly rejected null hypotheses, and therefore, a method is needed to reduce the chance of receiving false-positive results (*i.e.* type I errors). Several different methods can be applied to control for FDR, however given the overlapping time periods examined in this study, a method is needed which can deal with FDR under the assumption of positive dependence. Therefore, in **step 4**, the 'Benjamini–Hochberg–Yekutieli' procedure was applied to the trend-testing output from each individual 'analysis set' (Benjamini and Yekutieli, 2001). An 'analysis set' corresponds to a group of tests which are expected to exhibit mutual positive dependence, which in this case are the 12 overlapping periods over which each hydrometeorological variable was tested for the different annual and seasonal periods (these periods are detailed in the **Section 6.2.2**).

Following the application of this procedure to all the hydrometeorological data considered; a number of significant trends were detected. These trends are then considered against the historical land-cover changes which occurred in spatial and temporal proximity with these detected trends. Based on these findings, possible drivers of the detected trends are discussed, in particular for the observed trends in streamflow and baseflow.

4.2 Eco-Hydrologic Modeling

Eco-hydrologic processes are dependent on the quantity, quality, timing, and location of water; which are in turn impacted by numerous environmental variables, such as land-cover/use, geology, soils, climate, topography, and anthropologic impacts. Spatially-distributed and process-based eco-hydrologic models are designed to simulate the complex interactions between water and ecosystems, through a combined representation of hydrologic, hydraulic, water quality, and/or ecologic model components (Brewer *et al.*, 2018). This combined representation makes them well-suited for applications related to eco-hydrologic processes and HES assessments, such as scenario analysis, payments for watershed services, and spatial planning applications (Guswa *et al.*, 2014).

A key criterion in the selection of an eco-hydrologic model is the level of model complexity to utilize. Greater model complexity, through increased spatial and process representations, comes with a trade-off in terms of higher operational complexity, increased input data/calibration requirements, increased risk of over-parameterization, and greater model uncertainty (Beven, 2012). Uncertainty in eco-hydrologic models are function of many factors, including input data, model structure, and model parameters (Abbaspour *et al.*, 2008). While some degree of uncertainty is inherent to all models, less complex models will typically have lower uncertainty than more complex models containing numerous parameters (Beven, 2012). Model selection should not therefore follow a 'more complexity is better' approach, but rather be adapted to fit the objectives of the model application and required level of model output detail.

The decision of which level of model complexity to use will in part be a function of the amount of data available for a proposed study site, as a lack of data can be a constraining factor for the use of models with high data-input requirements. In data constrained study sites, the selected eco-hydrologic model must be capable of use with limited input and have a flexible model structure to represent a range of potential processes (Guswa *et al.*, 2014). Ultimately, the model utilized must be capable of representing changes in eco-hydrologic dynamics at the spatial and temporal scale relevant for the application, while minimizing the "signal-to-noise" ratio due to sources of model uncertainty (Brewer *et al.*, 2018; Guswa *et al.*, 2014).

A wide range of hydrologic models are available which could be applicable to the research goals in the Vouga basin (i.e. spatially explicit scenario simulations in a large basin), each of which has their own relative strengths and weaknesses (Brewer *et al.*, 2018; Devia *et al.*, 2015). The model selected for use in this research is the Soil and Water Assessment Tool (SWAT), which is detailed in the following section.

4.2.1 The Soil and Water Assessment Tool (SWAT)

Among different basin scale eco-hydrologic models, the **'Soil and Water Assessment Tool' (SWAT)** has arguably been the most widely used for HES assessments (Duku *et al.*, 2015; Francesconi *et al.*, 2016; Lüke and Hack, 2017; Vigerstol and Aukema, 2011). According to the SWAT literature database, there have been 89 journal articles published with the keyword of 'ecosystem services' to date, with the first papers on the topic appearing in 2005 (https://www.card.iastate.edu/swat_articles/). More broadly, SWAT is one of the most widely used models for landscape scale eco-hydrologic simulations, and has been applied to a wide number of different climate zones and application contexts worldwide (Gassman *et al.*, 2007). SWAT is a semi-spatially distributed and process-based model, which was originally designed as a tool to assess different agricultural practices, and has since developed to cover a wide range of processes and applications (Krysanova and Arnold, 2008; Neitsch *et al.*, 2009). For HES-specific studies and applications, SWAT has most frequently been used to model provisioning services (*i.e.* streamflow quantity) and to a lesser degree regulating services (*i.e.* water quality), with some studies also considering supporting and cultural HES (Francesconi *et al.*, 2016).

SWAT functions by dividing the watershed into *n* number of sub-basins, based on the topographic features of the watershed and the specifications of the modeler (*i.e.* minimum drainage area). Within the sub-basins, the landscape is broken up into individual hydrologic response units (HRUs), which are lumped land areas with a unique combination of land-cover, soil, and slope. The underlying assumption behind the HRU concept is that differences in these characteristics will result in significantly different hydrologic behaviors. The basic element of the model is the calculation of the water balance, which is broken into two components: 1) the land phase of the hydrologic cycle, which quantifies the amount of water and matter generated from each sub-basin, and 2) the routing component, controlling the movement of water to the watershed outlet. Once a water balance acceptable to the modeler is achieved, other elements associated with watershed-scale hydrologic processes can be considered through application of different watershed states/scenarios, including: vegetation conversion impacts, waterborne loads of sediment/nutrients/pesticides, alternate land-management scenarios, and many other potential options. SWAT simulates the main transformation and transport processes for both nutrient and pesticides, making it well suited for simulating the dynamics of agro-chemical inputs. Nitrogen is partitioned into inorganic and organic forms by the model, and nitrogen can be input by fertilizer, manure, plant residue, and rain; and is removed by plant uptake, leaching, volatilization, denitrification, runoff, and erosion (Neitsch *et al.*, 2009)

SWAT is best suited for making projections over relatively large temporal scales, it is not intended for detailed analysis of single events (*i.e.* sub-daily), such as flood-induced streamflow and sedimentation. In addition, the level of spatial discretization in SWAT makes it poorly suited for representing processes and landscape features operating within the sub-basin scale (*e.g.* riparian filters or vegetation strips), although the aggregated response of these processes at larger spatial scales can be estimated.

A full description of the SWAT model is provided by the theoretical documentation of (Neitsch *et al.*, 2009), which gives details of the processes represented in the version of SWAT used in this research. In this thesis, the SWAT model is utilized for assessing nitrate fluxes in the Vouga basin in **Sections 7 and 8**.

4.2.2 SWAT Modeling "Best Practices Guide"

The majority of SWAT modeling procedures used in this dissertation follow standard approaches utilized in most SWAT model applications, and therefore are not discussed in detail. However, several of the modeling methods utilized in this study deviate from "normal practice" in order to address the specific challenges of this study site and/or to test alternative approaches which may be otherwise advantageous. To this end, the following section details these advanced methods, to serve as a "**best practices guide**" which may be of interest to other SWAT model users. The topics covered include:

- Soil Data Modification
- Fertilization Date Modifications
- Objective Function Selection
- Pareto Parameter Set Selection
- Ensemble Model Predictions

4.2.2.1 Soil Data Modification

A lack of adequate soil data is a common challenge in eco-hydrologic modeling applications having a spatially explicit component. Soil data may be lacking in scale or detail to adequately represent the hydrological processes of interest for a given study site or may be only available at a spatial scale that is not commensurate with other spatial inputs (*e.g.* digital elevation map, land-cover/land-use map). In such a case, it may be advantageous to increase the spatial resolution of the soil data set by using associated landscape data and characteristics as a proxy to estimate properties relevant to hydrological processes (Abbaspour *et al.*, 2008). This approach was applied to a sub-basin of the Vouga basin by Tavares Wahren *et al.* (2016), who used the Soil Land Inference Model (SoLIM) in conjunction with field data collected from soil profiles, which allows for the generation of a spatial model to predict soil characteristics at different landscape positions. This type of method has significant potential for soil mapping applications, however it is also is heavily dependent upon the density and distribution of the soil samples used as input.

Where an adequate number of existing samples is not available and/or are infeasible to collect (*i.e.* in a large basin), then the use of a predictive spatial model will not be a viable method. In this case, a more simplified approach can be applied using more commonly available data, if it can be linked with an understanding of the site characteristics and how they relate to the properties of interest in mapping. This type of approach was utilized in the current study, to improve the soil data resolution with respect to the depth of the impervious layer within the soil, which is a property deemed critical to hydrologic processes in the Vouga basin. The details of this approach are provided in **Section 7.2.3**.

4.2.2.2 Fertilization Date Modifications

When simulating the growth of the agricultural crops in SWAT, the user must define the date fertilization operations will occur, which is commonly done by setting specific dates within the growth cycle for each crop being simulated. While this is a straightforward and logical method to set the fertilization dates, it can lead to two potential sources of error in estimates of plant growth and fertilizer export.

The first issue is that this method does not take any consideration of the weather conditions and/or soil moisture levels at the time of fertilization. This can lead to fertilization operations occurring during very wet conditions, during which there is a much higher potential for applied fertilizer to be washed off from the fields where fertilizer is applied. This will lead to increased rates of fertilizer export and reduced plant growth, and is a situation which would clearly be avoided by an actual farmer. The second issue is that fertilizer operations for a given crop are carried out uniformly on the same date throughout the entire basin, regardless of the size of the region simulated. This leads to a large influx of fertilizer on the same date, which in turn has a high potential for export on those days. These operations should be distributed over a period of a few days, to better reflect the normal variability of timing between different agricultural operators. This would better represent a real-world situation, which would also distribute the export risk potential over several days.

Given these issues, SWAT model users who are assessing agricultural production and/or fertilizer export should check their fertilization schedules against the moisture conditions for each part of the simulated region with a different precipitation source. In cases where there are high levels of moisture, the user should move the operation to a new date, within a reasonable window of time. For the current study, a threshold of 5 mm precipitation within a period of 3 days before or after the targeted fertilization date was applied, and the date was moved if needed to move outside of this window. These thresholds are unlikely to be appropriate at all locations, however, and would need to be customized to the specific characteristics of any given site. A more sophisticated method of adjusting agricultural management operations in SWAT has recently been developed in an R-package by Schürz *et al.* (2017), which uses a detailed rule based system to modify operation dates. This method is recommended for SWAT users who are proficient in the R programming language, as it avoids the need to manually modify the operation dates within the SWAT model files, which is both time consuming and prone to error. However, the more simple threshold method was applied in the current study, as both this and following steps of the modeling procedure were conducted prior to the availability of the Schürz *et al.* (2017) method.

4.2.2.3 Objective Function Selection

A key decision that must be made in all hydrologic modeling applications is the selection of the objective function(s) which will be used to evaluate model performance. All objective functions have relative strengths and weaknesses, which should be recognized by the model operator, and compensated for when possible. Perhaps the most commonly used objective function types are correlation-based measures, such as the Nash-Sutcliffe Efficiency (NSE) or Coefficient of Determination (CoD), which are based on the summation of squared residuals between the model and observed data. Despite their widespread use, these measures are known to be oversensitive to extreme values, and therefore have a bias towards models which match peak flows (Legates and McCabe, 1999). Another commonly used type of objective functions are measures of absolute error, such as Bias or Percent Bias (PBIAS). A potential problem with these types of metrics is the tendency to over-predict model performance in cases of off-setting model error (*i.e.* if a positive model error is followed by an equivalent negative model error, the two errors would offset, and the result would be a perfect performance value).

One method of compensating for the weakness of a specific objective function is the use of multiple objective functions having complementary strengths/weaknesses. An example of this could be the use of a correlation-based measure (*e.g.* NSE) in conjunction with an absolute error measure (*e.g.* PBIAS) to try to capture multiple perspectives of the model's behavior. The downside of this approach is that the use of multiple objective functions complicates the selection of the best performing parameter sets, which can't be selected by ranking performance on a single measure. This is particularly problematic if model performance is to be assessed on additional non-hydrologic performance indicators (*e.g.* nutrient fluxes, sediment loads, *etc.*), which will further complicate parameter set selection.

An objective function approach which could be applied to achieve the complementary benefits of using multiple objective functions, without adding additional metrics, is the use of a single objective function which integrates multiple metrics into a single performance value. An example of this type of objective function is the Kling–Gupta Efficiency (KGE), which aggregates model performance on measures of correlation, bias, and variability within a single metric (Gupta *et al.*, 2009; Kling *et al.*, 2012). By using these three elements, KGE can capture both the temporal dynamics (*i.e.* correlation) as well as the distribution of flows (*i.e.* bias and variation) with a single value.

The primary disadvantage of using a relatively recently developed objective function, such as KGE, is the lack of familiarity and widespread usage by hydrologic modelers. The lack of familiarity can make the interpretation of model performance more difficult both for the model operator and potential audience, while the lack of a large body of prior studies using the same metric makes comparisons against previous research more challenging as well. By comparison, more commonly used metrics have developed standardized guidelines of performance (*e.g.* Moriasi *et al.*, 2007), which have a great deal of appeal for comparing models across study sites (although the validity of this approach is not clear).

While the challenge of selecting an appropriate objective function to evaluate hydrologic flows is substantial, selection of a metric to measure non-hydrologic model outputs, such as nutrient or sediment fluxes, is even more of challenge. The cause of this difficulty is that there is typically far less observed data for these types of variables, when compared to streamflow. Unless there is a purpose-built data collection campaign for a given study site, the best temporal resolution that a modeler can often expect for such variables are monthly or bi-weekly values.

This lack of data makes the use of correlation-based metrics very unreliable, given that there are so few data points for comparison. In the case where the observed data is available at one measurement per month, then the ratio of modeled-to-observed data will be around 30 to 1, leading to a large mismatch between the two datasets for comparison. In addition, given the high day-today variability in variables such as nutrient fluxes, there is a high probability that the measurements on a given day will not match with model outputs due to relatively short temporal offsets, rather than a lack of adequate process representation by the model.

An alternative type of performance metric which can be used in this type of case involves the removal of the temporal component to the data, and basing the comparison strictly upon the cumulative distribution function of the two data-sets. An example of this type of approach is the use of a Kolmogorov–Smirnov test (KS), a nonparametric test which compares a sample distribution against a reference distribution, to determine the likelihood that the sample is equivalent to the reference. This test can be modified for use as an objective function by quantifying the distance between the empirical distribution of the sample (*i.e.*

the observed data set) and the cumulative distribution function of the reference distribution (*i.e.* the model output).

The advantage of this approach is that by transforming the data into distribution functions, the observed and the modeled values can be directly compared, despite the mismatch in the number of contributing values. In addition, by removing the temporal component, the problem of poor performance due to small temporal offsets is removed, however, this also means that this metric has no sensitivity to the timing of modeled flows. Therefore, this metric is best suited for matching the overall distribution of the magnitude of flows in the observed data, with no consideration for the temporal component.

The Kling-Gupta Efficiency (KGE) and the modified Kolmogorov–Smirnov (KS) test are utilized as the primary objective functions in this research, which are discussed further in **Section 7.4**.

4.2.2.4 Pareto Parameter Set Selection

As stated previously, when multiple objective functions are used to evaluate model performance, the question arises of how to rank the performance of different parameter sets. One method of using multiple objective functions in a selection is to assess their efficiency using Pareto optimization. Pareto optimization ranks every parameter set on two or more selection criteria, and identifies those parameter sets where it is impossible to improve one criterion without making one of the other performance criteria worse. All parameter sets which meet this definition are part of the Pareto front, and can be considered to represent an optimal trade-off point between the different criteria used.

The advantage of using Pareto optimization for parameter set selection is that it provides an objective way of selecting among many different parameter sets, which may be very similar in performance on one or more of the criteria being utilized (*i.e.* equifinality). This process will function best if the criteria being used evaluate contradictory aspects of model performance (*e.g.* high and low flow prediction), or on different components of model performance (*e.g.* hydrologic and matter fluxes). The more independent and differentiated the criteria are, then the greater potential for the Pareto optimization to find meaningful trade-off points in model behavior.

In this research, Pareto optimization was used to select parameter sets from the calibration of the SWAT model, using the Kling-Gupta Efficiency (KGE) to evaluate hydrologic performance and the Kolmogorov–Smirnov test (KS) to evaluate how well the model represents nutrient fluxes. Further details on this calibration procedure and the results of the Pareto optimization are provided in **Section 7.4.1**.

4.2.2.5 Ensemble Model Predictions

When using a model calibration method that identifies multiple parameter-sets which are considered to provide an equally good representation of the target processes (*e.g.* Pareto optimization), the result is the generation of multiple independent model outputs. However, a multitude of predictions is not useful for many practical uses of model output (*e.g.* planning applications), and therefore the multiple individual predictions will need to be merged into a single ensemble prediction. An ensemble prediction represents a single combined prediction that is comprised of the individual contributors, which can be generated either with equal or differentiated weighting between each member. In the case of using a Pareto optimization approach to select the contributing parameter sets, for example, each member it considered equivalent, and therefore would typically receive an equal weight in the final prediction.

The primary advantage of using an ensemble modeling approach is that the multiple contributing members will offset the risk of a poor prediction, due to the misidentification of a single "best" parameter set. In the best-case scenario, the different contributing parameter sets will help capture different attributes of model behavior that might be missed by any single parameter set, leading to a more thorough representation of the target process (*e.g.* different flow magnitudes). This could be a particular advantage in cases where multiple criteria are used to select the contributing parameter sets, and therefore may provide better representations on different model components. Additionally, by providing a range of different model predictions, an inherent measure of predictive uncertainty is provided, depending on the degree of variation between the representations of the contributing parameter sets.

It is important to note, however, that an ensemble prediction will not necessarily generate a more accurate model prediction, but rather a more reliable prediction. Given multiple contributing parameter sets, it is possible that anyone of the individual members may be clearly preferential to all others, in which case the use of an ensemble prediction would make the final prediction *worse*. However, since there is no way of identifying *which* parameter set this would be, then simply knowing it is possible given perfect information is not practically useful. Therefore, a more useful way of thinking about an ensemble prediction is as a strategy of risk mitigation, to avoid the risk inherent in the selection of a single parameter set, which comes at the expense of potentially discarding a single best performing parameter set.

An ensemble modeling strategy is applied in this research, to generate a single model prediction from the multiple parameter sets identified in the Pareto optimization approach discussed in the previous section. The details and results of this approach are discussed further in **Section 7.3**.

4.3 Ecosystem Service Assessment

A model-based assessment of changes in ecosystem services under different potential options involves **(1)** the generation of scenarios to represent the targeting changes, and **(2)** the quantification of the amount of change for both directly modeled variables, and potentially for additionally derived variables as well.

4.3.1 Scenario Testing

The use of eco-hydrological models to examine potential options can help make the concept of ecosystem services 'operational' for decision makers, by allowing for the representation of different management alternatives through the simulation of scenarios of interest. Scenarios allow for the evaluation of potential policy actions, changing conditions (*e.g.* climate change), or to simulate the impact of extreme scenarios to explore boundary conditions (*e.g.* simulate total afforestation/deforestation). Scenarios are typically carried out by first calibrating the model to current conditions using observed data, and once satisfactory model performance has been established, the model inputs can then be modified to represent different scenarios. This process provides a way to anticipate the impacts of potential management decisions or to simulate historical conditions outside of the observed data range.

In this research, the SWAT model was calibrated and implemented to simulate the existing hydrologic/nutrient conditions in the Vouga basin **(Section 7)**; and then this base model was used to generate alternate scenarios for reduced fertilizer inputs in the lowland agricultural regions of the basin. The details of these scenarios are discussed further in **Section 8.2.**

4.3.2 Model-Based Ecosystem Service Assessment and Valuation

Model-based ecosystem service assessment and valuation can be carried out following two different types of approach: (1) using integrated models, which have both biophysical outputs and valuation methods within a single model; or (2) through non-integrated model based approaches, in which a model is used to generate the biophysical outputs, and the valuation is generated through post-processing of data (Guswa *et al.*, 2014).

Bagstad et al. (2013) compared the available tools for using an integrated modeling approach, which provide both ecosystem service quantification and valuation. From the tools compared, several models were identified which are both in the public domain and are appropriate tools for basin scale scenario assessments, including: ARIES, Co$ting Nature, EcoServ, InVEST, LUCI, MIMES, and SolVES. These models have high potential for these types of applications, as they are generalizable (*i.e.* not site-specific), are applicable at the landscape scale, and are not restricted in their use by commercial licenses. Of these models, ARIES and InVEST have been the most widely applied and both cover a wide range of ecosystem services through various modules (Bagstad *et al.*, 2013).

An alternative to this type of 'integrated model' approach is the use of an eco-hydrologic model to independently estimate changes in ES, with valuation conducted afterwards through the application of post-processing methods. The SWAT model has been widely applied following this approach, primarily for estimates of changes in provisioning or regulating HES, however no standardized approach has yet emerged (Francesconi *et al.*, 2016). Vigerstol and Aukema (2011) compared different tools for modeling HES, with comparisons drawn between traditional hydrological models (*e.g.* SWAT) and integrated ecosystem services assessment and valuation models. Their findings suggest that traditional hydrologic tools can provide more detailed, and potentially accurate, assessments than the integrated ES models considered (*e.g.* InVEST). However, the integrated ES models are typically more accessible to non-experts and have lower data requirements to operate.

This is also supported by the findings of Lüke and Hack (2017), who found that SWAT provided more detailed model results when compared to the InVEST or RIOS models, but that SWAT required significantly more time and expertise to operate. They therefore suggest using the integrated models in cases of limited time, data, or expertise. A further approach which could be applied is to use a simpler model as a "screening tool" (*e.g.* the RIOS model, which is designed to locate preferential areas for the maintenance/restoration of multiple HES), with the more detailed assessment conducted using a model such as SWAT or InVEST.

This research applied a non-integrated approach to the assessment and valuation of HES, based on the use of the SWAT model to generate output from alternate scenarios, which is covered further in **Section 8**.

4.3.3 Financial and Economic Valuation of HES Changes

In using a non-integrated assessment approach (*i.e.* based on the SWAT model), biophysical outputs are generated directly from the model, while any additional outputs of interest must be derived independently. To assess the impacts of different scenarios, it is necessary to estimate both the direct financial changes that are expected to be experienced by stakeholders, and the potential changes in the economic value of HES (which will also be experienced by stakeholders). The estimation of financial changes under different scenarios can be calculated by applying a **partial budget analysis** approach. This method evaluates the financial effects of incremental changes in an agricultural operation, by estimating how revenues and expenses will change under various scenarios. This approach only considers resources or other components which are directly affected by changes in agricultural operations, and doesn't consider any wider impacts of management alterations, such as the effect on the agricultural market.

Changes in the economic value of HES can be estimated using a wide range of different methods, with selection dependent upon the type of analysis and the type of the ecosystem service being considered (see **Section 2.6**). For an eco-hydrologic model-based ecosystem service assessment, methods which are based on an analysis of market values are well suited, given that they can be more directly estimated from biophysical model outputs. For the case of estimating the change in HES value due to alterations in water quality, the potential change in water treatment costs for the water resource users can be used as proxy for the change in HES value. For example, the 'Replacement Cost' could be estimated, which represents the lowest cost alternative which could provide the same service as the HES being considered.

This research applies a partial budget analysis approach to estimate the change in financial expenses under different agricultural fertilization scenarios and considers different household water treatment costs as a proxy for the change in the economic value of the HES. The details and results of this analysis are discussed in **Section 8.2**.

5 Vouga Basin Description and Background

5.1 General Characteristics

The study region for this research is the Vouga River basin, located in the north-central region of Portugal (Figure 1), with a total drainage area of 3,635 km^2 and a main channel length of 148 km. The river terminates at the Ria de Aveiro, a shallow estuary-coastal lagoon which extends approx. 45 km north-south, and 10 km east-west, which is connected to the Atlantic Ocean by a single tidal channel.

Figure 1. Location of the Vouga Basin (outlined in red) within the Iberian Peninsula.

The north-central region of Portugal is categorized as a wet Mediterranean climate zone with oceanic influences, with a wet period typically ranging from October to April, and a dry warm period ranging from June to September. Figure 2 provides the mean monthly precipitation and temperature recorded at an upland gauge within the Vouga basin ('Campia' gauging station) from 1971 to 2000, which shows the distinct offset between precipitation and temperature which is characteristic of Mediterranean climate zones.

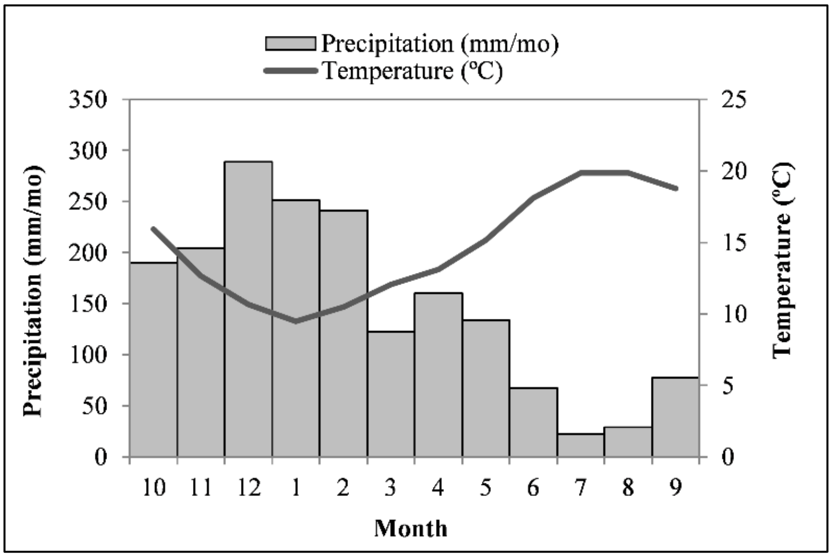


Figure 2. Mean monthly precipitation and temperature recorded at the Campia gauge from 1971 to 2000 (SNIRH, 2013).

Based on the FAO–UNESCO (1988) soil classification system, a large portion of the Vouga basin soils consists of Humic Cambisols, which are characterized by a sandy-loamy, organic matter rich cambic horizon in the upper part of the mineral soil and with a more sandy, less weathered subsoil (Rocha *et al.*, 2015; Stefanova *et al.*, 2015). Podzols are prevalent in the southern lowland portions of the basin, while Fluvisols are dominant around the confluence of the Cértima and Águeda rivers, and towards the outlet of the Vouga river (Stefanova *et al.*, 2015). Other soil types with smaller areal coverage include Regosols and Solonchaks (Rocha *et al.*, 2015; Stefanova *et al.*, 2015). In the upper parts of the basin, areas with steep slopes typically have very shallow, more stony soils (depths < 30 cm; Leptosols), while on plateaus and in slope hollows the soils are somewhat deeper and better developed (Tavares Wahren *et al.*, 2016).

The Vouga basin has relatively distinct geologic/topographical regions, which have a strong impact on the hydrologic behavior of the different regions of the basin. The upland region of the basin is dominated by low permeability geology (*e.g.* schist, greywacke, quartzite, mica schist, gneiss) located on steep mountainous slopes (Rocha *et al.*, 2015; Silva *et al.*, 2002; Stefanova *et al.*, 2015). In this portion of the basin, the low permeability of the underlying geology, in combination with the highly seasonable precipitation patterns, results in large seasonal differences in flow magnitudes, and annual streamflow totals are typically dominated by extreme events (Silva *et al.*, 2002). Partly due to these factors, the Vouga basin has a high flood frequency, and is characterized as having one of the highest flood risk potentials in northern Portugal (Santos *et al.*, 2018). By contrast, the lowland region of the basin is dominated by geologic formations with medium to high permeability (*e.g.* siltstone, sandstone, limestone, dolomite, sand and alluvium; (Rocha *et al.*, 2015), including areas of karstic geology.

5.2 Land-Cover/Land-Use Change History

The Mediterranean region of Europe has undergone significant land cover changes over its long history of human habitation, with only ~ 4.7 % of primary vegetation unaltered (Geri *et al.*, 2010). In recent decades, some of the most significant trends in land-cover/land-use in the Mediterranean region have been: increased rural abandonment, a decrease in traditional agricultural/pastoral activities, and widespread planting of fast-growing tree species (Geri *et al.*, 2010; Serra *et al.*, 2008). This large-scale transformation is certain to have altered hydrologic processes at multiple scales, and gaining a better understanding of the effect of these changes is critical for predicting the impact of future land-cover changes, particularly given concerns over potential water shortages in this region due to changing temperature and rainfall regimes (Giorgi and Lionello, 2008).

The north-central region of Portugal is representative of these wider landscape changes, as it has undergone substantial land cover/use changes over the past centuries, which have fundamentally altered its vegetative landscape. From the 1800s until the 1980s, this region had a general trend towards both increased agricultural and forest land cover, with reductions in natural vegetation types (*e.g. mato* shrublands and low-density oak forests). The effect of these changes on the spatial patterns of forestry and agriculture in the Vouga are apparent in the current land-cover patterns of the Vouga basin (Figure 4). This aggregated land-cover map depicts the clear concentration of agriculture (and settlements) in the southern portion of the basin, while the central and northern regions are dominated by forestry.

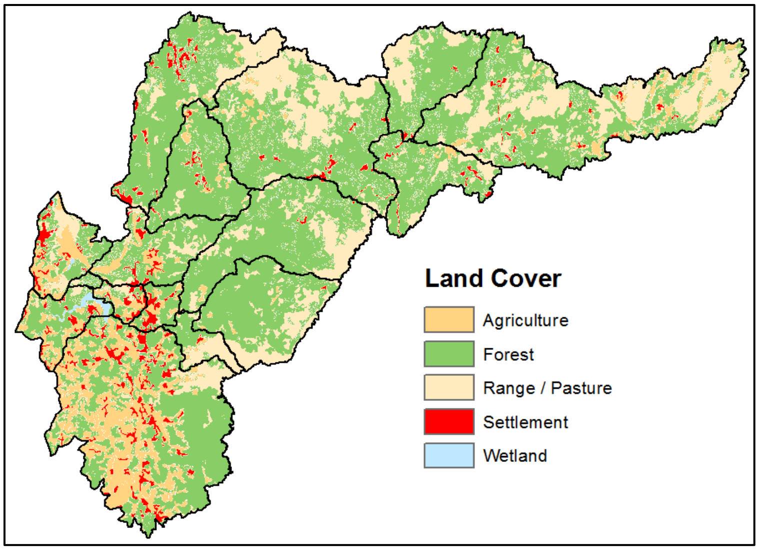


Figure 3. Land-cover map of the Vouga basin with aggregated land-classes. The overlying black lines are the sub-basin boundaries from the SWAT model delineation (see section 7.2.1 for more detail).

5.2.1 Forestry

Since the end of the 19th century, forest land-cover has greatly increased in Portugal, with coverage increasing from 7% in the 1870s to 35% in 2015 (EASAC, 2017). In north-central Portugal, the most significant forest transition was from traditional rural agro-silvopastoral being replaced by plantation tree species (Jones *et al.*, 2011; Moreira *et al.*, 2001). One of the key drivers behind this change was the enactment of legislation in 1938 which encouraged afforestation of areas classified as 'uncultivated/ wasteland', which often consisted of areas of shrublands (*i.e. mato*), mountain ranges, and sand dunes (Coelho *et al.*, 1995; Estêvão, 1983; Ferreira *et al.*, 2000; Jones *et al.*, 2011; Silva *et al.*, 2004).

The primary plantation tree species initially established during this period was *Pinus pinaster*. However, beginning in the 1970s *Eucalyptus globulus* became the preferred species due to its faster growth and higher profitability, which was cultivated primarily for use in the paper pulp industry. During this period, eucalypt plantations began to replace pine forests following their harvest, as well as being widely introduced into remaining areas of shrublands and in recently burned areas (Jones *et al.*, 2011). This regional trend of afforestation of shrublands with *Pinus pinaster*, followed by a secondary transition from *Pinus pinaster* to *Eucalyptus globulus* plantations, is representative of the land-cover changes in the Vouga basin. The hydrologic impacts of this transition are examined in detail in **Section 6**.

In addition to the potential hydrologic impacts of this land-cover change, widespread afforestation of the region of Portugal has also been responsible for an increase in fire frequency and severity (Shakesby, 2011). Portugal consistently has among of the highest rates of wildfire in Europe, both in terms of number of events and area burned (EEA, 2016). Figure 4 shows the burned area of a heavily forested sub-basin of the Vouga (Águeda watershed) from 1975 to 2010, during which a total of 30,790 ha burned, with some single years having wildfire effecting over 10 % of the entire sub-basin (*i.e.* 1986 and 1995; Instituto da Conservaçao da Natureza e das Florestas, 2014). On the national level, 2017 represented an exceptionally severe fire season, with a total burnt area of ~540 thousand ha, which is 498% of the average from the previous decade (San-Miguel-Ayanz *et al.*, 2018). This included a large fire in the north-central region (~65 km south-east of the Vouga basin) which began on June 17th, resulting in major property damage and 66 fire related deaths.

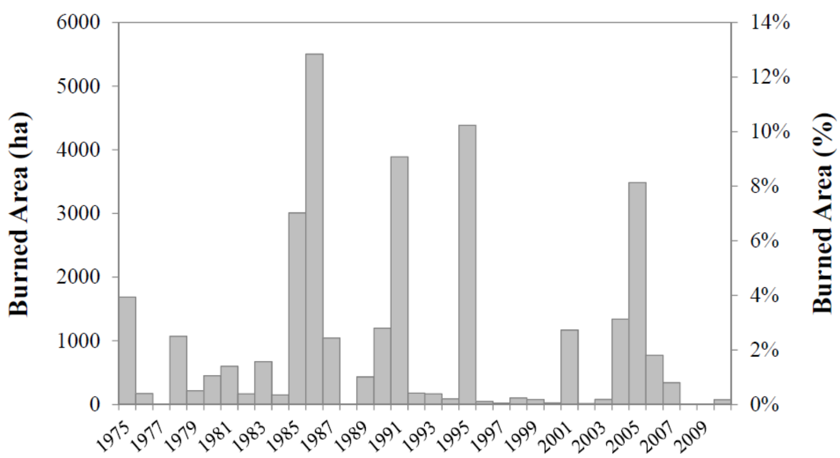


Figure 4. Burned area in the Águeda watershed from 1975 to 2010 (area of 404 km^2) Source: Instituto da Conservaçao da Natureza e das Florestas, 2014).

Wildfire can have significant short-term impacts on hydrologic functioning, primarily by decreasing infiltration potential and increasing surface runoff and soil erosion (Malvar *et al.*, 2011; Prats *et al.*, 2012). In addition to these well-established wildfire impacts, burned forests may also contribute to water quality problems through pollutants carried in post-fire ash; and in contrast to the relatively low export of nutrients from forested areas, forest fires may lead to occasional high exports of nutrients, as well as other pollutants (Nunes *et al.*, 2017). Wildfire can also be a significant driver in land-cover change, by promoting the conversion of vegetation types. In this respect, wildfire has been a major driver of land-cover change in north-central Portugal, partially due to natural succession processes, and in part by encouraging land-owners to convert from pine to eucalypt plantations in the post-fire period, thereby accelerating the existing land-cover change trends.

5.2.2 Agriculture

The proportion of land under agricultural production in Portugal has varied significantly since the beginning of the 20th century, with periods of both expansion (until the mid-960s) and contraction (1986-2006; Jones *et al.*, 2011). Jepsen et al. (2015) characterized the transitions in European land-management regimes since the year 1800, which have varied significantly depending upon socio-economic conditions. According to their classification, northern Portugal is currently in the 'Industrialization' stage of agricultural production, which is characterized by specialized commercial production, and high inputs of fertilizers and pesticides. By contrast, many EU countries are classified as being in the 'Environmental Awareness' stage, which is characterized by attempts to reduce environmental impacts through the establishment and implementation of agro-environmental policies (Jepsen *et al.*, 2015). The most current EU 'Environmental Implementation Review Country Report' for Portugal highlights that despite significant improvements in the last decades, Portugal still faces many challenges in implementing and enforcing environmental policies (European Commission, 2017a).

The primary threat to freshwater from agricultural production comes in the form of diffuse (*i.e.* non-point) pollution, which effects 46% of water bodies in Portugal, compared to 27% for point-source pollution (European Commission, 2017a). In December of 2014, the Rural Development Programme (RDP) for mainland Portugal was adopted by the European Commission, which defines how 4.2 billion € of public money will be allocated over the period from 2014 - 2020 (European Commission, 2017b). A major goal of the RDP is the restoration, preservation, and enhancement of ecosystems related to agriculture and forestry; which receives approximately 26% of the overall budget (€1.1 billion; European Commission, 2017b), and approximately 72% of this allotment is to be used to incentivize farmers to use environmental /climate-friendly land management practices.

Some of the objectives of this component of the RDP are to include approximately 35% of the agricultural area in Portugal under contracts for Agri-Environment Commitments, Organic Farming, or Natura 2000 (European Commission, 2017b). This funding allocation marks a substantial commitment to improving the environmental sustainability of Portuguese agricultural operations. However, other efforts have been lacking. For example, the current status of the EU Water Framework Directive (WFD) mandated 'River Basin Management Plans' (RMBPs) for Portugal have been deemed to have deficiencies by the European Commission, which limits their utility in assessing the status of Portuguese water bodies (European Commission, 2017a).

In terms of water quality in Portugal, one of the main issues which has been highlighted is nitrate pollution, as according to the last available report on the ‘Nitrates Directive’ (from 2008 – 2011), nitrate levels were elevated in 20% of monitoring stations (European Commission, 2017a). With respect to compliance, the need for better balanced fertilization and compliance with the 170 kg/ha/year obligation were highlighted (European Commission, 2017a). The topic of nitrate water pollution from diffuse sources is examined in detail in **Sections 7 and 8**, which investigates the relationship between agricultural fertilizer application and HES.

6 *Time series Analysis of the Hydrologic Ecosystem Service Impacts of Afforestation in the Águeda watershed*

6.1 *Introduction*

The north-central region of Portugal underwent significant changes in land-cover change in the 20th century, which parallel many of the changes seen throughout the Mediterranean region during this time (Geri *et al.*, 2010). The Águeda watershed, located in the Caramulo mountain range within the Vouga basin, is representative of the landscape changes which occurred in the north-central region of Portugal (detailed in **Section 5.1**). With respect to forested land-cover, one of the most significant has been the widespread transition from traditional rural agro-silvopastoral activities to a landscape dominated by plantation forests, in particular with the tree species *Pinus pinaster* and *Eucalyptus globulus* (Jones *et al.*, 2011; Moreira *et al.*, 2001).

This afforestation is expected to have altered hydrologic processes at multiple scales, although the impacts of these changes are not yet fully understood. Both of these tree species have relatively high consumptive water demand due to increased evapotranspiration and, thus, the potential to substantially reduce local water availability. Bosch and Hewlett (1982) estimated that pine and eucalypt forests cause an average decrease of over 40 mm/yr in water yield per 10% change in land cover, while Farley *et al.* (2005) reported that afforestation with pines and eucalypts can lead to reductions in streamflow of 40% (± 3%) and 75% (± 10%), respectively. Rodríguez-Suárez *et al.* (2011) found that afforestation with *Eucalyptus globulus* caused a drop in water table depth as well as a decrease in streamflow during the summer period, which they attributed to the higher transpiration capacity of the eucalypt plantations compared to the original crop lands.

Water losses to the atmosphere from canopy interception are a further important component of water use by Mediterranean forests. Interception rates have been found to vary widely in this region, depending on the tree species, canopy density, and climatic conditions. With respect to *Pinus pinaster*, Ferreira (1996) reported interception rates of 15-18% of rainfall in the Águeda watershed (mean precipitation ~ 1,700 mm/yr), while Valente *et al.* (1997) found a similar rate of 17% in a drier region of central Portugal (mean precipitation ~ 600 mm/yr). For *Eucalyptus globulus*, both Ferreira (1996) and Valente *et al.* (1997) observed lower rates, amounting to 10-14 % and 11 % of rainfall, respectively.

By contrast, much higher interception rates have been found for other tree species in different parts of the Mediterranean, with values near and even exceeding 50% of rainfall. For example, Scarascia-Mugnozza *et al.* (1988) found canopy interception rates of 68 % for a mature *Quercus cerris* forest in central Italy (mean precipitation 1,006 mm/yr), Iovino *et al.* (1998) found rates of 58% for a mature *Pinus nigra* forest in southern Italy (mean precipitation 1,179 mm/yr), and Tarazona *et al.* (1996) observed rates of 48% for a mature *Pinus sylvestris* forest in northern Spain (long-term mean precipitation of 895 mm/yr and 1,253 mm/yr).

A further hydrologic factor relevant to afforestation in north-central Portugal is the potential for impacts on soil water repellency (SWR). Both pine and eucalypt tree species can promote SWR in the topsoil due to the considerable amount of resins, waxes, and aromatic oils contained in their organic matter (Benito and Santiago, 2003; Doerr and Thomas, 2000; Ferreira *et al.*, 2000; Keizer *et al.*, 2005; Shakesby *et al.*, 2000). SWR is a key factor in triggering land degradation processes due to reductions in infiltration capacity and increased overland flow (Benito and Santiago, 2003; Doerr and Thomas, 2000; Keizer *et al.*, 2005; Shakesby *et al.*, 2000).

While SWR is frequently associated with post-fire soil conditions, Doerr *et al.* (1996) demonstrated that SWR is a widespread characteristic of both burned and unburned soils in the Águeda watershed during dry periods, in particular for stands of *Eucalyptus globulus*. Santos *et al.* (2013) examined temporal patterns in topsoil SWR in the Águeda watershed between July 2011 and June 2012 in unburnt pine and eucalypt plantations. Their findings suggested that the breakdown of SWR following dry summer conditions occurs through different mechanisms in the pine and eucalypt stands. In the pine stands, SWR breakdown occurred from the top-down (*i.e.* vertically downwards), while in the eucalypt stands, breakdown occurred from the bottom-up (*i.e.* vertically upwards). Unpublished results indicated that this contrast reflected varying infiltration patterns, with infiltration occurring relatively slowly (*i.e.* matrix flow) in pine stands, as opposed to much faster (*i.e.* macropore flow) in eucalypt stands. This contrast in infiltration patterns appeared to be a product of SWR induced alterations in flow pathways.

Additionally, the magnitude of any changes in forest cover will largely depend upon what point of the species life-cycle and/or the cycle of the plantation a change occurs. The establishment and harvesting of forest plantations is a disruptive process in itself (in particular with regards to potential for soil erosion), which occurs in the study area approximately every 8 to 12 years for eucalypt plantations, and every 35 to 50 years for pine plantations (Nunes *et al.*, 2017).

Despite the well-documented potential for hydrologic impacts from afforestation in the Mediterranean region, there has been little investigation into the long-term effects in north-central Portugal. This is in part due to a lack of long-term streamflow records that allow for historical analyses. A notable exception to this lack of data is the Águeda watershed in the Caramulo Mountains, where streamflow data records are available from 1936 until the present. Afforestation/deforestation studies typically focus on small paired watersheds, of which one has undergone abrupt and well-recorded changes in land cover (*e.g.*

Bosch and Hewlett, 1982). By contrast, this study is conducted on a meso-scale watershed (404 km^2), where afforestation has occurred progressively over an extended period. Furthermore, the present study lacks a nearby watershed to serve as a paired site, which has a similarly long data record, similar physical-environmental characteristics, or a land use history without similar land cover changes (*i.e.* to serve as a control site).

6.1.1 Watershed Description

The Águeda watershed is located in the uplands of the Vouga basin, in the Caramulo Mountains of north-central Portugal (Figure 5). From the streamflow gauging point of Ponte Águeda, the watershed area is approx. 404 km^2. The Águeda River is a left bank tributary to the Vouga River, which terminates at the coastal wetland of the Ria de Aveiro lagoon. This region of Portugal is located in a wet Mediterranean climate zone, with pronounced seasonal differences in temperature and precipitation between dry summer and wet winter seasons (Figure 2). The Serra do Caramulo Mountains, which forms the source area of the Águeda river network, receives a substantial amount of annual rainfall, which can range from 1,000 to 2,500 mm/yr. Topographically the landscape is dominated by steep hill-slopes with stony and shallow soils (< 0.5 m), which have a long history of anthropogenic impacts. These shallow soil were classified by Ferreira *et al.* (2000) as stony, sandy loam, weakly structured Umbric Leptosols.

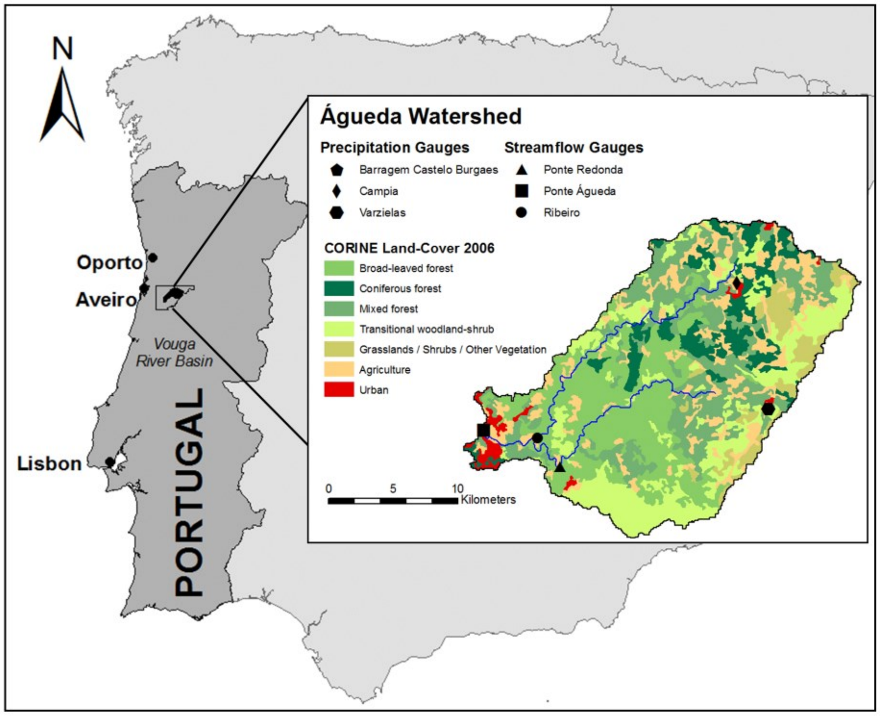


Figure 5. Location and land-cover/land use map of the Águeda watershed.

North-central Portugal has undergone substantial land-cover/use changes over the past centuries, following a general trend towards both increased agricultural and forest land cover, with reductions in natural vegetation types (*e.g. mato* shrublands and low density oak forests). With respect to forested land-cover, the trend in this region was primarily the afforestation of former shrublands with *Pinus pinaster*, followed by a secondary transition from *Pinus pinaster* to *Eucalyptus globulus* plantations. Based on this regional pattern and afforestation maps available for the wider area (*i.e.* Serra do Caramulo Mountains; Rego, 2001), a general timeline of land-cover change in the Águeda watershed during the period of investigation was approximated, which is summarized in Table 3.

Table 3. Land-cover periods and dominant afforestation trends in Águeda watershed from 1935 to 2010 (Rego, 2001).

Land-Cover Period	*Time Period*	*Dominant Afforestation Trend*
P1	**1935 - 1950**	Large-scale replacement of shrubland with *Pinus pinaster.*
P2	**1950 - 1970**	Continuing afforestation with *Pinus pinaster,* but at a slower rate.
E1	**1970 - 1990**	Rapid reforestation with *Eucalyptus globulus* (particularly post-1986 wildfire), replacement of *Pinus pinaster.*
E2	**1990 - 2010**	Relatively stable forested area, with continued replacement of *Pinus pinaster* with *Eucalyptus globulus.*

The current land cover in the Águeda watershed reflects this large-scale transition towards eucalypt forests. According to the Corine Land Cover classification of 2006, approx. 46% of the watershed was covered by broad-leaf forest - which is predominantly eucalypt (Corine Land Cover, 2010). Other land-cover types with significant areal coverage in 2006 include: 22% mixed forest (mostly mixed stands of eucalypt and pine), 14% agriculture, 10% pine forest, 6 % *mato* shrubland, 2% urban, and 1% grasslands (Figure 5).

6.1.2 Research Objective

To assess the hydrologic impacts of afforestation in the Águeda watershed during this time period, this study adopts a data-driven and exploratory approach, using multiple trend analyses on the 75-years of hydrometeorological data available from 1936 to 2010. This assessment is conducted over the entire data record as well as over multiple (overlapping) sub-periods for both annual and seasonal trends. The significant trends detected through this analysis are then considered with respect to the regional afforestation trends, and discussed in the context of previous field-studies conducted in this watershed. Therefore, the objective of this study is to apply a trend-testing methodology to a long-term data set in a watershed which has undergone progressive afforestation over a 75-year period, to assess what significant trends can be detected, and to relate these changes to the afforestation which has occurred there. To this end, the following hypotheses are tested:

> **Hypothesis 1a:** The large-scale afforestation with pine and eucalypt species which occurred in the 20^{th} century in the Águeda watershed has led to a statistically significant reduction in in-stream water availability.

Hypothesis 1b: The Águeda watershed meets the "prerequisite conditions" proposed by Andréassian (2004) needed to see a significant change in water availability due to changes in forest cover.

6.2 Data

For the Thiel-Sen/Mann-Kendall test used in this study (detailed in **Section 4.1.1**), trend testing was conducted over both annual and seasonal time periods. The seasonal breakdown corresponds to the prevailing precipitation patterns of the study site, which consists of i) a 'Wet Season' from October to January when the largest amount of precipitation occurs, ii) a 'Transitional Season' from February to May when precipitation rates are reduced, and iii) a 'Dry Season' from June to September when precipitation is lowest. Due to gaps in the streamflow record (discussed further in **Section 6.3.1**), the hydrologic years 1999/2000 through 2002/03 were unavailable for the trend testing for both the annual and seasonal time periods, and the hydrologic years 1954/55 and 1975/76 were unavailable for the annual and transitional season. In addition, the trend tests were not conducted during the 'Dry Period' for streamflow (and therefore also baseflow), due to the uncertain data quality during these months.

6.2.1 Hydrometeorological Variables

Hydrometeorological records for the Águeda watershed were compiled from hydrological year 1935/36 (Oct 1st 1935 to Sep 30th 1936) until hydrological year 2009/10, for the variables: precipitation, temperature, potential evapotranspiration, streamflow quantity, streamflow yield, baseflow quantity, and baseflow index. Table 4 provides an overview of the hydrometeorological variables used in this study and their data source.

Precipitation data were obtained from the Campia rain-gauge, of the Sistema Nacional de Informação de Recursos Hídricos (SNIRH, 2013), which consists of 24-h rainfall totals collected at 9:00 each day. The SNIRH provides a reliability ranking for the data in the range of 5 – 15, for which Campia is ranked as 14 (highly reliable). Data gaps occurred with the greatest frequency between 1997 and mid-2003, which were filled using linear regression with the nearby rain-gauges Varzielas ($r^2 = 0.82$) and Barragem de Castelo Burgães ($r^2 = 0.79$).

Table 4. Summary of hydrometeorological variables.

Hydrometeorological Variables			
Variable	**Description**	**Data Source**	**Unit**
P	Precipitation	SNIRH Gauge Data	mm
T	Temperature	IPMA Gauge Data	ºC
PET	Potential Evapotranspiration	Thornthwaite Equation	mm
Q	Streamflow Quantity	SNIRH Gauge Data	mm
Q_{yld}	Streamflow Yield	$\sum Q_{mm/}\sum P$	%
BF	Baseflow Quantity	Recursive Digital Filter	mm
BFI	Baseflow Index	$\sum BF_{mm/}\sum Q_{mm}$	%

Temperature data was also compiled using data from the Campia location, from the gauge of the Instituto Portugues do Mar e Atmosfera (IPMA, 2014). When data from Campia was not available, the time-series gaps were filled using linear regression with the temperature gauge Coimbra ($r^2 = 0.93$), which is part of the Global Historical Climate Network available at the National Climatic Data Center (NCDC).

Potential evapotranspiration (PET) was estimated using the Thornthwaite equation (Thornthwaite, 1948), using the temperature data from the gauge Campia. The Thornthwaite equation was selected to estimate PET, as opposed to more sophisticated equations (*e.g.* Hargreaves, Penman–Monteith) as there was insufficient data available over the entire time-series to support calculations from these equations. Another option which was considered for estimating long-term PET values is the gridded Penman–Monteith based dataset available from the Climatic Research Unit (CRU) at the University of East Anglia (Harris *et al.*, 2014).

To assess the suitability of this dataset to the study watershed, the monthly PET values of the CRU data and the locally derived Thornthwaite values were compared against locally derived Penman-Monteith values, over the period of January 2002 to September 2010. This assessment indicated that the locally derived Thornthwaite values are better correlated than the gridded CRU dataset with local Penman-Monteith values. This may be due to the mountainous terrain of the study watershed, and the relatively large grid size of the CRU dataset (0.5 degrees) being unable to capture smaller scale impacts on PET. Based on this assessment, the locally derived Thornthwaite PET values were identified as the most reliable and representative data source available for assessing long-term trends.

Streamflow data consists of daily average discharge measurements from the gauging station Ponte Águeda from SNIRH (2013). This station was operational from June 1935 until the end of September 1990, and was then reactivated in October 1999. Streamflow for the interim period (1990/91 until

1998/99) was estimated using linear regression with the upstream gauges Ribeiro ($r^2 = 0.76$) and Ponte Redonda ($r^2 = 0.75$). However, the streamflow estimates from the hydrologic years of 1999/2000 through 2002/03 were eliminated from the dataset due to low data quality, owing to the absence of an adequate stage-discharge curve during this period.

In addition, a number of smaller streamflow gaps occurred throughout the daily streamflow dataset. When they occurred during periods with little or no precipitation, the gaps were filled by fitting a logarithmic decay curve (traditional linear reservoir with a semi-log fitting) to the streamflow recession. If gaps occurred during a precipitation event, then this approach was not applied and the gaps were left unfilled. If the number of gaps was > 5% of the total record, then the entire period was removed from analysis, which was the case for the hydrologic years 1954/55 and 1975/76.

Finally, data for the driest months of the year (*i.e.* June to September) during the period from before 1963 and after 2004 had very high uncertainty, due to unreported and variably occurring impoundments of streamflow during these months. Therefore, this 4-month period had to be removed from the streamflow analysis for the entire data record, to keep the inter-annual comparisons consistent. After the streamflow gaps were filled, the ratio of precipitation which becomes streamflow was calculated, to allow potential changes in the streamflow-precipitation relationship to be assessed. This ratio is defined as the 'streamflow yield', which is the total streamflow divided by total precipitation, with the period of summation determined by the period being considered (*i.e.* the annual or the seasonal ratio).

The final data set utilized in this study is a baseflow time-series calculated with the Eckhardt digital filter using the daily streamflow dataset (Eckhardt, 2005). Baseflow corresponds to the portion of streamflow which does not come directly from a precipitation event, and can be used as a proxy of the sustained streamflow contribution from slow-flow pathways. The relative proportion of baseflow from each day of streamflow was estimated, which was then aggregated to the time periods used for analysis. To assess the baseflow time-series calculated using the Eckhardt digital filter, a supplementary data set from 2001 to 2009 was also utilized, which calculates baseflow contribution using conductivity data from the SNIRH streamflow data using the 'Conductivity Mass-Balance' method (Stewart *et al.*, 2007).

6.2.2 Periods of Analysis

For each hydrometeorological variable, the trend testing procedure was applied over 12 different time-periods with varying start/end dates and lengths. The longest period tested contains the entire 75-year data record (hydrologic years 1936 - 2010), followed by two periods of 50 years, three periods of 35 years, and six periods of 25 years. These overlapping periods of different lengths aim to thoroughly sample the potential range of years, while still allowing enough years of data to produce a robust significance test within each test period (*i.e.* a minimum of 25 years). Figure 6 provides an overview of the testing periods, and their temporal correspondence with the afforestation periods shown in Table 3.

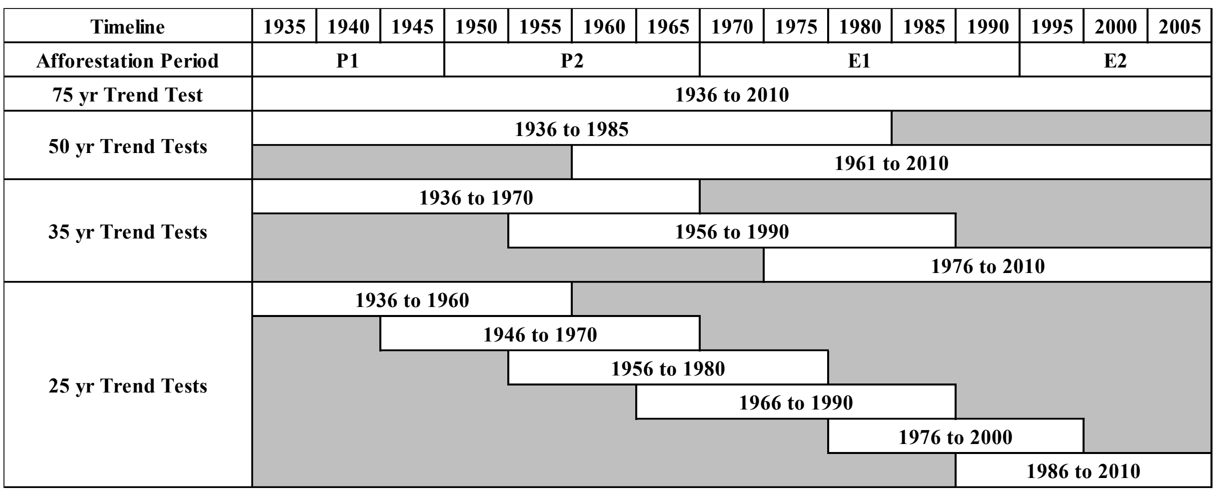


Figure 6. Timeline of the trend-testing periods and their correspondence with the different afforestation periods in the Agueda watershed: P1 = large scale pine afforestation; P2 = slower pine afforestation; E1 = rapid eucalypt expansion; E2 = slower eucalypt expansion period.

6.2.3 Seasonal Breakdown

To characterize the hydrometeorological conditions of the three seasons' used in this study; the median values of the hydrometeorological variables during the study period are presented in Table 5. This summary shows the strong climatic pattern in the watershed, with distinctly contrasting precipitation, temperature, and potential evapotranspiration values between seasons. With respect to streamflow, the values are similar during the wet and transitional seasons, however both streamflow yield and baseflow index are higher during the transitional season, which reflects the sustained streamflow carried over from the wet season precipitation, and the lower proportion of streamflow coming directly from precipitation events.

Table 5. Seasonal and annual median values of the hydrometeorological variables in Águeda watershed from 1936 - 2010.

		Median Values: 1936 - 2010						
Season	**Months**	**P (mm)**	**T (ºC)**	**PET (mm)**	**Q (mm)**	**Q_{yld} (%)**	**BF (mm)**	**BFI (%)**
Wet	Oct - Jan	965	11.7	145	301	30 %	149	55 %
Transitional	Feb - May	626	12.6	198	281	43 %	184	63 %
Dry	Jun - Sep	193	19.3	390	NA	NA	NA	NA
Annual	All*	1,787	14.7	732	565	36 %	320	59 %

* The months of June to September are not included for Q (mm), Q_{yld} (%), BF (mm), and BFI (%).

6.3 Results

6.3.1 Elimination of Dry Season Streamflow

The months of June to September had to be removed from all streamflow analyses, due to uncertainty related to variable seasonal impoundments during this part of the year. To quantify the percentage of streamflow that this excluded from the analysis, an assessment was made over the years when streamflow impoundments did not occur (45% of years). During these years, approx. 6.5% of streamflow occurred between the months of June to September (Fig. 7, monthly mean values presented).

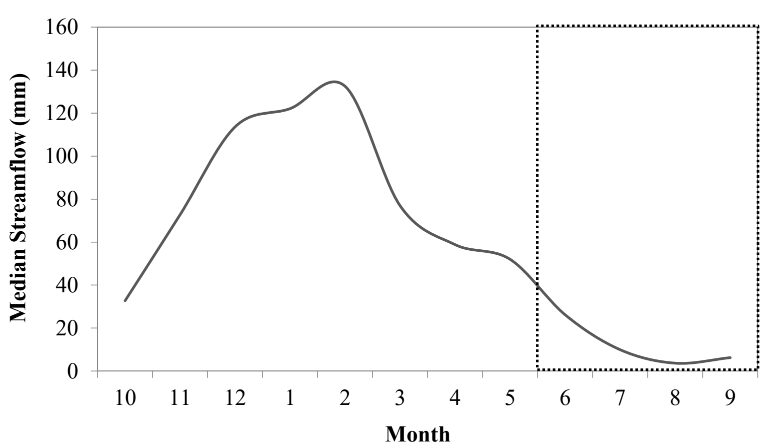


Figure 7. Monthly mean streamflow during the years without seasonal impoundments; the boxed-off period (June - September) indicates the period removed from the streamflow and baseflow analysis.

6.3.2 Assessment of the Baseflow Calculations

The baseflow index used in this study is estimated by the Eckhardt digital filter, which contains two parameters: BFI_{max} (maximum value of the baseflow index) and a (a filter parameter). These parameters were set at $BFI_{max} = 0.80$, and $a = 0.98$, based on testing of different recommended values provided by Eckhardt (2005). To provide a check on the baseflow values estimated using this method, the results were then compared against baseflow values calculated using conductivity data from 2001 to 2009 with the 'Conductivity Mass-Balance Method' (Stewart *et al.*, 2007).

At the monthly time-scale, the two compared baseflow data-sets have a Pearson's correlation coefficient of 0.96 for all months (Fig. 8a), and 0.83 for months with < 100 mm of baseflow (Fig. 8b), which indicates that the Eckhardt method agreed well with the more empirical Conductivity Mass-Balance Method. This, in itself, does not confirm the accuracy of the baseflow values utilized, but it does indicate their consistency over the study period, and thus their suitability for the time-series trend analysis.

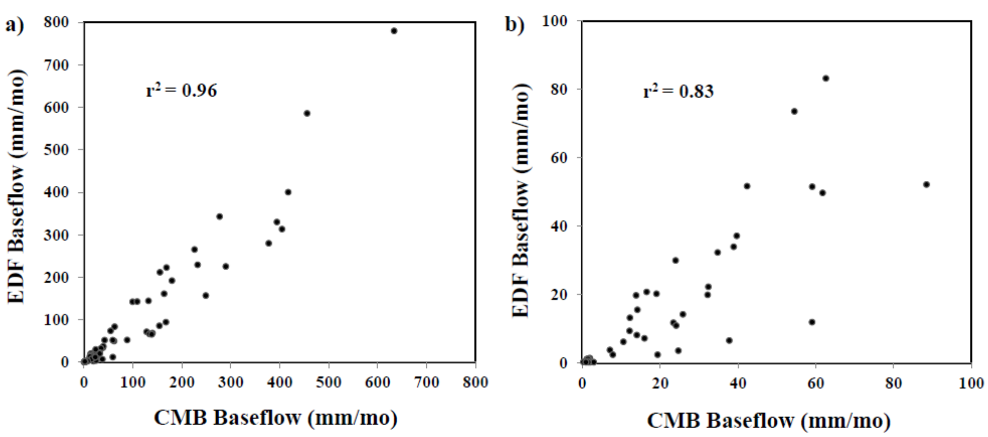


Figure 8. Monthly plots of baseflow from the Conductivity Mass-Balance (CMB) and Eckhardt digital filter calculations; 8a includes all months ($r^2 = 0.96$) and 8b includes months with < 100 mm of baseflow ($r^2 = 0.83$).

6.3.3 Thiel-Sen/Mann-Kendall Trend Testing Results

The results for the Thiel-Sen/Mann-Kendall trend tests for the variables of precipitation, temperature, potential evapotranspiration, streamflow yield, and baseflow index are presented by Fig. 9. Trends which were found to be statistically significant are indicated in the figure with the dashed lines.

For the precipitation data, three significant trends were identified during the transitional season. All trends corresponded to decreases in precipitation: –7.9 mm/yr trend over the 50 years from 1961 to 2010, –11.3 mm/yr trend over the 35 years from 1976 to 2010, and –14.3 mm/yr trend over the 25-year period from 1976 to 2000. These trends indicate that there was a pattern of decreasing precipitation totals during the transitional season (February - May) starting during the P2 land-cover period, and this pattern continued through the E1 and E2 land-cover periods (*cf.* Table 3).

Three significant trends were also found for potential evapotranspiration (PET) during the transitional season: a –0.8 mm/yr trend over the 50 years from 1936 to 1985, a –1.3 mm/yr. trend over the 25 years from 1956 to 1980, and a 1.7 mm/yr trend over the 25-year period from 1976 to 2000. Therefore, the PET data shows a pattern of negative trends throughout the P1, P2, and into the E1 land-cover periods, which reverses and becomes positive during the E1 period and into the E2 land-cover period (*cf.* Table 3).

For the streamflow data, no significant trends were found for either streamflow totals or streamflow yield. No significant trends were found for baseflow quantity either; however a number of significant trends appeared for baseflow index (BFI). For the annual test period, four significant trends were found in total: including significant positive trends of 0.16%/yr for the 35-year period from 1936 to 1970 and of 0.31%/yr for the 25-year period from 1946 to 1970; and negative trends of –0.22%/yr for the 35-year period from 1956 to 1990 and a –0.46%/yr trend for the 25-year period from 1966 to 1990. Two significant trends were found for BFI during the wet season: a 0.28%/ yr trend for the 35-year period from 1936 to 1970 and a –0.33%/yr trend for the 25-year period from 1966 to 1990. Therefore, the BFI data showed an overall pattern of positive trends during the P1 and P2 land-cover periods, which reverse to negative trends during the P2 period and throughout the E1 land-cover period (*cf.* Table 3).

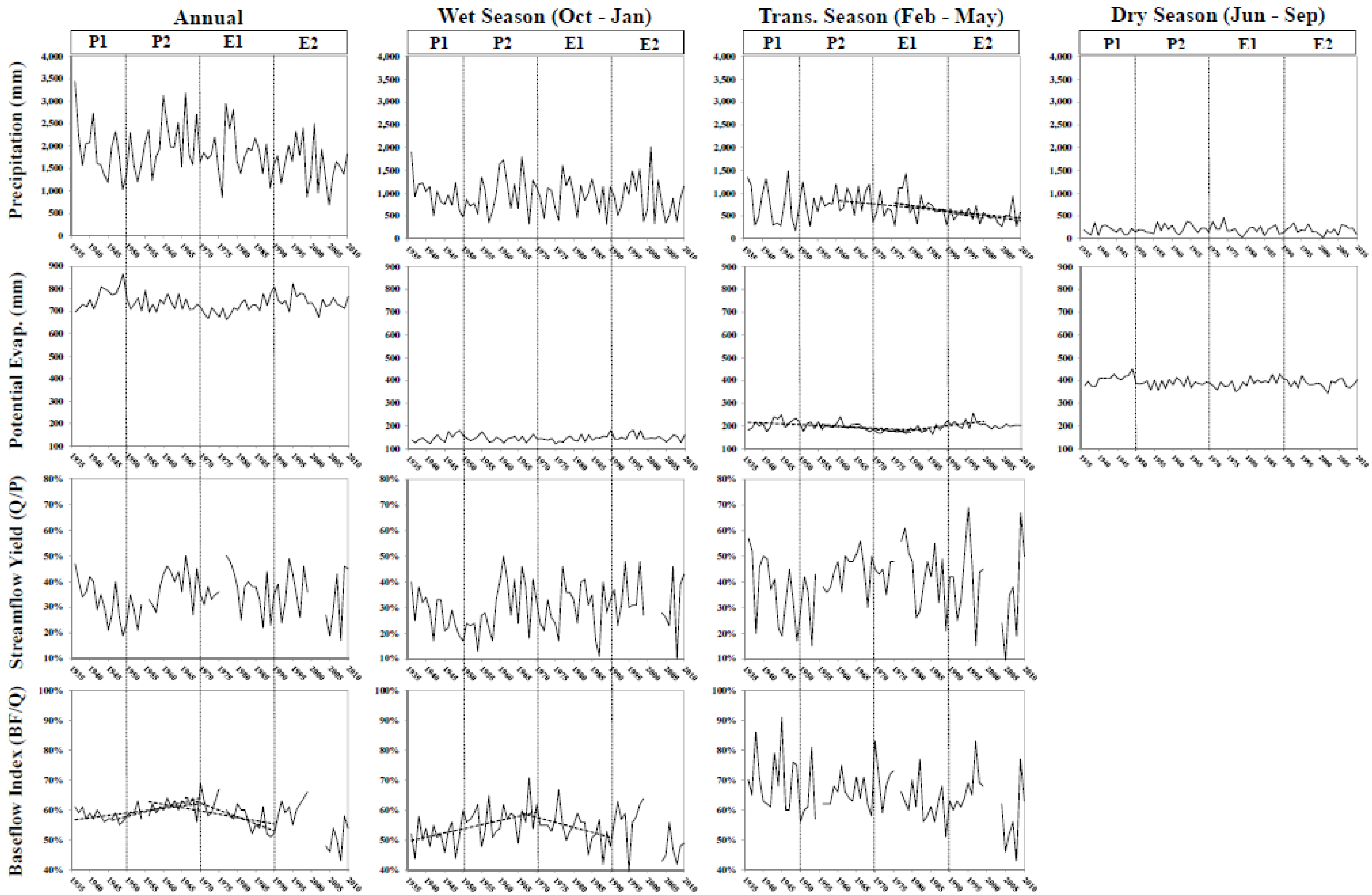


Figure 9. Summary of the trend-testing results, with the afforestation periods (P1, P2, E1, E2: *cf.* Table 3) overlain for comparison. Significant trends are indicated with dashes lines.

6.4 Discussion

6.4.1 Streamflow Trends

The streamflow tests revealed that there were no significant trends for either the total quantity or yield over any of the periods tested (Fig. 9). These results therefore contrast with the overall pattern found in meta-analysis studies dealing with the hydrologic impacts of afforestation/deforestation, which indicate that afforestation tends to reduce streamflow (*e.g.* Bosch and Hewlett, 1982; Brown *et al.*, 2005; Farley *et al.*, 2005). However, there are a number of individual cases within these meta-analyses studies which show contrasting trends to the overall pattern. These cases are difficult to directly compare to the current study, however, as most were conducted at the plot to micro-catchment scale, and investigated sites which underwent relatively rapid land-cover change. By contrast, this study was conducted on a mesoscale watershed (404 km^2), which underwent relatively gradual land-cover changes over a 75-year period. In this case, any potential changes in hydrologic processes are likely to be far more diffuse and difficult to detect, when compared to the paired catchment studies.

Despite this limitation, some comparisons can be made to sites with similar site conditions, in terms of having winter-dominant precipitation and shallow soils. Across a number of catchments with winter-dominant rainfall, Brown *et al.* (2005) found that afforestation led to much larger proportional reductions in summer flows compared to winter flows, which they attributed to the afforestation-induced changes in interception and evapotranspiration. Among these catchments, those of Gallart *et al.* (2001) and Lewis *et al.* (2000) demonstrated the importance of soil depth in controlling the hydrological response of Mediterranean mountain catchments in the Pyrenees and California, respectively, which is reflective of the soil conditions found in the Águeda watershed. Other studies with somewhat similar site conditions (*i.e.* Bari *et al.*, 1996; van Lill *et al.*, 1980) were conducted at very different temporal and spatial scales than the present study, making comparisons to their findings difficult. In spite of the lack of comparable studies for direct comparison, the absence of a marked reduction in streamflow was an unexpected finding, given the large-scale of afforestation which has occurred in the Águeda watershed.

A potential explanation for this lack of observed impact could be the presence of off-setting climatic trends over the same period. Either an increase in water availability due to higher precipitation (P) and/or a reduction in atmospheric demand due to lower potential evapotranspiration (PET) could compensate for any land-cover induced changes. While no significant trends were found for either P or PET at the annual time scale, or during the wet or dry seasons, significant trends were found during the transitional season, which may have impacted water availability.

With respect to increasing water availability during the transitional season, negative trends in PET were found for the periods 1936 - 1985 and 1956 - 1980 (Fig. 9). These trends occur primarily during the periods of pine afforestation (P1, P2) and partially during the transition to eucalypt (E1; *cf.* Table 3). The trends in PET would lead to a reduction in atmospheric demand during this period, and therefore could be responsible for offsetting an increase in consumptive demand that occurred from afforestation.

With respect to reductions in water availability during the transitional season, negative trends in P were found for intervals from 1961 to 2010, 1976 to 2010, and 1976 to 2000; and a positive trend in PET was found from 1976 to 2000 (Fig. 9). These trends may indicate movement toward a relatively more arid environment, which could therefore lead to a reduction in water availability. However, no corresponding reductions in streamflow were found during this period. This lack of change is particularly noteworthy given that these trends occurred during the eucalypt afforestation periods (E1, E2; *cf.* Table 3), which would also be expected to increase consumptive demand, and would therefore amplify, rather than offset, an increase in atmospheric demand.

Given the lack of significant climate trends at the annual time scale, and the contrasting findings during the transitional season, offsetting climatic trends do not appear to be an adequate explanation for the overall lack of observed streamflow changes in the Águeda watershed. However, given that the observed climate trends occurred during the transitional season, there may have been streamflow impacts during the (following) dry season. This can only be speculated on however, since no assessment can be made on streamflow during the dry season, due to the limitations in the streamflow data (*i.e.* the summer streamflow impoundments). Therefore, no comparison could be made with the findings of Rodríguez-Suárez *et al.* (2011), who found dry season reductions in the water table and streamflow discharge following afforestation with eucalypt; or to Brown *et al.* (2005) who found that afforestation led to much larger proportional reductions in summer flows compared to winter flows.

An alternate explanation for the lack of streamflow change could relate to the specific characteristics of the watershed, which may make it less responsive to changes in forest land-cover than would typically be expected from the literature. With respect to watershed characteristics, Andréassian (2004) identifies several prerequisites conditions necessary to observe hydrologic impacts, including soil, climatic, and eco-physiological factors.

With respect to soil conditions, the characteristics of the soils of the Águeda watershed may be a key factor in the lack of a reduction in streamflow. Under conditions of well-developed soils, the deeper rooting depths of trees will give greater access to soil moisture, allowing for more transpiration, resulting in higher water consumption. However, the soils of the Águeda watershed tend to be very shallow, being typically < 1 m deep and often as shallow as 20-30 cm (Santos *et al.*, 2013). These depths are less than the maximum rooting depth of pine and eucalypt tress, and therefore are likely to be a constraint to deep rooting for both species (Canadell *et al.*, 1996). In addition, the schist and granite bedrock in this watershed is relatively impermeable and cannot easily be penetrated by tree roots, which restricts the access of tree species to groundwater reserves as well. Therefore, the capability of the fast-growing pine and eucalypt trees to access deeper sources of soil moisture than the original shrub and slow-growing tree species is likely much less relevant in this watershed than it would be in a location with deeper soils. In the case of the Águeda watershed, the most important soil-related factor in water consumption appears to be the low moisture storage capacity of the soils, severely off-setting the potential impact of widespread planting of trees with higher water consumptive capacity.

A second factor which could contribute to the lack of reductions in streamflow is the Mediterranean climate regime of the study area. In all Mediterranean-type climates, the period of peak sunlight and temperature, and therefore potential evapotranspiration, is out of phase with the maximum precipitation period (Brown *et al.*, 2005). Given the low amount of summer precipitation and the shallowness of soils in this watershed, there will typically be little soil water available for summer evapotranspiration (David et al., 1994; Doerr and Thomas, 2000). In this regard, the climatic conditions of the Águeda catchment may have an amplifying effect on the impacts of the shallow soils, by further reducing the higher evapotranspiration potential of fast-growing trees species.

With respect to eco-physiological conditions, the specific land-cover changes in the Águeda watershed may also be a factor in the lack of an observed reduction in streamflow. One of the primary drivers of increased consumptive water use by tree species is their typically high canopy interception capacity (Domingo *et al.*, 1994; Scarascia-Mugnozza *et al.*, 1988; Tarazona *et al.*, 1996; Valente *et al.*, 1997). In the Águeda watershed, however, the interception rates appear to be comparatively low for pine and eucalypt species (Coelho et al., 2008; Ferreira, 1996; Valente et al., 1997), while the interception capacity of Mediterranean shrublands can be relatively high. Garcia-Estringana *et al.* (2010) found that Mediterranean shrub species can have interception capacities similar to those of forests.

In addition, interception rates are particularly high in shrublands growing in dense stands (Llorens and Domingo, 2007). These characteristics apply to the '*mato*' shrubland that was the most common vegetation type in the Águeda watershed prior to pine afforestation, as it has a relatively high leaf-area index and the tendency to grow in very dense stands (Asner *et al.*, 2003). By contrast, given the poor soil conditions of the study site, the densities of the tree plantations are not as high as they could be on well-developed soils. Average tree density from unpublished plot assessments put the density of unevenly spaced eucalypt stands (< 15-yr old) at 1,600 trees/ha, of evenly spaces eucalypt stands on terraces (< 5-yr old) at 1,500 trees/ha, of eucalypt on flat terrain (< 5-yr old) at 2,600 trees/ha, and of unevenly spaced pines (< 30-yr old) at 500 trees/ha. Therefore, the land cover/use change from shrubland to pine/eucalypt forest might not have resulted in large changes in either transpiration rates or canopy interception rates.

This review of the site characteristics of the Águeda watershed indicates that it does meet the "prerequisites conditions" identified by Andréassian (2004) which are needed to observe afforestation-driven streamflow changes at the watershed scale. Given this lack of these prerequisites conditions, and the absence of offsetting climate trends as an alternative explanation, the streamflow findings of this study appear to be primarily a function of watershed characteristics, with soil properties as the most important factor.

6.4.2 Baseflow Trends

No significant trends were found for total baseflow quantity (BF) over any of the periods or seasons tested. However, a number of trends appeared for baseflow index (BFI), for both the annual data and the wet season data, which includes both positive and negative trends over different parts of the data record.

Positive trends in BFI were found from 1936 to 1970 for the annual data and for the wet season, and from 1946 to 1970 for the annual data (Fig. 9). These trends correspond with the pine afforestation land-cover periods P1 and P2 (*cf.* Table 3). These trends could be an indication that the pine afforestation promoted slower flow pathways, by increasing the amount of water entering the soil matrix *via* infiltration, and reducing surface flow and fast subsurface flow (*i.e. via* macropores). However, given that previous studies in Águeda watershed have found soil water repellent (SWR) conditions in pine stands (during dry periods), pine afforestation would not normally be expected to increase matrix infiltration at this site (Keizer *et al.*, 2005; Santos *et al.*, 2013). However, the land-cover state during the initial conversion to pine forests were significantly different from the land-cover during these studies, which may have led to a more positive impact on infiltration rates. This is due to the ground preparation and planting operations used, which would have the effect of breaking-up the repellent topsoil layer and creating sinks for overland flow, both of which would promote infiltration. This effect would be reduced over time, and eventually SWR would recover in established stands.

Negative BFI trends were found from 1956 to 1990 for the annual data, and from 1966 to 1990 for the wet season (Fig. 9). These time periods correspond with the early part of the P2 land-cover period, and the entirety of the first eucalypt afforestation period (E1, *cf.* Table 3). Therefore, the negative BFI trends occur during the period when *Pinus pinaster* plantations had reached greater maturity and (after logging) were being rapidly replaced with *Eucalyptus globulus*. The reductions in baseflow during this period may therefore be related to soil water repellency (SWR) in the established pine stands and the newly established eucalypt stands. An increase in SWR could lead to an increase in quick flow, particularly *via* fast sub-surface flow from macropore infiltration, and lead to more rapid conversion of precipitation into streamflow.

The temporal correspondence between the significant trends in BFI and land-cover changes which could affect hydrologic flow pathways indicate there may be a relationship between afforestation and changes in baseflow index in the Águeda watershed. These findings are further supported by field studies conducted in the watershed, which show the strong impact of SWR in pine and (particularly) eucalypt stands on hydrologic flow pathways (Santos *et al.*, 2013). However, given that there is no field data available to verify the site conditions during the time of the observed trends for this study, the attribution of the changes in BFI to land-cover change is necessarily speculative. To test this hypothesis, further field studies would be needed to examine baseflow dynamics under land-cover conditions which replicate the historic conditions.

6.5 Conclusion

This study did not detect statistically significant – negative or positive – trends in streamflow quantity or yield in the Águeda watershed over the 75-yr period examined, despite the large scale afforestation with *Pinus pinaster* and (later) *Eucalyptus globulus* which has taken place there. Hypothesis 1a stated:

> **Hypothesis 1a:** The large-scale afforestation with pine and eucalypt species which occurred in the 20^{th} century in the Águeda watershed has led to a statistically significant reduction in in-stream water availability.

Based on these finding, **hypothesis 1a is rejected.**

While these findings differ from the general conclusion of afforestation/deforestation meta-analysis studies, such as Bosch and Hewlett (1982), Brown *et al.* (2005), and Farley *et al.* (2005); they do support the assertion of Andréassian (2004) that there are prerequisite climatic, pedological, and eco-physiological watershed conditions that are necessary to observe hydrologic impacts at the watershed scale. These conditions are not present in the Águeda watershed, and the lack of soil moisture holding capacity is likely the primary controlling factor. Hypothesis 1b stated:

> **Hypothesis 1b:** The Águeda watershed meets the "prerequisite conditions" proposed by Andréassian (2004) needed to see a significant change in water availability due to changes in forest cover.

Based on these finding, **hypothesis 1b is rejected.**

With respect to baseflow trends, the initial conversion from more natural land-cover types (*i.e. mato* shrublands, low density oak forests) to pine plantations appears to have had a significant – initial – positive impact on baseflow index (increasing baseflow), while the substitution of pine plantations by eucalypt plantations had a negative impact on baseflow index (decreasing baseflow). The positive trends are attributed to the impact of the site preparation methods applied during the initial pine planting on soil infiltration capacity, while the negative baseflow trends are attributed to the onset of soil water repellency (SWR) under the mature pine and eucalypt stands. Therefore, from the standpoint of promoting well-regulated streamflow (*i.e.* higher baseflow) the impacts of the afforestation with pine were generally positive, while those of re-/afforestation with eucalypts were generally negative.

The variability in impacts between different species is an important consideration from a policy perspective, as it highlights that it is not enough to consider simply the effects of a forest land-cover change, but that the specific characteristics of the forest types must be accounted for. While in this this historical case the impacts of the pine afforestation was primarily positive, and the eucalypts was negative, it is important to stress that the antecedent land-cover to their planting in the study catchment was unequal. Pines were primarily replacing naturally occurring shrublands, which was followed by the replacement of the planted pines by eucalypts. Therefore, a direct comparison between the impacts of widespread planting with pine or with eucalypt cannot be drawn from this study. In addition, these baseflow findings are based on a statistical/historical analysis, with no field data available for validation. To further test this hypothesis, field studies would be needed to examine baseflow dynamics under different land-cover conditions replicating the historic conditions. Despite these caveats, these findings indicate the potentially significant impacts that forested land-cover change can have on hydrologic flow patterns. From a policy perspective, this highlights that to adequately understand potential impacts of a forested land-cover change, it is not sufficient to consider only the spatial area modified, but to consider the specific climatic, pedological, and eco-physiological conditions of the site.

7 SWAT Model Assessment of Nitrate Fluxes in the Vouga Basin

7.1 Introduction

The land-use/land-cover patterns of the Vouga basin are characterized by distinct spatial and temporal patterns. S**ection 6** considered the provisioning HES (*e.g.* water quantity) impacts of the historical land-cover changes, which consisted of a transition away from mixed land-use patterns, and towards a distinct pattern of forestry dominated land-use in the middle/upper basin, and agricultural land-use in the lower basin. **Section 7** moves the spatial focus of the research from these upland regions, up to a basin wide assessment of water and nitrate fluxes, and the temporal focus moves from considering historical impacts to that of present-day conditions.

7.1.1 Nitrate Water Pollution and Agriculture

Water quality is strongly tied to land cover and land use, and in particular with agricultural practices. Nitrate (NO_3^-) is one of the most common water contaminants, and due to the low sorption of this anion in soils it is highly susceptible to leaching. The main non-point source of nitrate pollution is from the use of nitrogen-based fertilizers in agricultural production (Moss, 2008). Plants have a limited capacity for nitrogen uptake within a given period of time, and the uptake efficiency of fertilizers tends to be relatively low, and as a result, far larger quantities of fertilizer are frequently applied than are ultimately taken up by crops (FAO, 2015). Largely as a result of this large-scale application of fertilizers, reactive nitrogen has become far more abundant in the environment, and excesses of nitrogen are now nearly as common as deficits (Sutton *et al.*, 2011).

Nitrogen application rates have decreased across much of Europe in the last decades, which has been attributed to factors such as the introduction of agro-environmental policies (*e.g.* Nitrates Directive), the breakdown of socialism (in eastern Europe), and changes in nitrogen use efficiency (Jepsen *et al.*, 2015; Levers *et al.*, 2016). Levers *et al.* (2016) found corresponding trends of increasing crop yields and decreasing nitrogen application rates in the EU over the last 20 years, which implies a decoupling of crop yields from nitrogen inputs. This decoupling has been attributed to an improvement in nitrogen management (Lassaletta *et al.*, 2014), and/or or the intensification of production onto more fertile areas leading to more efficient production (Jepsen *et al.*, 2015). Despite these improvements, however, it is still estimated that less than half of the reactive nitrogen added to cropland globally is converted into harvested products, with the remainder being lost to the environment (Lassaletta *et al.*, 2014).

Excess nitrate is exported off agricultural sites through surface and sub-surface hydrological fluxes, in particular during precipitation events or during irrigation. Nitrate ions can move downward freely with drainage water, which make them easily leached from the soil with vertical sub-surface flow to groundwater. Agricultural soils in general, and in particular those with high hydrologic conductivity and high water inputs, are therefore very prone to nitrate leaching.

The consumption of nitrate enriched water can pose a serious health threat, both to humans and livestock (Di and Cameron, 2002; Moss, 2008). Excess nitrate is also damaging to ecosystems, as excessive nitrates in surface waters can lead to the explosive growth of algae, leading to the depletion of oxygen (*i.e.* anoxia), particularly in restricted waterways, such as coastal and estuarine water bodies. In addition to this immediate impact, the repeated occurrence will alter the health, numbers, and diversity of plant and animal species in effected ecosystems, leading to long-term alterations in system functioning (James *et al.*, 2005).

Given these risks to health and natural ecosystems, there have been substantial efforts to regulate permissible levels in most developed countries. In the European Union (EU), there are a number of policy directives which address water quality and have a bearing on the regulation of nitrate in water bodies. The most critical of these policies with respect to nitrate from agricultural sources, are the Nitrates Directive (91/676/EEC), the Water Framework Directive (2000/60/EC), and the Groundwater Directive (2006/118/EC). In terms of strict limits, these directives set the maximum acceptable concentration at 50 mg/l (equivalent to 11.3 mg/l of nitrate-N), which is similar to the limits established in the United States (44 mg/l nitrate, 10.0 mg/l nitrate-N).

7.1.2 Nitrate Water Pollution Risks in the Vouga Basin

The Vouga basin contains a number of different land-cover/land-use types, which would be expected to have varying degrees of nitrate export potential. Despite the overall mixed land-use of the basin, there are clear patterns of land-cover in the basin, with some areas dominated by forested land-cover and others by agricultural activities. Figure 10 shows the percentage of agricultural land-use, broken down by sub-basin, which demonstrates a strong concentration of agriculture in the southern basin, where most of the sub-basins have around 30 - 40% agricultural cover.

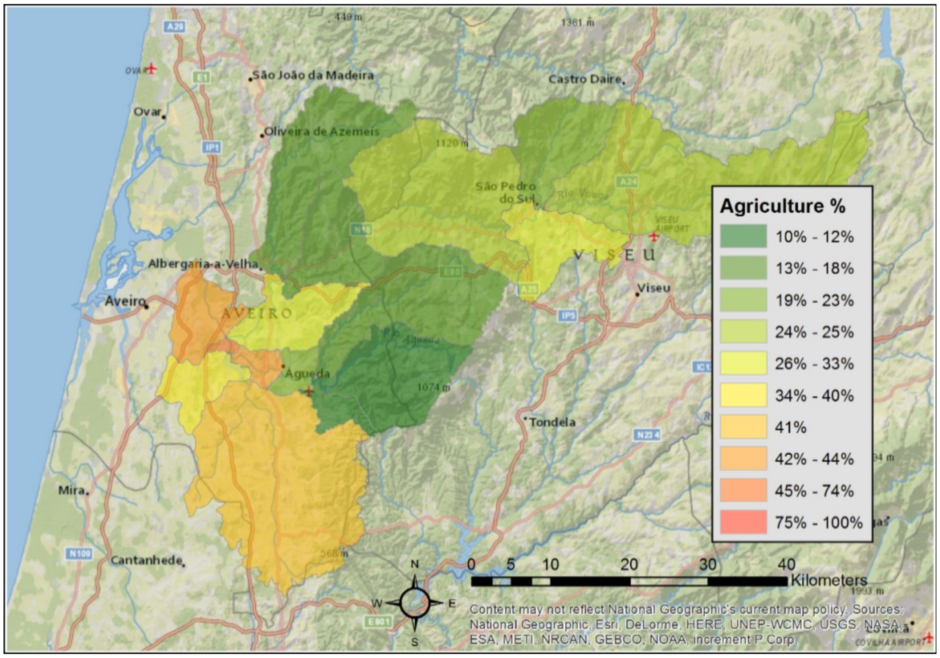


Figure 10. Percentage of agricultural land-use per sub-basin in the Vouga basin.

Within the main agricultural production areas, there are two crop types which are particularly relevant for nitrate export; intensively cultivated and fertilized corn (maize) and vineyards. The vineyards within the Vouga are part of the Bairrada wine growing region, which is listed as a *Denominação de Origem Controlada* (DOC). Vineyards in Mediterranean regions frequently have high agrochemical input requirements, given that they are often grown in soils with relatively low nutrient and organic matter content levels and vines are often also susceptible to pests and diseases (Serpa *et al.*, 2017). Rocha *et al.* (2015) examined the impact of the cultivation of these crop types in the Vouga basin and found high nitrate exports from the current level of fertilization from both types.

There are several key water bodies within the Vouga basin which could potentially be at risk from nitrate pollution from this intensive agricultural area. The surface water body within the closest proximity to this area, is the 'Pateira de Fermentelos', a shallow freshwater lake and surrounding wetland, which has a highly variable seasonal areal coverage, ranging from approx. 3 to 5 km^2 (Fig. 11; Ferreira *et al.*, 2010). The Pateira is the largest natural freshwater lake on the Iberian Peninsula, and constitutes one of Portugal's most important wetland areas for wildlife, in particular for migrating bird species (Ferreira *et al.*, 2010; Sena and de Melo, 2012). Given the surrounding prevalence of agricultural and urban land-cover types, the Pateira has experienced ongoing problems with the accumulation of contaminants from both point (industrial and domestic) and diffuse (agricultural) sources. Roebeling *et al.* (2016) found that while the current status of surface waters in the Pateira is good from a chemical perspective, it is only moderate from an ecological perspective. Due to the risk of nutrient accumulation, the Pateira is at high risk of eutrophication, and it as well as the main contributing stream (*i.e.* the Cértima) has been the focus of a number of previous studies (Cerqueira *et al.*, 2005; Ferreira *et al.*, 2010; Oliveira *et al.*, 2012; Sena and de Melo, 2012).

A second key water body is the 'Ria de Aveiro', a shallow estuary-coastal lagoon (Figure 11). The Ria is primarily fed by the Vouga river, as well as several other smaller river systems (*e.g.* Antuã, Caster, Boco), and is connected to the Atlantic ocean by a single tidal channel, which constrains the circulation of lagoon waters (Lopes *et al.*, 2005). The Ria is a highly productive ecosystem, and historically large amounts of sea grasses and algae were annually collected from the inner areas of the lagoon (Silva *et al.*, 2002)). The Ria now provides an important habitat for many bird species, and is an important component of the local economy (*e.g.* tourism, aquaculture, recreational fishing, salt collection). The area surrounding the Ria de Aveiro has a relatively high population density, as well as heavy utilization for agricultural and industrial activities. This has resulted in significant inputs of nutrients and other contaminants, and given the high ecological productivity of the Ria, the lagoon is under considerable threat of organic enrichment and eutrophication.

The third water body to consider is the interconnected network of regional groundwater aquifers, which include the 'Aveiro Quaternary', 'Aveiro Cretaceous', and the 'Bairrada Karst' aquifers (Gooch, 2015; Sena and de Melo, 2012; Serpa *et al.*, 2017). Within the Vouga basin, the recharge area of the 'Aveiro Cretaceous' aquifer is located directly to the west/southwest of the Pateira de Fermentelos (Sena and de Melo, 2012); while the 'Bairrada karst' aquifer is located directly in the central portion of the Cértima watershed (Serpa *et al.*, 2017). Given that the geology of this area consists largely of highly permeable sandstones, and that this area is under heavy agricultural production, these aquifers may be vulnerable to pollution from surface water sources. Serpa *et al.* (2017) examined the export of agrochemicals from a small sub-catchment of the Cértima watershed under different climate and land-use scenarios, and found relatively low concentrations of nitrate in-stream, but a much higher export of nitrate into groundwater. This may be a reflection of the highly porous geology of this part of the Vouga basin, and an indication of the potential for groundwater pollution.

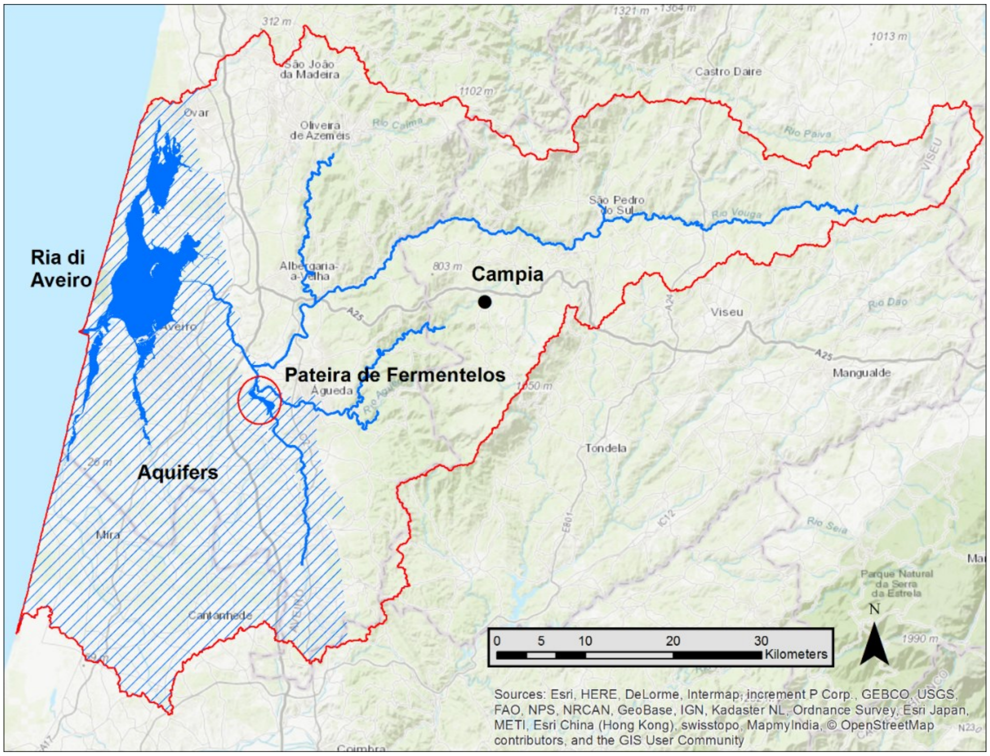


Figure 11. Stream network, major hydrologic features, and the 'Campia' precipitation gauge in the Vouga Basin. The area with hatched lines represents the area overlying groundwater aquifers.

7.1.3 Research Objectives

The focus of this research topic is to examine how current agricultural practices in the Vouga basin are impacting water quality (specifically nitrate) at the basin scale. This assessment is made using the SWAT eco-hydrologic model, which was set-up, calibrated, and applied to the Vouga basin using a number of advanced modeling methods, intended to improve the hydrologic simulations at this study site. The first objective is to examine how nitrate export varies between different parts of the basin, to determine the main nitrate export regions and flow pathways. The second part of this topic assesses nitrate export at the scale of hydrologic response units (*i.e.* a distinct combination of land-cover/land-use, soil, and slope class), to determine which water bodies are at the greatest risk from nitrate pollution (*i.e.* the Pateira de Fermentelos (inland lake), the Ria de Aveiro (coastal lagoon), and the groundwater aquifers. To address these questions, the following two hypotheses are considered:

> **Hypothesis 2a:** The highest rates of nitrate export will occur in the agricultural lowlands, and the primary flow pathway will be *via* surface flows.

Hypothesis 2b: The water body in the Vouga basin at the highest risk of diffuse nitrate pollution is the Pateira de Fermentelos (inland lake), followed by the groundwater aquifers, and lastly the Ria de Aveiro (coastal lagoon).

7.2 Model Setup

The following section details the SWAT model setup, which forms the foundation for the analysis in **Sections 7 and 8**.

7.2.1 Basin Delineation

The Vouga basin was delineated in SWAT from the last streamflow gauging point before the Vouga River enters the Ria de Aveiro ('Frossos' gauge). Delineation from this point captures the main river channels, but excludes the coastal plains which lie outside of the drainage area of the Vouga River, but instead drain directly to the Atlantic Ocean. Given that the focus of this research was primarily on the main channel, the lowland coastal areas were excluded from the SWAT model setup. Figure 12 shows the outline of the delineated area in orange, with the excluded lowland areas outlined in yellow. The main channel network is outlined in blue. This delineation resulted in a total of 19 sub-basins with a total of 2,298 km^2, an elevation range from 16 to 1,110 m asl, and a mean elevation of 360 m asl. There are a total of 1,273 hydrologic response units (HRUs) in the basin, as a result of the combination of the land-cover, soil, and slope classes, which is detailed in the following sections.

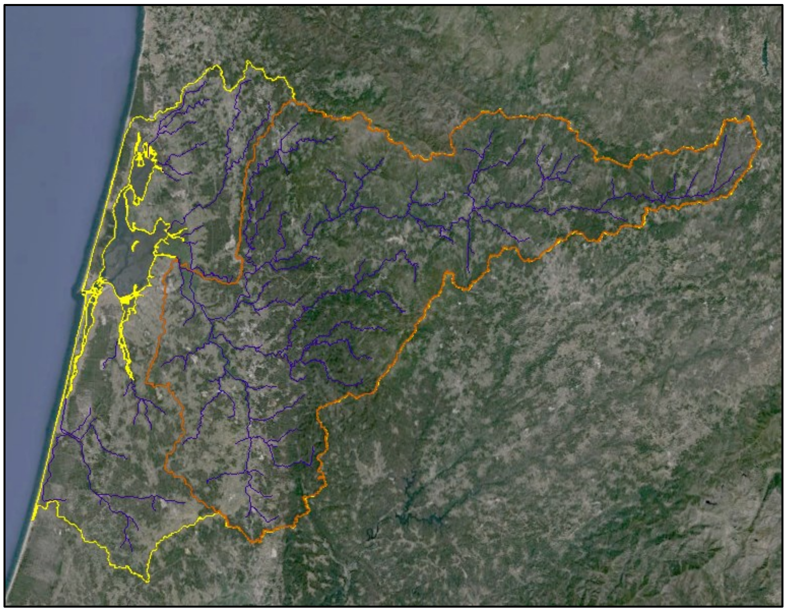
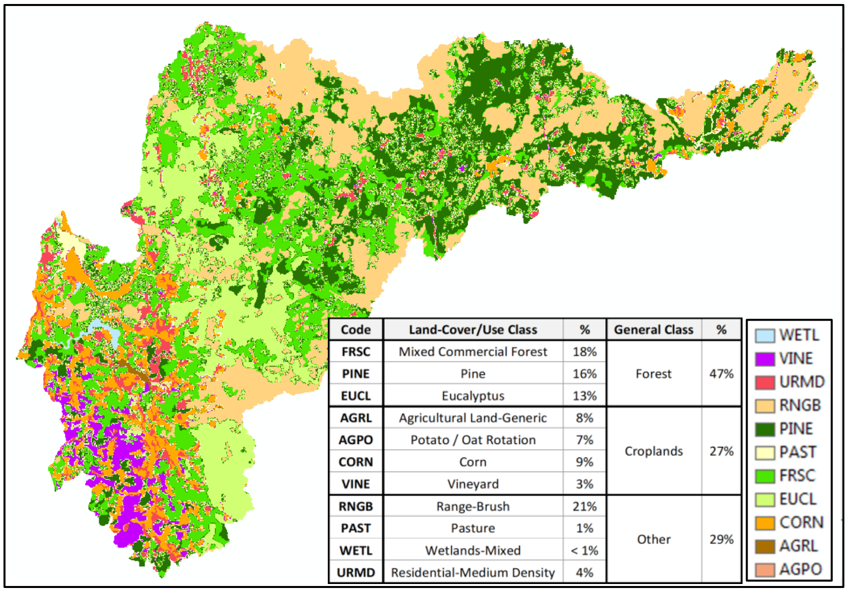


Figure 12. SWAT delineation of the Vouga basin, the included area is outlined in orange, the excluded area is outlined in yellow, and the river channel network is in blue.

7.2.2 Land-Use Class Definition

To define the hydrologic response units (HRUs), the user of SWAT must define the land-cover classes, soil classes, and slope classes. Eleven land-cover classes were defined (shown in Fig. 13), which are based on the Corine Land Cover classification (Corine Land Cover, 2010), with modifications to better represent the regional land-cover characteristics (Rocha *et al.*, 2015).



Code	Land-Cover/Use Class	%	General Class	%
FRSC	Mixed Commercial Forest	18%	Forest	47%
PINE	Pine	16%		
EUCL	Eucalyptus	13%		
AGRL	Agricultural Land-Generic	8%	Croplands	27%
AGPO	Potato / Oat Rotation	7%		
CORN	Corn	9%		
VINE	Vineyard	3%		
RNGB	Range-Brush	21%	Other	29%
PAST	Pasture	1%		
WETL	Wetlands-Mixed	< 1%		
URMD	Residential-Medium Density	4%		

Figure 13. Land-cover/use classes in the Vouga basin.

7.2.3 Soil and Slope Class Definitions

The soil data available within the study area are based on the FAO–UNESCO (1988) soil classification system, which primarily consists of Eutric Fluvisols (Je), Humic Cambisols (Bh), and Gleyic Podzols (Pg). As discussed in **Section 4.2.2.1**, this base soil data was modified using ancillary spatial information, to better define the depth of an impervious soil layer in the landscape, as this is a critical hydrologic characteristic of this study area.

The depth of the impervious layer was defined based on the underlying geologic type, with a depth set at 1.0 m beneath the bottom of the soil profile for areas which are underlain by granitic or schist bedrock, while no impervious layer was set for areas underlain by sandstone. A further proxy used for this layer is the presence of pine forest in the upper watershed, in which case the impervious layer was set to 0.5 m below the soil profile. The presence of pines was used as a proxy in this case, as at this location the pine forests tend to be grown on steep slopes, with very shallow soils above granitic/schist bedrock. The left side of Fig. 14 shows the impervious layer, where the blue area has no impervious layer set (sandstone), the yellow area has an impervious depth of 1.0 m (schist or granitic), and the red area has an impervious depth of 0.5 m (pine forest on schist or granitic).

To generate the final soil layer, the impervious layer was merged with the base soil layer to create a total of 9 soil classes. The final soil layer is shown on the right side of Fig. 14, where the first two letter of the soil class indicate the geologic type: granitic (GR), schist (SC), or sandstone (SS); the next two letters indicate the base soil class, and the presence of a 'P' at the end indicates pine forest (*e.g.* GRJeP).

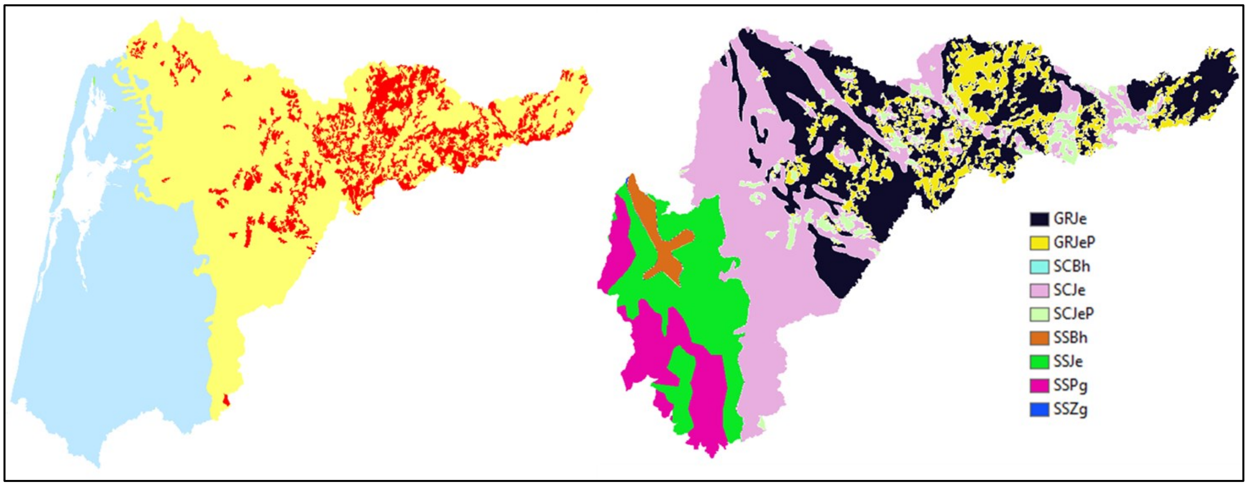


Figure 14. *Left*: The impervious layer map of the Vouga basin. *Right*: The final soil layer map.

The final component of the hydrologic response units are the slope classes assigned to the landscape. Five slope classes were defined at this site, with break points set at 3.0%, 8.5%, 17.5%, 32.0%, and > 32.0%. These slope classes are based on increments at which the slope which are anticipated to influence flow patterns.

7.2.4 Additional Set-Up Details

In addition to the mandatory set-up steps detailed, a number of additional details and features of the basin were included in the model set-up, including:

- A range of hydrometeorological stations in proximity to the basin were utilized, including: 11 precipitation gauges, 4 temperature gauges, 3 solar radiation gauges, and 3 wind gauges. Each sub-basin uses the gauge which is located closest to the sub-basin center.
- Elevation bands were set to account of orographic precipitation and temperature reductions. For every 100 m elevation gain, there is an additional 85 mm precipitation and a reduction of 0.6 °C temperature.
- Point source inputs to the main channel were set for two water treatment plants, at Fermentelos and Assequins Redonda; and one reservoir was defined, at Burgães.

- The default stream channel widths defined in SWAT are much too wide, so they were adjusted to reasonable widths, based on estimates from satellite images.
- Potential evapotranspiration was calculated using the Hargreaves equation, as the values produced by Penman-Monteith were unrealistic.

7.2.5 Management Operations

Detailed management schedules were set-up for the three agricultural land-classes of corn, vineyards, and a rotation of potato/oat. Corn and vineyards are the main crop types of interest for this study, while the potato/oat rotation and generic agricultural land-cover class are included to provide a baseline from other agricultural activities. The management schedules contain the planting, tillage, fertilization, and harvest dates for each crop, and are based on the values of Rocha *et al.* (2015), with further modifications.

However, by default SWAT does not account for the weather conditions during period around fertilization (discussed in **Section 4.2.2.2)**, which can potentially lead to fertilization taking place during periods of excess moisture. This will result in an unrealistically high risk for fertilizer export, as in reality a farmer would not apply fertilizer during a period of excess moisture. To address this issue, a threshold of 5 mm precipitation within a period of 3 days before or after the targeted fertilization date is set, in which case the fertilization date is moved to a drier date.

To examine the impact of this modification on nitrate export rates, a test was run using sample data, both with and without the date modifications. Figure 15 shows the results of the comparison for surface, leached, lateral, and groundwater export, respectively, with each dot representing a single HRU, where the original fertilization date is on the x-axis and the modified date is on the y-axis. In most cases the export values fall along the 1-to-1 line, however in a many cases the values are located to the right of the 1-to-1 line, indicating a that original fertilization date produced higher exports. Given this, the fertilization date modification appears effectively reduce nitrate export in many cases, that is presumably due to unrealistic behavior.

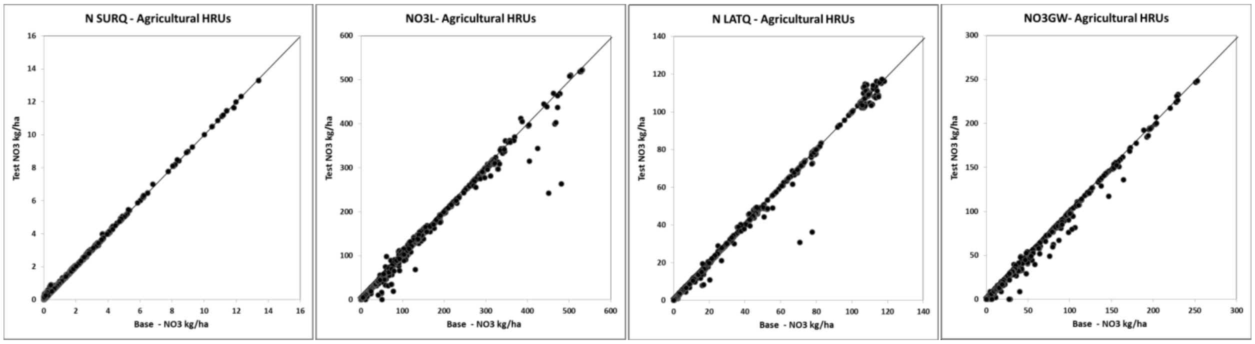


Figure 15. Comparison of HRU-scale nitrate export in the Vouga basin for surface, leached, lateral, and groundwater, between the original fertilization date (x-axis) and the modified date (y-axis).

7.3 Model Calibration

7.3.1 Basin Regionalization

A total of 9 streamflow gauges are available during the targeted time period which had enough data for use in calibration. Several preliminary model runs were carried out using all of these gauges, in order to test different parameter ranges and to get an understanding of the basins hydrologic behavior. These preliminary calibration efforts found that there was distinctly different hydrologic behavior throughout different regions of the basin; which are attributed to the differences in the geologic, topographic, and vegetative characteristics; leading to contrasting flow pathways and hydrologic behavior.

To better represent the behavior of the different parts of the basin in model calibration, the basin was divided into three distinct regions, as shown in Fig. 16. The upland of the basin consists primarily of granitic and schist geology, with steep topology, and is heavily forested (with large areas of pine). The midland of the basin has similar geology as the upland, but has more mixed forest and eucalypt coverage. The lowland area is very distinct from the other two regions, with primarily sandstone geology, much flatter terrain, and is dominated by agricultural land-cover. Notably, the lowland basin also contains a significant area of karstic and other highly porous geologic types.

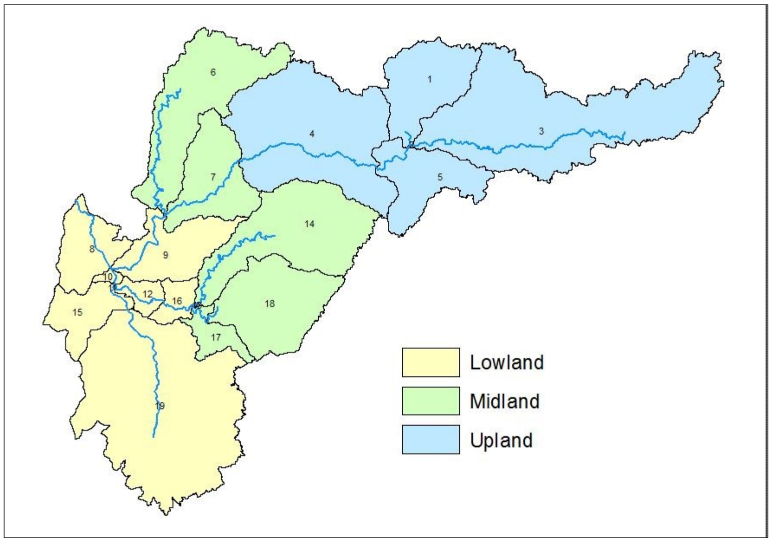


Figure 16. Division of the Vouga basin into three landscape regions.

Within each of these regions, several streamflow and nitrate gauges were examined for data quality and model performance in the preliminary model simulations. Based on this, one gauging station was selected as representative for each region, which was used in further in model testing. Further testing found an additional distinction in the hydrologic behavior in the lower basin, with respect to the areas with karstic geologic structures. To account for this, the sub-basins in this part of the basin (#15 and #19) were parameterized independently from the rest of the lowland basin.

7.3.2 Model Parameterization

The parameters considered in model calibration are provided by Tables 6 and 7. Table 6 presents the 'global parameters' which were calibrated the same across all regions. These parameters control aspects of nutrient cycling, soil water movement, and surface runoff; which are not expected to vary significantly in their function between the different regions. Table 7 provides the 'regional parameters' which were calibrated independently within each region. These parameters control the shallow aquifer, transmission loss, and the aquifer recharge; all of which are expected to vary between the regions, given the differences in geology and topography. Some of the regional parameters maintain the same calibration range between regions, while others were assigned different ranges, in cases where it was justified based on preliminary model. The most significant change was the very high ranges assigned to the karstic region for several of the parameters, which was done to try to simulate the very high porosity and subsurface flow in this type of geologic structure.

Table 6. Global parameters used in calibration, with their ranges and a short description.

Global Parameters	*Calibration Range*	*Parameter Definition*	*Model Usage*
N UPDIS	10 - 30	Nitrogen uptake distribution parameter	Plant Nutrient Uptake
CDN	0 - 2	Rate coefficient for denitrification	Denitrification
SDNCO	0.95 - 1.01	Threshold value of nutrient cycling water factor for denitrification to occur	
CMN	0.0001 - 0.001	Rate coefficient for mineralization of the humus active organic nutrients	Mineralization
RSDCO	0.01 - 0.1	Rate coefficient for mineralization of the residue fresh organic nutrients	
NPERCO	0 - 1	Nitrate percolation coefficient	Nitrate Transport
SOL AWC	-0.15 - 0.15	Available water capacity	Percolation
SOL K	-0.15 - 0.15	Saturated hydraulic conductivity of first layer (mm/hr.)	Infiltration/Percolation
SURLAG	0 - 3	Surface runoff lag coefficient	Surface Runoff & Matter Transport

Table 7. Regional parameters used in calibration, with their ranges and a short description.

Regional Parameters	*Region*	*Calibration Range*	*Parameter Definition*	*Model Usage*
ALPHA_BF	All	0.01 - 0.99	Baseflow recession constant	Shallow Aquifer
GW_DELAY	All	0 - 31	Delay time for aquifer recharge	
GW_QMN	Upper & Middle	0 – 200	Threshold water level in shallow aquifer for base flow (mm H_2O)	
	Lower	50 – 300		
	Karstic	200 - 600		
GW_REVAP	All	0.02 - 0.2	Revap coefficient	
RCHRG_DP	Upper & Middle	0 – 0.25	Aquifer percolation coefficient	
	Lower	0.1 – 0.6		
	Karstic	0.4 – 0.9		
CH_K	Upper & Middle	0 – 100	Effective hydraulic conductivity of channel (mm/hr.)	Transmission Loss
	Lower	50 – 400		
	Karstic	300 – 3,000		
CH_N	All	0.01 – 0.3	Manning's "n" value for the tributary channels	Peak Rate/Channel Flow

The range of values tested in calibration were set based on the findings from preliminary model runs, and from available literature from SWAT studies in the same region (Nunes *et al.*, 2017; Tavares Wahren *et al.*, 2016). From these selected parameters, 3,000 parameter sets were generated using Latin Hypercube sampling, and the full calibration was run over the period 2004 to 2007, with one additional year prior to this period used as a model warm-up.

7.4 Results and Discussion

7.4.1 Pareto Optimal Parameter Set Selection

The results of model calibration are shown by Fig. 17, for sub 03 (upper-basin), sub 16 (middle-basin), and sub 15 (lower-basin), respectively. The x-axis shows the model performance on the Kolmogorov-Smirnov (KS) metric, which indicates how well the model represents nitrate loads (kg NO_3^--N). The y-axis depicts model performance on the Kling-Gupta Efficiency (KGE) metric, which indicates how well the model represents the streamflow time-series (cms). The KGE values shown are inversed (1 – KGE) for the purpose of the Pareto selection, so both objective functions are optimal at zero. Both axes are scaled from 1 (worst) to 0 (best), therefore, an optimal model would be located in the bottom left of the plotting space. Each individual black dot within the scatterplot is model performance for each individual parameter-set tested. The red dots are those which are identified as being Pareto optimal for each individual calibration site.

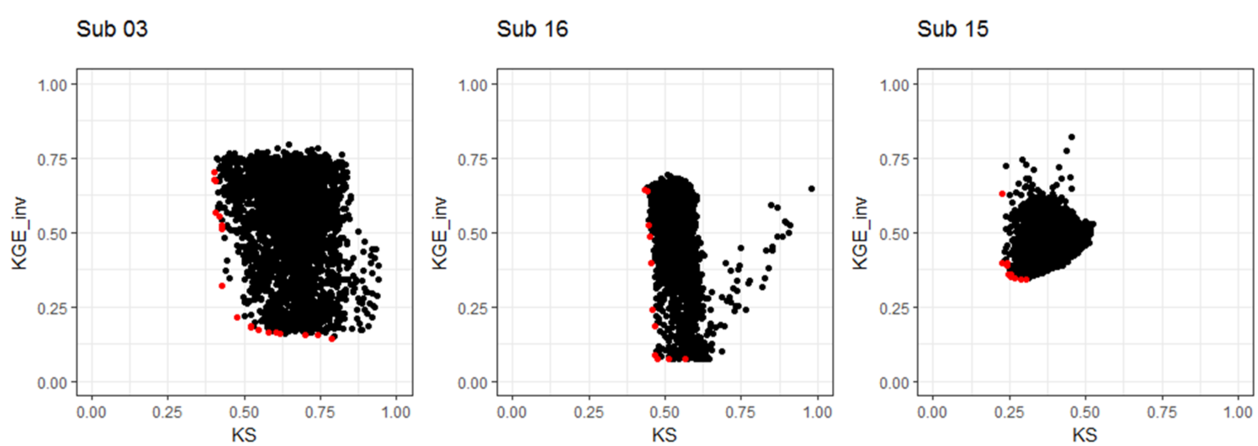


Figure 17. Pareto selection plots for the three calibration gauges in the Vouga basin, where both objective functions are optimized at zero. The selected parameter sets are highlighted in red.

The Pareto selection for sub 03 shows that parameter-sets were selected fairly equally along two long fronts of the distribution. A number of parameter sets were identified that fall along the left front of the distribution, which have gradually improving values for KS, which comes at the expense of reductions in KGE. A similar pattern follows at the bottom front of the distribution, where parameter sets were selected which have gradually improving values of KGE, coming at the expense of worse values of KS.

The selection for sub 16 shows a similar overall structure, but with slightly better values on KGE (*i.e.* closer to zero) and similar values of KS, but with less variability. Given the structure of the parameter-set distribution, a number of parameter-sets were selected along the left front of the cloud, with gradually increasing KS values and worsening KGE values. A smaller selection was made along the bottom front, with gradually improving KGE values and worsening KS values.

The structure of the parameter sets for sub 15 in markedly different from the other two locations, with a more rounded shape and shorter fronts. As a result, most of the parameter sets selected fall along the rounded front at the bottom left of the distribution, with a single outlier parameter set which is slightly better on KS, and worse on KGE. Overall, the KGE values at this site were worse than the other two locations, while the KS values were better.

The use of Pareto optimization for selecting parameter sets provides an interesting method of evaluating model performance, which has both pros and cons. On the pro side, the method provides an objective method of selecting parameter sets which have a mix of different trade-offs in their performance on the two metrics. On the con side, the selection can end up being affected (in a rather arbitrary way) by the shape of the distribution-cloud of parameter sets, which can end up including outliers (on one metric) that might otherwise be excluded. From these results, there is a clear case of equifinality of model performance on both metrics in sub 03 and 16, which leads to long vertical and horizontal fronts, which tends to then result in the selection of parameter sets which have a similar value on one metric, but an increasingly worse value on the other metric. This could be avoided by setting a minimum threshold value for one or both metrics (essentially cutting the distribution at selected points). This step was not utilized in this calibration, but could be worthwhile in a situation where the outliers are extreme.

7.4.2 Streamflow Calibration

Figures 18, 19, and 20 show the streamflow predictions for the selected parameter sets at each calibration gauge, with all streamflow quantities shown in m^3/s (cms). The blue lines represent the observed streamflow, the grey lines show the individual streamflow predictions, and the red lines show the ensemble model prediction.

For sub 03, the KGE value from the ensemble model is 0.83, over the relatively short period of time for which observed data is available. The model represents the observed flow pattern closely in most cases, with the clearest deviation being that the model has a number of peaks in streamflow around the end of 2005/start 2006, which do not appear in the observed data. This indicates that the model may be somewhat oversensitive to the production of peak flows, but otherwise the modeled hydrograph appears to be an adequate representation of the observed flow patterns.

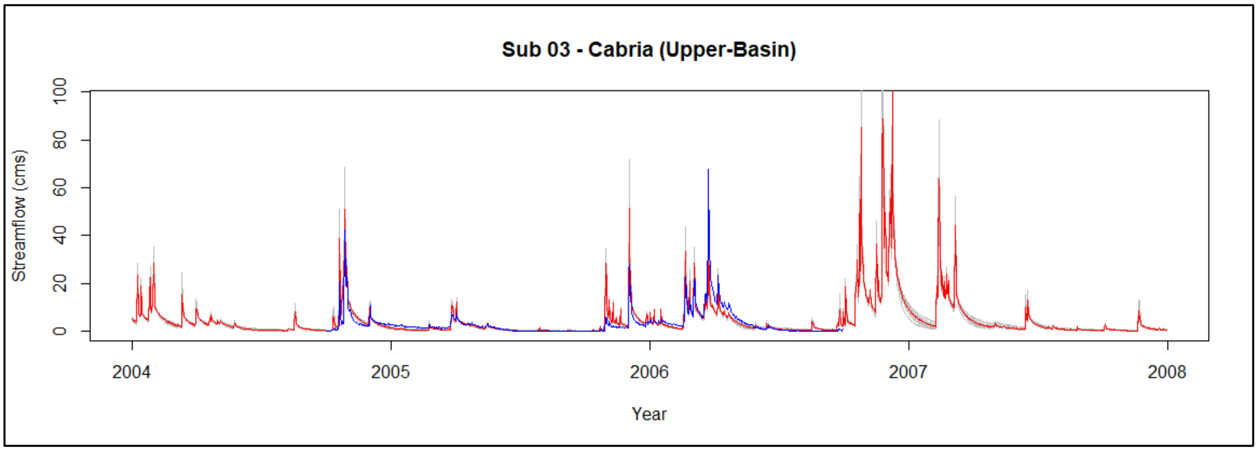


Figure 18. Time-series of the observed streamflow (blue), individual model predictions (grey), and the ensemble model prediction for sub-basin 03 (Cabria), which was used to calibrate the upper basin.

For sub 16, the KGE value from the ensemble model is 0.86, indicating a good fit of the model to the observed streamflow. The observed streamflow has some clear errors in the data in late 2004 and in parts of 2005, where there is an abnormal sustained peak flow period, and other periods of a sustained low flow which also appear abnormal. These errors are caused by occasional downstream impoundments of the stream (discussed in **Section 6.2.1**), and therefore they were removed from consideration in the calculation of the objective function. The main deviation of the model from the observed streamflow appears to be over-prediction during some of the streamflow recessions, which is most apparent in late 2006/early 2007.

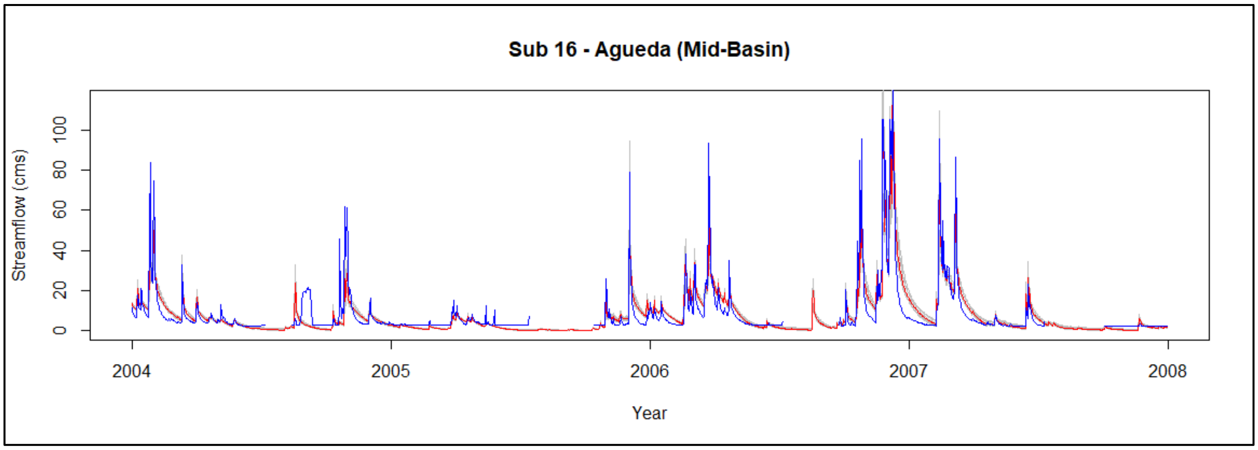


Figure 19 Time-series of the observed streamflow (blue), individual model predictions (grey), and the ensemble model prediction for sub-basin 16 (Agueda), which was used to calibrate the middle basin.

For sub 15, the KGE value from the ensemble model is 0.61, indicating a decent fit of the model to the observed streamflow, but noticeably worse than at the other two locations. The model has a marked difficulty to match the peaks in the observed streamflow, with both over-predictions at some points (*e.g.* 2004, early 2006 and 2007) and under-predictions at other points (*e.g.* late 2006 and late 2007). The model also shows considerably more variability in the individual predictions (the grey lines), with a larger spread of predictions, which is particularly visible in the peaks and streamflow recessions.

The difficulty in model behavior at this location is not completely unexpected, however, given a number of distinct difficulties with the gauge at this location. The gauge at this site is located directly after the Pateira de Fermentelos (a large freshwater body lake/lagoon), which clearly will disrupt both the stream level and timing of peaks and recessions which would occur in a normal stream channel. Additionally, the gauge is located shortly before the confluence with another stream (the Águeda), which will also impact the timing and level of streamflow at this location. Given these issues, use of this gauge for streamflow calibration would normally be avoided. However, there are few options for streamflow gauges in this portion of the basin, and even fewer which have sustained records for both streamflow and nitrate loads. Therefore, the decision was made to utilize this gauge, despite the difficulties with the location, and the resulting model appears to provide a reasonable representation of the hydrograph.

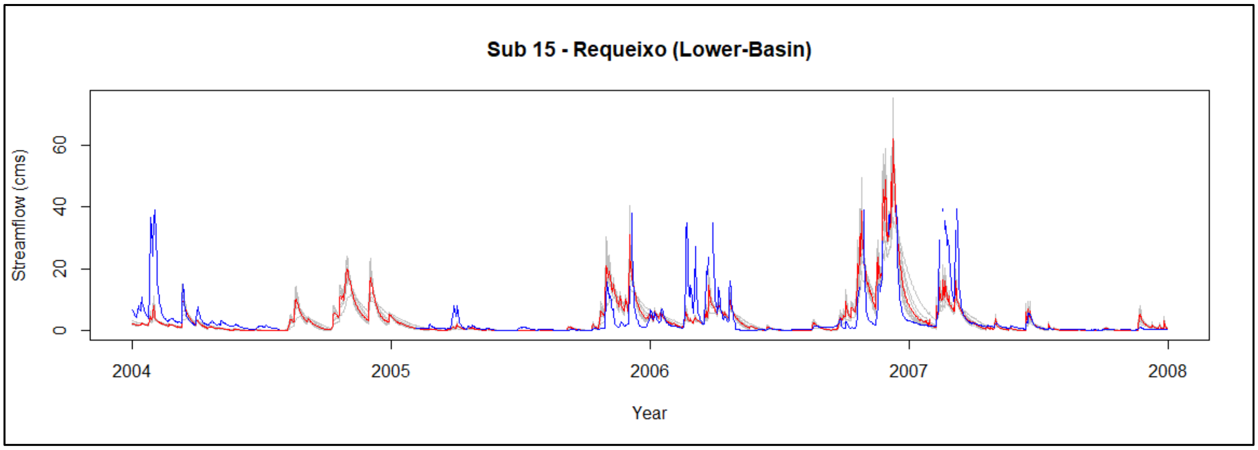


Figure 20 Time-series of the observed streamflow (blue), individual model predictions (grey), and the ensemble model prediction for sub-basin 15 (Requeixo), which was used to calibrate the lower basin.

7.4.3 Nitrate Load Calibration

The results of the nitrate calibration for the three calibration sites are provided by Figure 21, 22, and 23, which are the cumulative distribution functions of nitrate for the observed and modeled loads. The x-axis shows the total nitrate loads (kg NO_3^--N), while the y-axis represents the probability of exceedance. The blue line shows the values for the observed loads, the grey lines are the individual model predictions, and the red line is the ensemble model prediction. Given the mismatch between the observed data (1 value per month) and the model output (daily), the modeled line represents approximately 30 times more data points than the observed. This mismatch in the temporal resolution is the rationale behind using a cumulative distribution approach, as it puts both data sets into a comparable format, by removing the temporal element from the data.

In addition to nitrate loads (kg NO_3^-–N), nitrate concentrations were also determined and tested in calibration. However, given that the modeled concentration of nitrate is heavily dependent upon the modeled streamflow magnitude, it was determined that using the load provided a more independent means of assessing model behavior.

The plot for the upper-basin (Fig. 21, upper-left) shows that the observed and modeled loads are very similar (and low) up till about the 70th percentile. At this point, the modeled loads become substantially higher, and reach much higher peaks than the observed, which remain relatively low throughout. Based on this, the model seems to over-predict nitrate loads at this location. Part of this apparent over-prediction may be due to the low temporal resolution of the observed data, since with only a single daily value taken per month, there is a good chance of missing peak values. However, given that this issue would occur with all gauges and that they did not have the same degree of over-prediction it is unlikely that this explains it entirely. In this case, it may be that the amount of agriculture and/or fertilization levels in this sub-basin was over-estimated.

The plot for the middle-basin (Fig. 21, upper-right) depicts a much closer correspondence between the observed and modeled nitrate loads, with the most significant discrepancy being that the model under-predicts the observed at around the 90th percentile. The model also predicts much higher maximum load values, but this may be due to the low data resolution of the observed missing the highest actual values.

The plot for the lower-basin (Fig. 21, lower-left) shows a split fit to the observed data. The model has a systematic over-prediction of nitrate loads at the lower magnitudes; and at about the 80th percentile the lines cross, and at the model under predicts in the last 20th percentile. There is also a noticeably larger variability between the individual predictions, which can be seen in the spread of the individual (grey) lines after the 80th percentile. Despite the relative mismatch between the modeled and observed at this site, the overall approximation by the model of the cumulative distribution of the observed nitrate loads is still reasonable. Additionally, given the issues with the gauge at this location (discussed in **Section 7.4.2**), it is difficult to determine how much of this mismatch should be attributed to the model, and how much to the unreliable observed data.

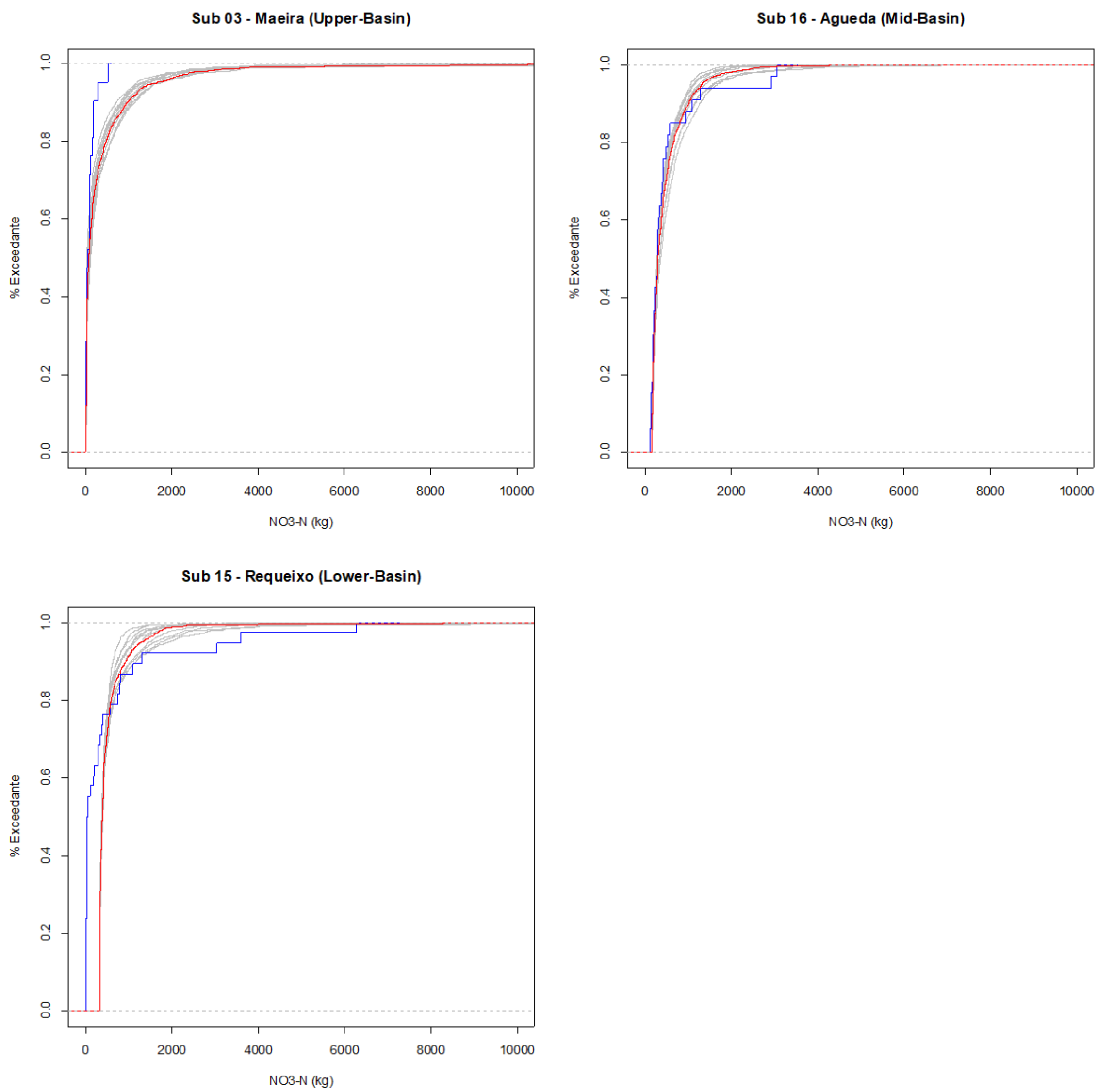


Figure 21 Cumulative distribution function of the observed and modeled nitrogen loads in upper-basin (top-left), middle-basin (top-right), and lower-basin (bottom-left).

7.4.4 Basin-Scale Water Fluxes

The parameter sets identified in the calibration process were then used to generate streamflow over the entire Vouga basin. Streamflow totals were aggregated to annual values (2004 - 2007), which showed consistent patterns of behavior across the different simulation years. The largest variability between years was in the total magnitudes of flow, due to precipitation differences. This was most apparent for the year 2007, which was significantly wetter than the other simulation years. However, the relative proportion of flow between sub-basin and between flow components did not vary significantly between years. To show the typical aggregated behavior across the 4-yr simulation period (2004 – 2007), the mean annual flow values are presented in Fig. 22.

The bar chart of the left side of Fig. 22 breaks down the different flow components into surface, lateral, and percolation. A clear pattern is obvious, where the upper and middle basin are dominated by a mix of surface and lateral flow, with very little percolation; while the lower basin is dominated by percolation, with some surface flow, and very little lateral flow. The right side of Fig. 22 shows the spatial pattern of the different components, with the amount of each flow type per sub-basin.

These differences clearly reflect the geologic and slope characteristics of the different basin regions. The upper and middle basin are dominated by geology with low permeability (*i.e.* granite and schist), and typically steep. In these basin regions, most of the water which infiltrates into the soil will be impeded by the impermeable layer at lower depths, which will drive lateral flow. By contrast, the lower basin is dominated by highly permeable bedrock (largely sandstone and karstic hydrogeology) on relatively flat terrain, which strongly promotes vertical downward flow. The lack of lateral flow indicated that most water that infiltrates the sub-surface ends up draining out of the soil profile, while the water which does not infiltrate becomes surface runoff.

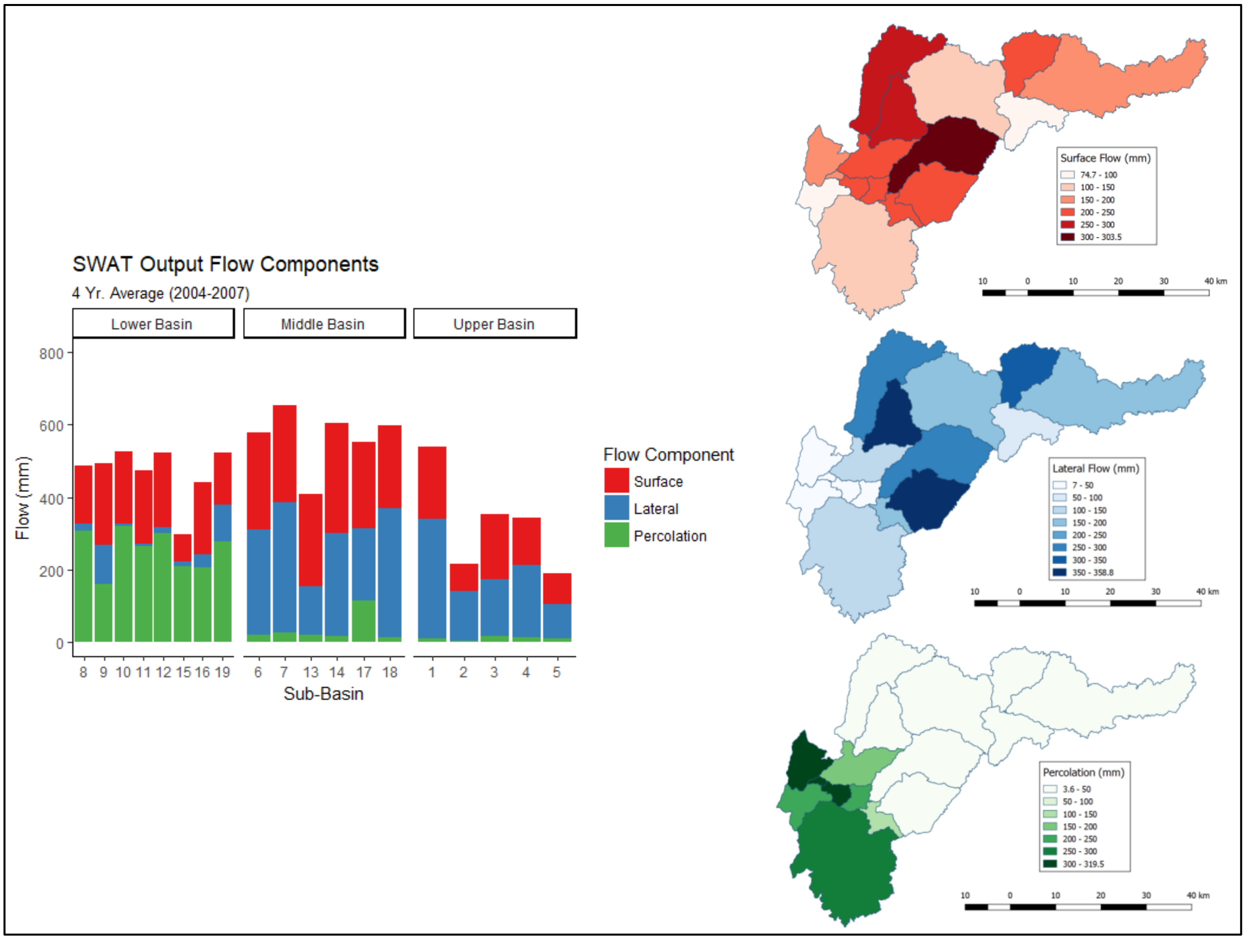


Figure 22. ***Left:*** **Bar-chart with a breakdown of the flow types by sub-basin and region in the Vouga basin.** ***Right:*** **The water flows mapped to their respective sub-basins.**

7.4.5 Basin-Scale Nitrate Fluxes

As with streamflow, the parameter sets identified in the calibration process were used to generate nitrate fluxes over the entire Vouga basin. The nitrate loads (kg/ha NO_3^--N) were also aggregated to annual values (2004 - 2007), and showed consistent patterns of behavior across the different simulation years. To show the typical aggregated behavior across the 4-yr simulation period (2004 – 2007), the mean annual nitrate loads are presented in Fig. 23.

The bar chart of the left side of Fig. 23 breaks down the different flow components into: surface, lateral, and leached nitrate. The patterns in the nitrate fluxes are parallel to the driving hydrologic flows, with the upper and middle basin dominated by a mix of surface and lateral flow, with very little leaching; while the lower basin is dominated by leaching, with very little surface or lateral flow. The right side of Fig. 23

depicts the spatial pattern of the different components, with the amount of each flow type per sub-basin. The primary difference between the patterns of streamflow and of nitrate is the much larger magnitude in the lower basin with respect to total nitrate loads. This is a reflection of the much higher ratio of agricultural land-use and fertilization that occurs in this portion of the basin. The intensive agricultural activity in this part of the basin, primarily with corn and vineyards, plus the porous bedrock present there, drives the high leaching rates seen in these sub-basins. These rates of nitrate leaching loss in the lower basin match well with reported values from other areas of intensive agricultural activities, with high rates of drainage (*e.g.* Di and Cameron, 2002)

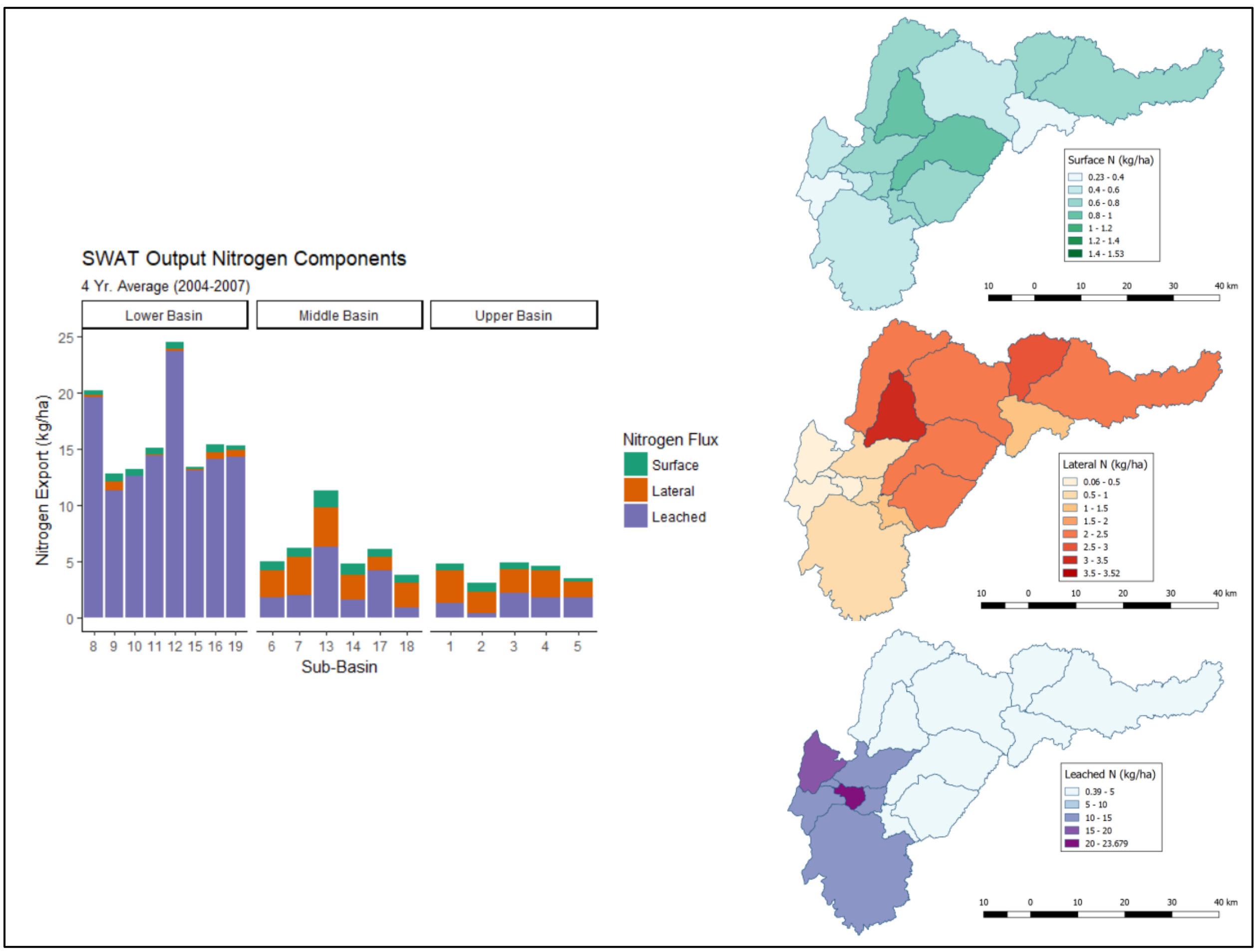


Figure 23. Left: Bar-chart with a breakdown of the nitrogen flux types by sub-basin and region in the Vouga basin. Right: The nitrogen fluxes mapped to their respective sub-basins.

While the nitrate load maps and bar charts indicate the strong concentration of leaching in the lower basin, the scaling by area tends to under emphasize the mass of leeched nitrate which is coming from the

Cértima sub-basin (the southernmost portion of the basin). Figure 24 presents the total nitrate leaching per sub-basin, which is approx. three to six times higher in the Cértima than in the other parts of the basin.

These rates of nitrate leaching, and the relative dominance of leaching as a flow pathway relative to surface or lateral flow, are in agreement with the findings of Serpa *et al.* (2017), which reported similar levels of annual nitrate leaching in the Cértima watershed (13.75 kg/ha), and relatively low nitrate export levels in surface and lateral flows. These levels of nitrate leaching are also in accordance with Moss (2008), who assert that approximately 25 kg/ha per year of NO_3^--N will leach from intensive arable systems.

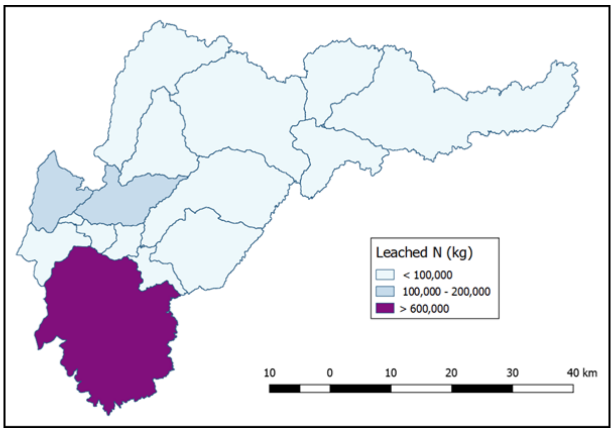


Figure 24 Nitrogen leaching per sub-basin (kg NO_3^--N).

7.4.6 HRU-Scale Drivers of Nitrate Fluxes

The basin-scale assessment provides an indication of the main regions and pathways of nitrate export, but it does not given inform on the drivers of the export behaviors. To better determine this, nitrate export needs to be examined at the scale of hydrologic response units (HRU; a distinct combination of land-cover/land-use, soil, and slope class, of which there are 1,241 in the Vouga basin). Looking at the relationship between HRU-scale factors and nitrate export should indicate the key landscape characteristics that drive nitrate export, as well as to determine the spatial distribution of export "risk-zones". This is addressed by looking at how the three export pathways (surface, lateral, and leaching) relate to the three HRUs characteristics (land-use, soil, slope), by looking at the distribution of annual HRU export values over the simulation period (2004 – 2007).

In Fig. 25 the distribution for surface nitrate export for each class of the three characteristics is presented. The land-cover comparison shows that the highest surface nitrate export is from urban areas (URBAN), with a few outlier HRUs for corn having relatively high values as well. This relatively high export levels from urban areas is likely driven by their high amount of impervious surface area. The soil class comparison exhibits that the highest surface N exports are from HRUs with the "Je" soil class (Eutric Fluvisols) which overlay granite (GRJe) and schist (SCJe). The slope class comparison shows no evident relationship between slope and surface nitrate export.

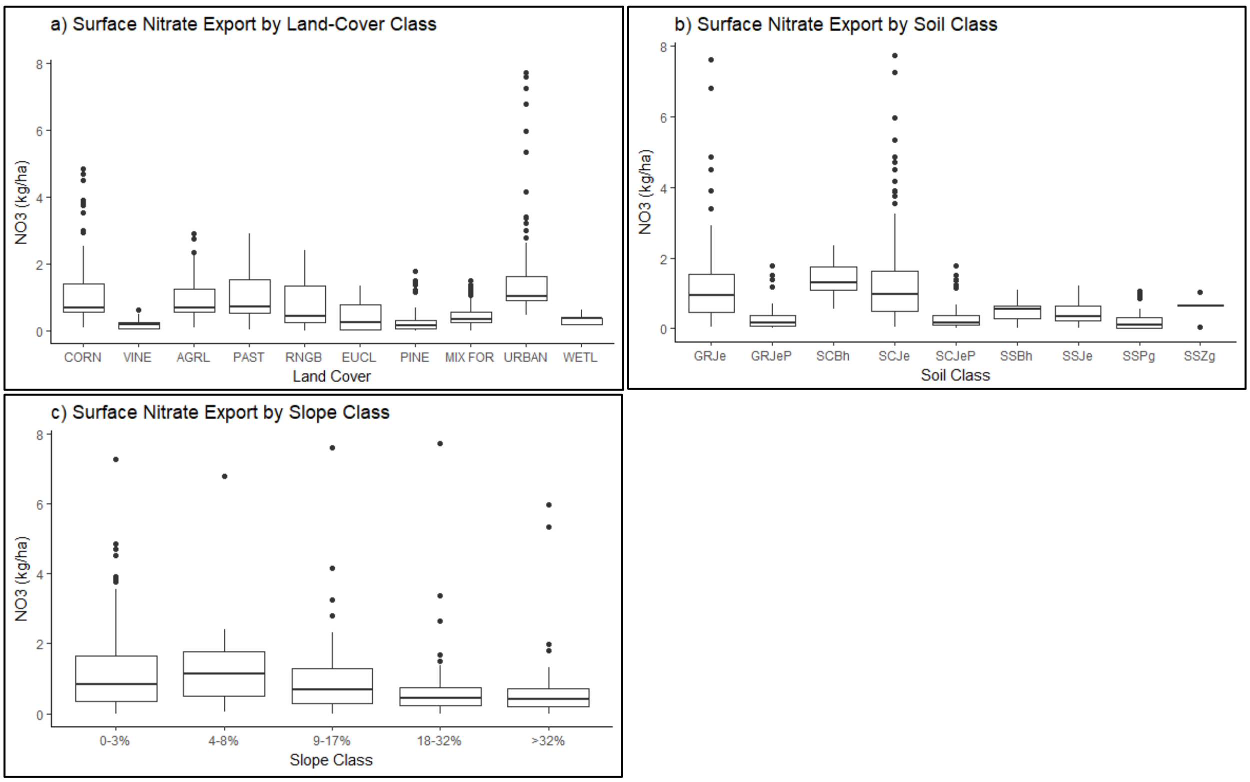


Figure 25. Surface nitrate export by (a) land-cover, (b) soil, and (c) slope class.

In Fig. 26 the box-plots of distribution for lateral nitrate exports are presented. The land-cover comparison shows that lateral nitrate export was highest from the three agricultural land-cover classes (CORN = corn, VINE = vineyards, AGRL = mixed agricultural use), with particularly high values from some corn HRUs. These higher values are certainly due to the large input of fertilizers these land-cover types receive. The soil class comparison shows that the highest lateral exports were overwhelmingly from some HRUs of the "Je" soils class (Eutric Fluvisols) which overlay granite (GRJe) and schist (SCJe). The slope class comparison demonstrates that lateral nitrate export generally increased with higher slopes. The soil and slope factors indicate nitrate being transported through water which has percolated through the soil column down to the impervious layer, and from there transported downslope.

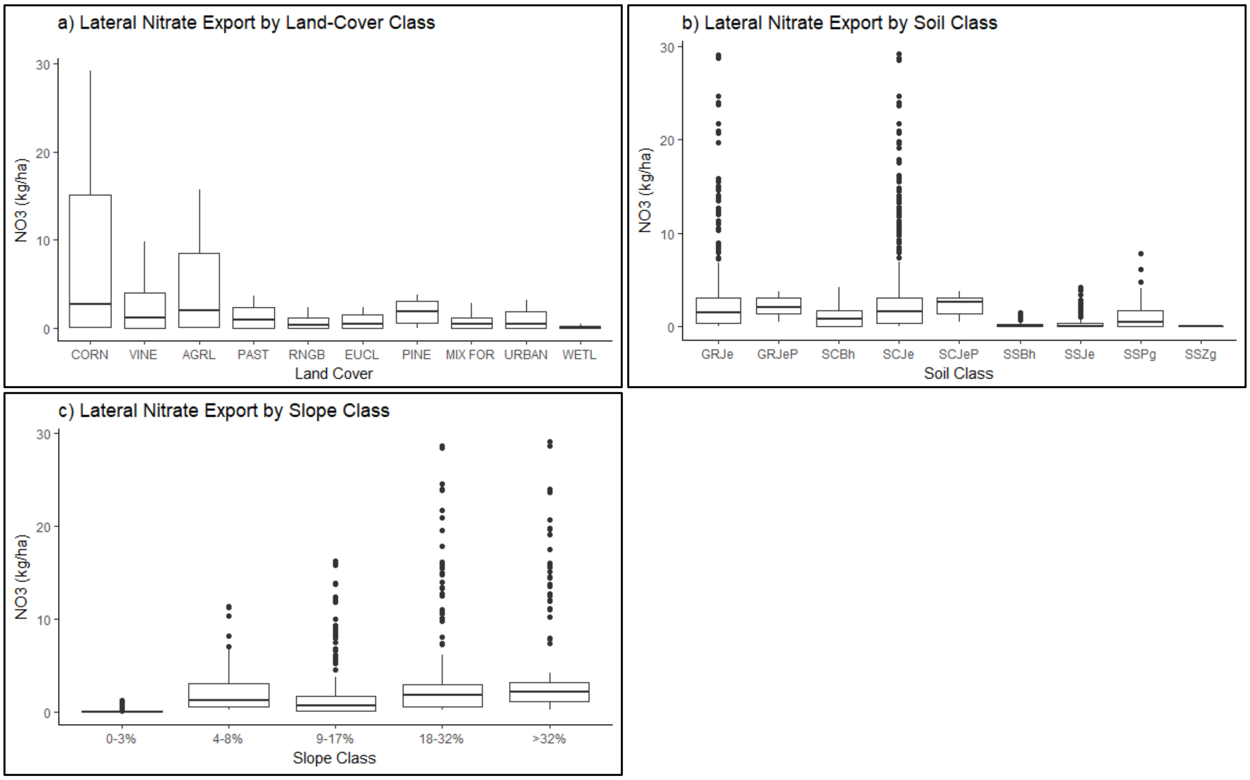


Figure 26. Lateral nitrate fluxes by (a) land-cover, (b) soil, and (c) slope class.

Figure 27 presents the box-plots of distribution for leached exports. The land-cover comparison demonstrates that leached nitrate was highest from the three agricultural land-cover classes, and was particularly high for corn HRUs. As with the lateral flow, this is a reflection of the high amount of fertilization these land-coves receive. The soil class comparison demonstrates that the highest soil classes were the Eutric Fluvisols (Je) which overlay sandstone (SSJe), and to a lesser degree over granite (GRJe) & schist (SCJe). Two other soils over sandstone, Humic Cambisols (SSBh) and Gleyic Podols (SSPg) also had relatively high median values. The relatively high permeability of sandstone (and lack of an impervious layer) drive the high leaching values on that geologic type, while the high values over granitic and schist geology was unexpected. The slope class comparison shows no clear relationship is evident between slope and nitrate leaching.

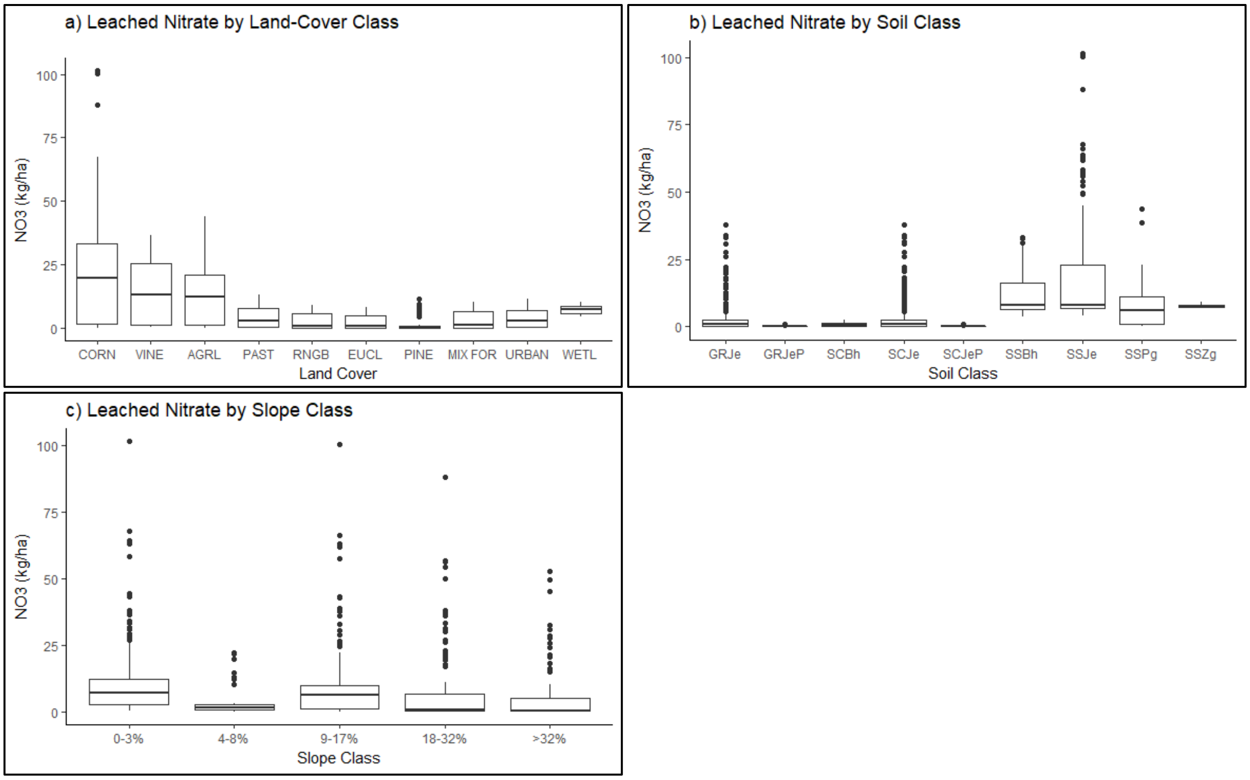


Figure 27. Leached nitrate fluxes by (a) land-cover, (b) soil, and (c) slope class.

By mapping nitrate export rates to their respective individual HRUs, the location of nitrate export “hotspots” is demonstrated in Fig. 28. This shows the concentration of high exporting HRUs in the Cértima (southernmost sub-basin), while the highest values are located in the areas near the main channel in the sub-basin adjacent to the north. Most of the other parts of the basin have relatively low levels of nitrate export, with the exception of some agricultural HRUs in the upper basin. These upper basin HRUs are located in sub-basin 03, which explains the high nitrate load values seen from the model at this gauge. This appears to be due to agricultural land-cover classes located on steep slopes with impervious bedrock, driving the high export rates. Given that these high values do not appear in the observed data, it is likely that the fertilizer rates applied at this location are a misrepresentation of the agricultural practices of the upland area, as the values applied in this study are based on reports from lowland agriculture in the region.

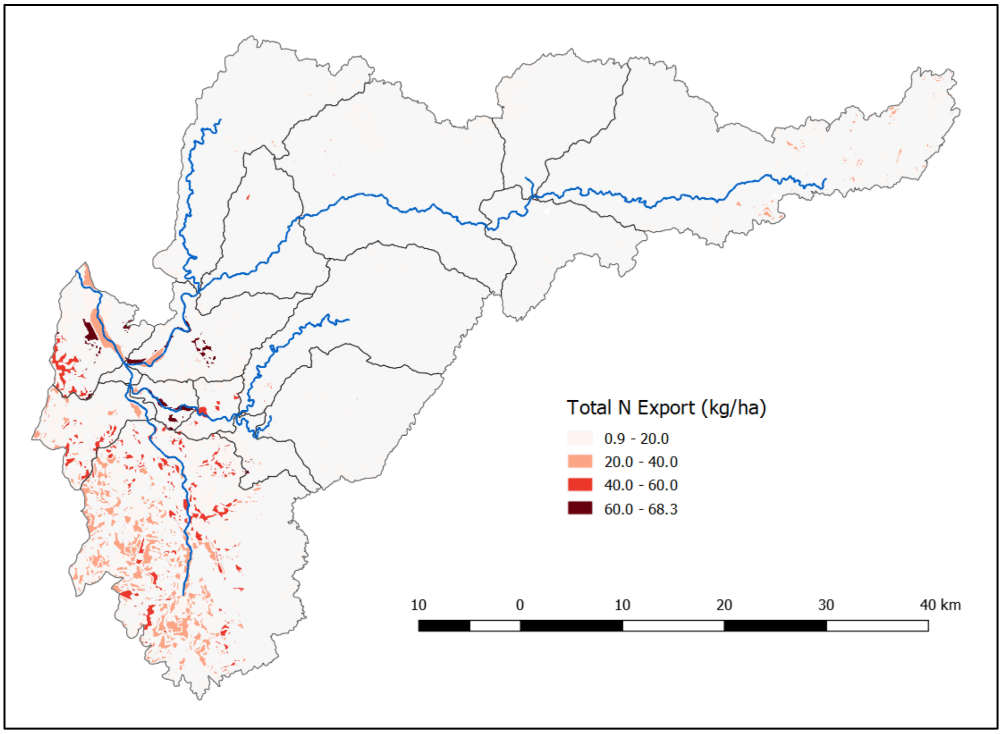


Figure 28. HRU-scale mapping of total annual nitrate exports.

7.5 Conclusion

The results of this section indicate that there is a high degree of variability in nitrate export from the different parts of the basin, with the highest rates coming from the lower basin, with particularly high total export from the Cértima watershed (the southernmost sub-basin). The main flow pathways for nitrate export in the lower basin is leaching, which is being carried by water percolating downwards; while in the middle and upper basin, the main pathway is lateral flow. At the HRU scale, the agricultural land-cover types consistently have the highest export for all pathways. Given that these areas receive the highest nitrate input, this is not surprising to find. For surface and lateral flow, the highest rates are from Fluvisols ('Je') soils overlying granitic and schist geology, with slope being a major control of lateral fluxes; while for leaching, the highest values are those which overlay sandstone geology. The location of the highest export areas are strongly concentrated in the lower basin region, with the highest rates of export associated with agricultural activities on 'Je' soils.

These findings help to address the two hypotheses proposed in this section:

> **Hypothesis 2a:** The highest rates of nitrate export will occur in the agricultural lowlands, and the primary flow pathway will be *via* surface flows.

Hypothesis 2a is partially accepted, as the highest nitrate export rates are clearly associated with the agricultural lowlands of the basin. However, the primary export pathway was not surface flow, but rather leached nitrate. This reflects the strong control of the geologic structure on promoting downward vertical water movement, in which the leached nitrate is exported. Even in the middle and upper basin, surface nitrate export was not a major component, as in this area the main pathway is through lateral flow. Based on these findings, surface nitrate export does not appear to be a major export pathway in any part of the basin.

> **Hypothesis 2b:** The water body in the Vouga basin at the highest risk of diffuse nitrate pollution is the Pateira de Fermentelos (inland lake), followed by the groundwater aquifers, and lastly the Ria de Aveiro (coastal lagoon).

Hypothesis 2b is partially accepted, however the area at highest risk based on these findings are the groundwater aquifers, followed by the Pateira de Fermentelos. While some nitrate is certain to be exported directly into the Pateira *via* surface and lateral flow, given its proximity to the intensive agricultural areas, this amount is far lower than the estimates of the leached nitrate that are exported to groundwater. However, an important consideration with respect to import risks to the Pateira is that it is not isolated from the groundwater supplies, but rather is hydrologically connected to sub-surface water bodies through a complicated network of aquifers (Sena and de Melo, 2012). The groundwater aquifers and the Pateira therefore cannot be considered in isolation of each other, and any the import of nitrate to one may also affect the other.

Overall, the Ria de Aveiro does not appear to be at risk from nitrate export from the main channel of the Vouga river. Although there is potential for moderately high in-channel nitrate exported from the basin lowland, these loads will be further diluted by streamflow coming from the upper parts of the basin at the river confluence shortly after the Pateira de Fermentelos. While this would not reduce the total load, it would be expect to substantially lower the concentration. This is supported by the findings of Silva *et al.* (2002), who found relatively low concentrations of nitrate entering the Ria from the Vouga (1.38 ± 0.24 mg/l). Despite this, there is also a great deal of the lowland area which is located around the Ria which was not considered in this study, which may be a source of both nitrate and other pollutants (*i.e.* mercury is a known risk for the Ria).

8 An Assessment of Nitrogen Fertilizer Reductions on Aquifer Pollution Risk in the Lower Vouga Basin

8.1 Introduction

8.1.1 Regional Aquifer System

A substantial portion of the coastal plain of north-central Portugal is underlain by the 'Western Hydrogeological Unit', an extensive network of overlapping groundwater aquifers. Within the boundaries of the Vouga basin, there are three aquifers which fall within the boundaries of the lower basin area: the Aveiro Quaternary aquifer (*Quaternario de Aveiro*), the Aveiro Cretaceous aquifer (*Cretacio de Aveiro*), and the Barraida karstic aquifer (*Carsico da Barraida*; Fig. 29).

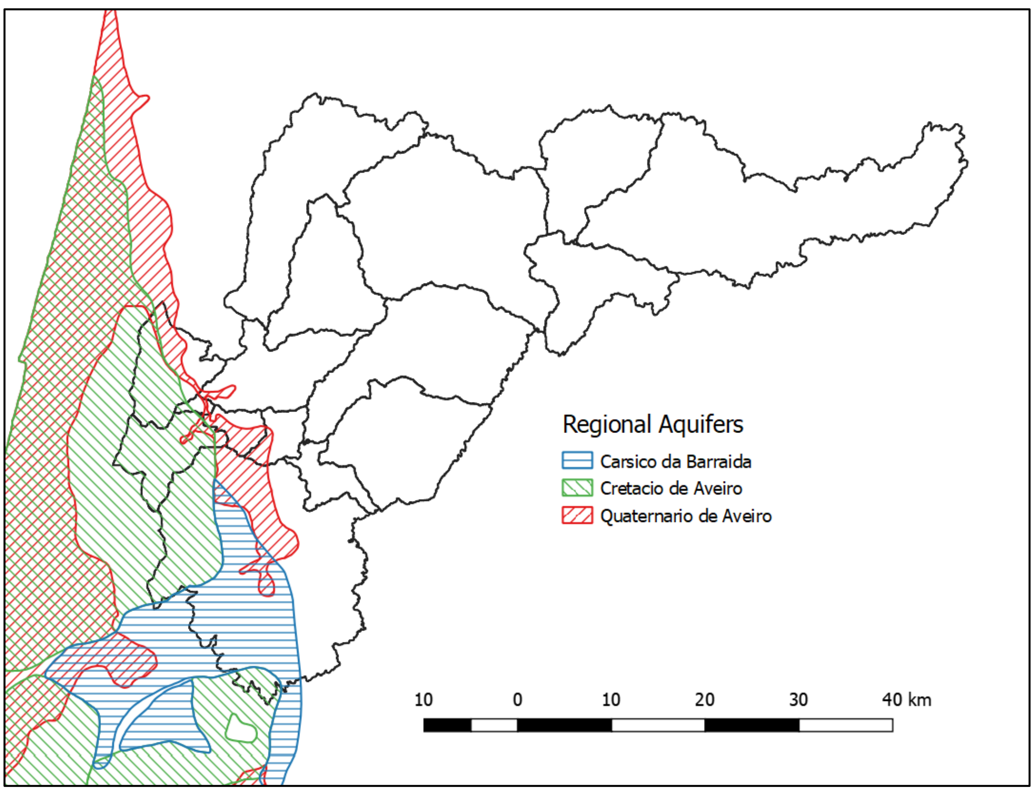


Figure 29. The location of the (overlapping) regional aquifers with respect to the borders of the Vouga basin.

The Aveiro Quaternary aquifer is the shallowest of the three aquifers, and is and mostly unconfined. This aquifer has historically been used by local populations and industries, however, increased water demand and concerns over contamination have led to greater concerns about its usage (de Melo and Silva, 2009). Given these concerns, there has been an increased reliance on the Aveiro Cretaceous aquifer, which is both deeper and confined for most of its extent. However, the Cretaceous aquifer is not confined in all parts of its eastern extent, much of which is located within the lowland portions of the Vouga basin. This lack of confinement is reflected in the water quality of the aquifer, which is mostly pristine in the western portions and has contamination issues in the eastern portion (de Melo and Silva, 2009). The third aquifer system, the Barraida karstic, overlaps with the southernmost part of the Vouga, and given its karstic geology, is very porous and susceptible to surface-groundwater interactions, and thus pollution from surface sources.

With respect to the Vouga basin, the location of these aquifers corresponds with the most intensive agricultural areas, which have the highest rates of nitrate leaching. Figure 30 shows a sub-set of the lower basin, which displays the spatial convergence of the modeled nitrate leaching (kg/ha/yr) and the underlying aquifer systems, based on the SWAT model simulations presented in **Section 7**.

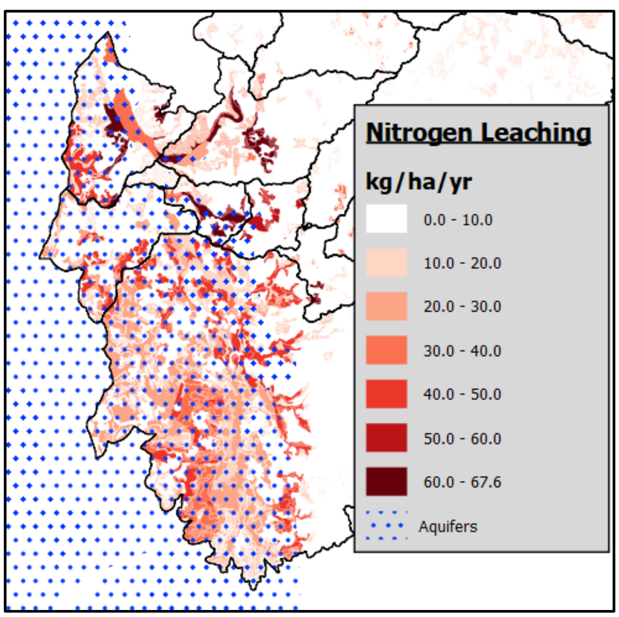


Figure 30 Annual nitrate-N leaching rates in the lower Vouga basin over the regional aquifers.

These results correspond with the findings from of the European Academies Science Advisory Council report on groundwater in the Southern Member States of the European Union (EASAC, 2018). This report assessed groundwater bodies for the purpose of the Water Framework Directive (WFD), and characterized them as being either: *at risk*, *under evaluation*, or at *no risk*; which with respect to their chemical status, the main contaminant of concern is nitrate and the mandated 50 mg/l threshold. Within the Vouga hydrographical region, one groundwater body was classified as *"At Risk"*, seven as *"Under Evaluation"*, and twelve as *"No Risk.* However, the specific water bodies that this refers to are unclear, as the report states: "*Unfortunately INAG (2005) does not specify the localization of the various groundwater bodies*" (EASAC, 2018).

These findings also support the conclusions of de Melo and Silva (2009), who report that there has been a general reduction in groundwater quality in the region, as well as specific concerns regarding poor water quality in the shallow aquifer and decisions to reduce its use as a drinking water source. Based on these findings and the SWAT modeling presented in **Section** 7, there is clear indication that this area is under a significant risk of groundwater pollution.

8.1.2 Nitrate Leaching Reduction Strategies

Once nitrate enters groundwater bodies they take a relatively long time to degrade under natural conditions, and therefore at high concentrations must be removed before being suitable for human consumption. Water treatment for removal of nitrate is relatively expensive, and therefore it is typically more efficient to prevent nitrate from entering water bodies in the first place, than it is to remove once already there. In the European Union (EU), there are several policy directives which address water quality and have a bearing on the regulation of reactive nitrogen in groundwater bodies, which initially included the Nitrates Directive (91/676/EEC) and the Water Framework Directive (2000/60/EC).

These directives set the maximum acceptable concentration at 50 mg/l (equivalent to 11.3 mg/l of nitrate-N). In 2006, the Groundwater Directive (GD) was established as a supplement to the WFD; which requires Member States to: (1) establish groundwater quality standards by the end of 2008; (2) carry out pollution trend studies; (3) reverse pollution trends so that environmental objectives are achieved by 2015; (4) operate measures to prevent or limit inputs of pollutants into groundwater; (5) make reviews of technical provisions of the Directive in 2013 and every six years thereafter; (6) comply with good chemical status criteria (based on EU standards of nitrates and pesticides and on threshold values established by Member States).

In this respect, there are two key factors controlling nitrate leaching rates: (1) the drainage volume from the soil to groundwater, and (2) the amount of nitrate accumulated in the soil above that needed for plant uptake (Di and Cameron, 2002). Drainage volumes are largely controlled by physical site conditions; such as climatic conditions (wet *vs.* dry climate), soil properties (coarse textured *vs.* fine textured), and the presence of preferred flow pathways (*e.g.* macropores, tile drainage systems). However, drainage rates can also be reduced by avoiding over-irrigation; and by controlling soil moisture levels during the periods of low evapotranspiration and high precipitation (*e.g.* the autumn-winter period in Mediterranean climate types).

In terms of management efforts that can be taken to reduce nitrate leaching, there are a number of agricultural best-management practices (BMPs) which can be considered, based on reducing the quantity of nitrogen-based fertilizers applied, and using farming techniques that limit nitrate export from the fields. (Ongley, 1996). The management of vegetation cover is important in this respect, to keep the soil covered with vegetation, in order to inhibit the accumulation of soluble nitrogen by absorbing mineralized nitrogen in soil microbial biomass and by this preventing leaching during precipitation events. Another important management consideration is on the period between crops, as the organic residue from harvesting may be mineralized into leachable nitrate; which can be reduced by planting of "green manure" crops, and by delaying the plowing of organic material into the soil (Ongley, 1996). Other simple measures, such as avoiding fertilization shortly before precipitation events, will also have beneficial effects on export rates.

However, given that in the case of leaching, the nitrate is already due to an existing accumulation within the soil profile, these BMPs may be of limited short-term use for reducing export rates. For example, in a SWAT model investigation comparing different agricultural BMPs, Ullrich and Volk (2009) found that while decreasing tillage intensity led to an overall reduction in nitrate export, it actually led to an increase in nitrate leaching due to the increase in groundwater recharge. This highlights the difficulty of controlling nitrate leaching through agricultural BMP, once there is a build-up of excess nitrate in the soil.

An alternative and straightforward method to controlling nitrate leaching is through land-use conversion to types less prone to nutrient export, such as forest land-cover types. While forest land-cover will not have the same buffering effect for leached nutrients as it can for surface flows, it can at least offset the total area of intensive export area, particularly if it is in areas of high risk. However, for many agricultural producers, sacrificing arable land for the sake of forest land-cover (even for other economic use, such as coppicing) may not be an attractive option. In the lowland areas of the Vouga basin there is a fair amount of forested land, but it tends to be grown on steeper slopes with poorer growing conditions, rather than on more viable area for cropland. It also tends to be grown in the outer edges of the sub-basins, away from stream channels, and in this respect it is in the wrong location from a water protection standpoint.

The most direct (and likely to be effective) method of reducing nitrogen accumulation in the soil is by reducing the amount of nitrogen-based fertilizers applied, given that any applied fertilizer is the primary source of excess soil nitrogen in most agricultural areas (Ongley, 1996). Di and Cameron (2002) found a quadratic relationship between annual leaching losses and the potentially leachable nitrogen, with the rate of fertilization being a prime control. In the Vouga basin, Rocha *et al.* (2015) investigated the effects of nitrogen fertilizer reductions, and the use of split and slow-release fertilizers, and found both approaches to be an effective method in controlling nitrate export.

8.1.3 Research Objectives and Hypotheses

This third research topic builds off of the base SWAT model of the Vouga basin established in **Section 7**, which identified the nitrogen "risk zones", and focuses on examining alternate fertilization scenarios in this portion of the basin. This study follows the approach of Rocha *et al.* (2015), and tests the effect of reduced agricultural intensity by running SWAT model simulations with reduced rates of fertilization, from the current rate down to 10%, in increments of 10%. The effect of this reduction is then assessed in terms of changes in nitrate export and crop yields, for the two main agricultural crops (corn and vineyards). The change in yield is then carried over into changes in agricultural profitability, using a partial budget analysis approach. In addition, the agricultural efficiency of the different HRUs is considered, in terms of crop yield *vs.* nitrate export, as well as the nitrogen use efficiency of the different crop types. Finally, estimates are provided of the potential economic impacts of nitrate pollution, by looking at example costs of different water treatment and pollution avoidance strategies.

To address these points, the following hypotheses are tested:

> **Hypothesis 3a:** There are differences in the agricultural efficiency of the different HRUs in terms of crop yield vs. nitrate export, which could be used to assist in identifying further management options.
>
> **Hypothesis 3b:** Fertilizer inputs could be reduced below current levels without substantially reducing crop yields and agricultural profits.

8.2 Results and Discussion

8.2.1 Fertilizer Reduction Scenarios: Corn

The fertilization schedules for corn were adapted from Rocha *et al.* (2015), following data from regional agricultural producers. The full fertilization rate (*i.e.* 100%) represents the average rate of fertilization based on self-reporting and is therefore an assumed “normal application rate”, which is a simplified approximation of the range of different quantities which would be applied by different producers. With respect to nitrogen-based fertilization of corn, an initial fertilization of 94 kg/ha of anhydrous ammonia (NH_4^+-N) and 33 kg/ha of nitrate-N (NO_3^-—N) are applied at the end of April; and a second round of 66 kg/ha of anhydrous ammonia (NH_4^+-N) and 33 kg/ha of nitrogen-N (NO_3^--N) is applied at the end of May. With respect to the 170 kg/ha/yr obligation of the European Commission (2017a), these values are 56 kg/ha over this limit (*i.e.* 226 kg/ha), and therefore can be considered to be quite high rates of application. Planting takes place in late April/early May, and the harvest occurs in early October. At each step in the reductions in fertilization intensity, these amounts were decreased in increments of 10%, along with the input of other fertilizer types (*e.g.* phosphorus-based) in parallel.

Figure 31 presents the change in crop yield (ton/ha) and nitrate leaching (kg/ha NO_3^--N) at the 10 levels of fertilization intensity. Using the 100% rate fertilization, the median yield is over 10 tons/ha, which follows a steady decrease with lower fertilization levels, down to a median value of around 2 tons/ha at 10% fertilization. The variation in yields within each increment is relatively high at the higher levels of fertilization, and becomes less at the lower fertilization levels. There is no apparent leveling off in crop yields at the higher fertilization levels, indicating that all modeled levels were effective in producing higher agricultural outputs.

Nitrate leaching shows a similar reduction to yields, with a median value around 30 kg/ha at full fertilization, and a median around 10 kg/ha at 10% fertilization. The variability in leaching rates within each increment were considerably higher for leaching than with yield, especially on the low end, with export values for some HRUs near zero at all fertilization levels. At the high end, leaching values reach over 60 kg/ha/yr at full fertilization rates. This indicates that there is a wide variation in the efficiency at which different HRUs are using the applied fertilizer. The overall reduction for leaching is also proportionally less than the drop for crop yield, which may be an indication of the accumulation of nitrogen in the soil, regardless of further input from fertilization.

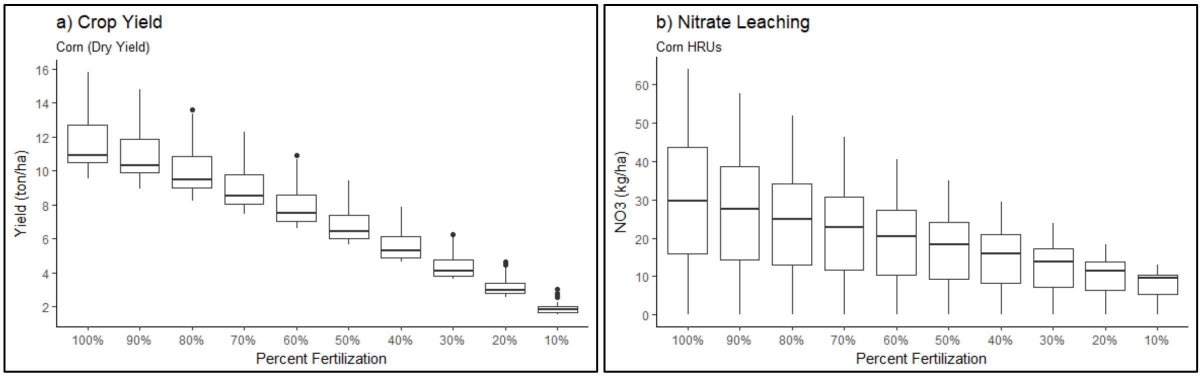


Figure 31. a) Crop yields and b) nitrate leaching at different fertilization rates in the lower basin corn HRUs.

To further consider the efficiency at which the corn crop is utilizing the applied nitrogen fertilizer, the nitrogen uptake ratio can be assessed (Fig. 32). This presents the ratio of nitrogen taken up by plants, relative to the amount applied as fertilizer. All values below the horizontal line (1.0) indicate that the plant is taking up less fertilizer than has been applied, and values above indicate that the plant is drawing more nitrogen from the soil than is applied. Figure 32 reveals that for all fertilization levels, except 10%, in the median HRU more fertilizer is being applied than is being taken up. This indicates that there will be a substantial accumulation of soil nitrate occurring in most HRUs, which will drive high rates of leaching when soil drainage occurs. Despite the consistency of the median rates, however, there is a wide range in uptake values, with each fertilization level having values both above and below the break-even point (1.0). This is a further indication of the variability in behavior of the different HRUs.

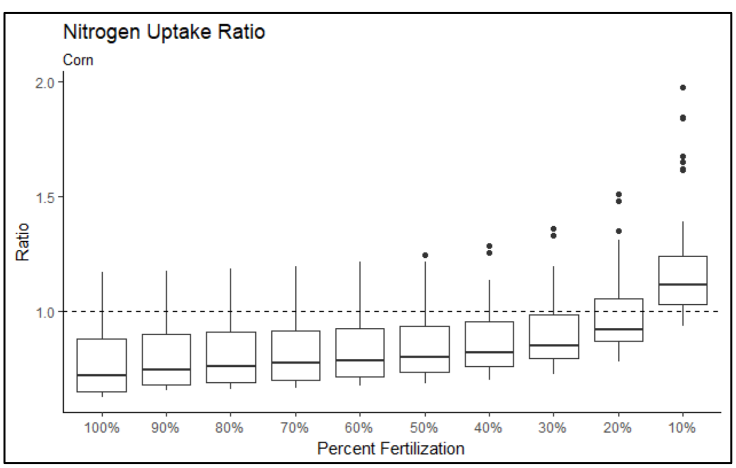


Figure 32. Nitrogen uptake ratio at different fertilization of corn crops. The horizontal line represents the equilibrium point between nitrogen application and uptake.

The final consideration for the corn crop at different fertilization levels is the estimate in profitability (€/ha). These estimates are made using partial budget analysis approach, a method to evaluate the financial effects of incremental changes in agricultural operations. The cost and price assumptions used in calculating profitability are provided by the Portuguese 'Instituto Nacional de Estatística' (INE, 2012), while the crop dry-to-wet yield ratios are provided by the FAO (Table 8), with all values in annual totals. From these values, the costs remain the same at all increment levels, with the exception of fertilizer costs, which are reduced at each increment, due to the need to buy less material. The increase from dry to wet yield is necessary to adjust the yield totals provided by SWAT (which are in dry yield) to the wet yield values utilized in crop prices.

Table 8. Cost and price assumptions used to estimate profitability of corn production.

Profitability Estimation Factors	*Value*
Cost of Equipment & Labor	€312
Cost of Materials	€210
Total Fixed Cost	***€521***
Fertilizer Cost (at 100% fertilization)	€314
Crop Price per Ton (3 yr. mean 2007 - 2009)	€168
Dry to Wet Crop Yield Increase	13%

Figure 33 reveals the change in profitability (€/ha) at the 10 levels of fertilization intensity. At 100% fertilization, the median profitability is around €1,200, which follows a steady decrease with lower fertilization levels, down to a median value of around €-200 at 10% fertilization. The variation in profits within each increment is relatively high at the higher levels of fertilization (ranging from around €1,000 to over €2,000 at the 100% level), and becomes less at the lower fertilization levels. This high variability reflects the large range in crop yields seen in Fig. 31. There is a slight leveling off in the median profitability from 90% to 100%, but otherwise the increase in profit is relatively steady. This indicates that increasing fertilization rates was increasingly profitable at all tested levels, while the slight leveling off suggests that profitability increases may not continue at higher fertilization levels than those tested.

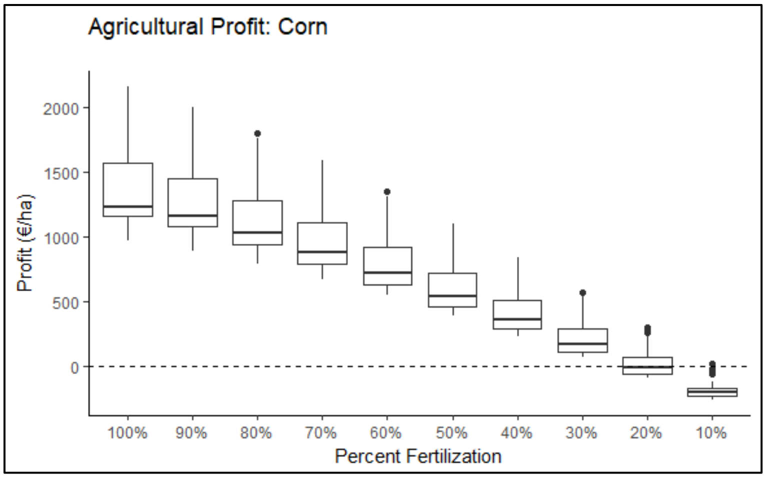


Figure 33. Agricultural profits at different fertilization rates in corn HRUs.

8.2.2 Fertilizer Reduction Scenarios: Vineyards

The fertilization schedules for vineyards were adapted from Rocha *et al.* (2015), following data from regional agricultural producers. As with corn, the full fertilization rate (*i.e.* 100%) represents the average rate of fertilization based on self-reporting and is therefore an assumed "normal application rate", which is a simplified approximation of the range of different quantities which would be applied by different producers. With respect to nitrogen-based fertilization of vineyards, 42 kg/ha of anhydrous ammonia (NH_4^+-N) and 42 kg/ha of elemental nitrogen (NO_3^--N) are both applied at the start of April. With respect to the 170 kg/ha/year obligation of the European Commission (2017a), these values are well below this limit (*i.e.* 84 kg/ha). The growing season commences in early March and harvest occurs in early October. At each step in the reductions in fertilization intensity, the fertilizer amounts were decreased in increments of 10%, along with the input of other fertilizer types (*e.g.* phosphorus) in parallel.

While the fertilization rates for vineyards are much lower than that of corn (and fall below the permissible EU limits), vineyard production in the Vouga basin is highly concentrated in the western and southern portions of the Cértima sub-basin (*c.f.* Fig 13). This area overlaps entirely with the regional groundwater system, and with a large portion of the Barraida karstic aquifer (*c.f.* Fig. 29). Given this, there is a substantial potential for groundwater contamination in this area, and the application of even moderate amounts of fertilizers may put them at risk.

Figure 34 shows the change in crop yield (ton/ha) and nitrate leaching (kg/ha N-NO_3^-) at the 10 levels of fertilization intensity. At 100% fertilization, the median yield is over 4 tons/ha, which follows a steady decrease with lower fertilization levels, down to a median value of around 1.5 tons/ha at 10% fertilization.

There is a gradual increase in crop yields from 30% to 90%, and then a larger increase towards 100%. This may indicate that yields would have continued to raise at higher fertilization rates.

Nitrate leaching shows a similar reduction to yields, with a median value around 27 kg/ha at full fertilization, and a median around 11 kg/ha at 10% fertilization. The variability in leaching rates within each increment were considerably higher for leaching than for yield, especially on the low end, with export values for some HRUs near zero at all fertilization levels. This indicates that there is a wide variation in the efficiency at which different HRUs are using the applied fertilizer.

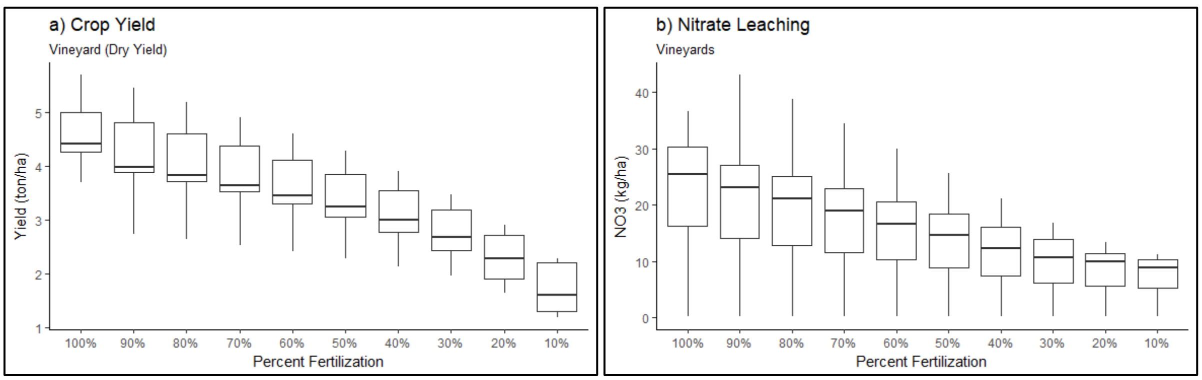


Figure 34. Crop yields and nitrate leaching at different fertilization rates in vineyard HRUs.

To further consider the efficiency at which the vineyards are utilizing the applied nitrogen fertilizer, the nitrogen uptake ratio is considered by Figure 35. This shows ratio of nitrogen taken up by plants, relative to the amount applied as fertilizer. All values below the horizontal line (1.0) indicate that the plant is taking up less fertilizer than has been applied, and values above indicate that the plant is drawing more nitrogen from the soil than is applied. Figure 35 reveals that at all fertilization levels the median HRU value is above the break-even point, indicating that more nitrate is being taken from the soil than is being applied (with very few HRUs below this line, even at the lower-tails of the distributions). This indicates that the vineyards had a higher nitrogen demand than was being met by the applied levels of fertilization and would deplete stored nitrogen in the soil over time.

The reason for the mismatch between the nitrogen demand by vineyards and the amount applied in the SWAT model simulations is unclear. One potential explanation is that the values reported by the regional agricultural producers are underestimates or are not an accurate representation of the rates used in the study site, which (based on Fig. 35) would be expected to be much higher. An alternative cause could be a misrepresentation of the parameterization of the nitrogen use efficiency, or other relevant parameters, in the vineyard crops, as represented in the SWAT model. However, given that the parameter values used in this study were adopted from previous studies applied in the same basin (*e.g.* Rocha *et al.* (2015)) it is unlikely that this behavior would not have been noticed by analyses, if this had been the case. Regardless, the amount of fertilizer applied in the SWAT model simulation should have been substantially higher, which presumably would have led to higher crop yield, nitrate leaching rates, and a more balanced ratio of nitrogen uptake to fertilizer inputs.

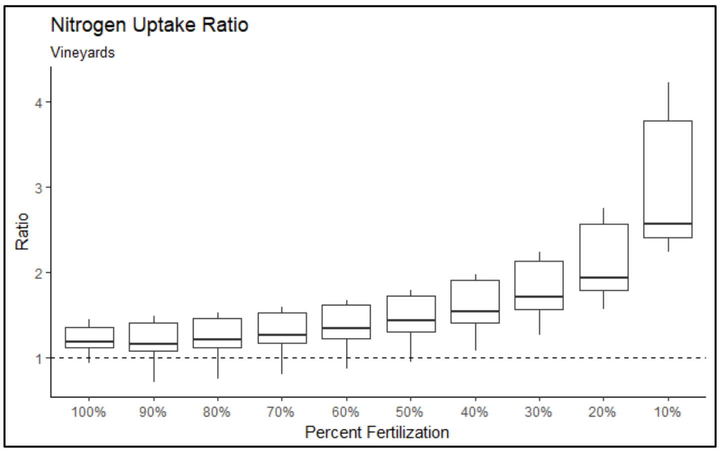


Figure 35. Nitrogen uptake ratio at different fertilization of vineyards. The horizontal line represents the equilibrium point between nitrogen application and uptake.

The final consideration for the vineyard production at different fertilization levels is the estimate of profitability (€/ha). These estimates are using the same partial budget analysis approach in **section 8.2.1**. The cost and price assumptions used in calculating profitability provided are in annual totals, which are provided by data from the 'Associação de Viticultores do Concelho de Palmela' (AVIPE) for the year 2007, while the crop dry-to-wet yield ratios are provided by the FAO (Table 9).

Figure 36 shows the change in profitability (€/ha) at the 10 levels of fertilization intensity. At 100% fertilization, the median profitability is around €650, which follows a steady decrease with lower fertilization levels, down to a median value of around €-1300 at 10% fertilization. The large negative profitability values are a reflection of the high fixed costs for vineyards, which are far higher than corn production. While all HRUs are profitable at the full rate of fertilization, at all other increments, at least some of the HRUs are not profitable; and at 50% and lower rates of fertilization, the median profitability value is negative. These relatively low profitability values are a reflection of the relatively low crop yields, which is likely due to the under-fertilization shown by Fig. 35. Given this, the profit estimations shown here are very likely to be substantially underestimated.

Table 9. Cost and price assumptions used to estimate profitability of corn production.

Profitability Estimation Factors	*Value*
Cost of Equipment & Labor	€982
Cost of Labor	€1200
Cost of Materials	€328
Total Fixed Cost	***€2510***
Fertilizer Cost (at 100% fertilization)	€185
Crop Price per Ton (3 yr. mean 2007 - 2009)	€420
Dry to Wet Crop Yield Increase	82.5%

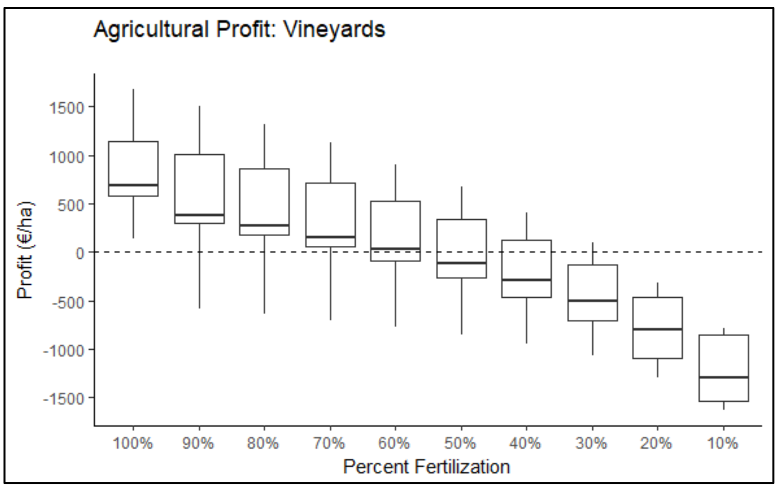


Figure 36. Agricultural profits at different fertilization rates in vineyard HRUs.

8.2.3 *Agriculturally Efficient/Inefficient HRUs*

The results from the previous sections indicate that there is a wide variation in the agricultural productivity of different HRUs in the lowland basin, with respect to crop yield versus nitrate leaching. To examine this relationship further, the crop yields are plotted against the total nitrate export (*i.e.* leached, lateral, and surface), which is shown in Fig. 37. Total nitrate was used rather than only leached in this case, to provide a more even representation between HRUs, regardless of their relative proportions of nitrate export pathway types.

These plots show that there is a clear negative relationship between crop yield and nitrate export for both crops. In the most efficient cases for corn, there are HRUs which produce over 16 tons/ha of yield, while exporting less than 10 kg/ha of nitrate, while the least efficient HRUs produce under 10 ton/ha while exporting over 60 kg/ha. For vineyards, the most efficient HRUs produce over 5.5 tons/ha and export under 5.0 kg/ha, while the least efficient HRUs produce under 3.5 tons/ha yield and export over 35.0 kg/ha of nitrate. From a management perspective, the identification of the most and least efficient HRUs would be useful in determining the locations with the most potential for management activities, perhaps by discouraging production in the least efficient areas or targeting them for BMP implementation.

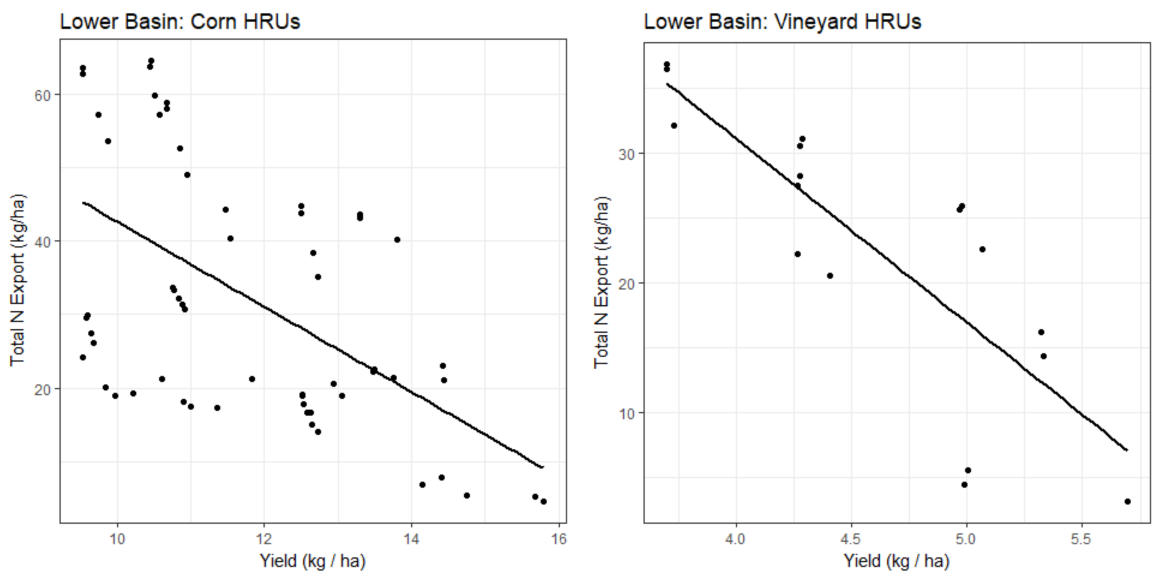


Figure 37. Scatter-plot showing the relationship between crop yields (kg/ha) and total export of nitrate (kg/ha).

8.2.4 Hydrologic Ecosystem Services Impacts

The findings of the preceding sections demonstrate that the intensive agricultural activities in the Vouga basin have a high potential for contaminating local groundwater aquifers, and that this risk could be reduced through lower fertilization rates, but that this would come at the cost of agricultural productivity and profitability. In a fundamental sense, this represents a trade-off between the regulatory HES benefits of water quality protection provided by these groundwater aquifers (in a pristine state), in exchange for increased agricultural output. To assess this loss of regulatory HES in a more concrete manner, the economic costs associated with elevated levels of groundwater pollution are worth considering. Specifically, what is the lost value of these groundwater aquifers as a drinking water supply, and what would be the cost to replicate the same service? This provides an indication of the 'Replacement Cost', which is the lowest cost alternative which could provide the same service as an unimpaired aquifer (*cf.* Table 2). In the lower Vouga basin, this change in HES value can be assessed in terms of the past, present, and potential future impacts.

In terms of the past effects of the impaired groundwater in this region, it is useful to consider that this area was until relatively recently more extensively utilized as a drinking water supply (de Melo and Silva, 2009). In recent years, there has been a move away from sourcing drinking water in this area and a new water supply facility was established in a more inland part of the basin (where the water source is primarily surface water from the plantation forested part of the basin), at a cost of approx. €2.5 million (http://amcv.pt/sistema/descricao-do-sistema/). This findings of this study has demonstrate that there is a high probability of large-scale groundwater nitrate contamination in the lower basin of the Vouga, which is supported by previous studies indicating similar concerns (de Melo and Silva, 2009; Sena and de Melo, 2012; Serpa *et al.*, 2017). And while the re-location of the water supply cannot be attributed solely to degradations of the water quality in these lower-basin aquifers, given the high risks of nitrate contamination, it is reasonable to assume that such a concern was a factor in the decision to relocate drinking water supplies. Therefore, the expense of building a new supply facility was at least in some degree incurred in order to replace the provisioning HES of a reliable drinking water supply which was previously being provided by the lowland aquifers.

Additionally, while re-locating water supplies can be an effective, if expensive, measure to avoid nitrate contaminated water bodies, this does not resolve the local aquifer contamination issue. Much of the lower Vouga basin is quite rural, and there are presumably many households and agricultural producers who rely upon private wells or small local providers, which are still utilizing the aquifers there. In this case, these users would be at significant risk of consuming nitrate contaminated water, particularly for wells drawing from the shallow aquifer.

The costs for an individual household to mitigate the risks of nitrate contaminated water can be substantial, (assuming that an individual is even aware of potential contamination). "*The California Nitrogen Assessment*" provides a range of the estimated cost for different treatment and avoidance strategies to deal with nitrate contamination, which have been reported from various locations within the United States (Tomich *et al.*, 2016). A summary of these values is provided by Table 10, which provides the median value (at a conversion rate of €0.86 to $1.00) from the different price estimates. The capital costs represent the initial cost needed to install a new system, while the service cost is the annual upkeep of the same system. The annualized cost provides an estimate of the annual cost, when the capital cost is spread over the period of the life expectancy of the installed capital (and therefore can capture the benefits of installing a more expensive but longer-lived system).

Table 10. Annual costs per household of alternative nitrate treatment and avoidance strategies, based on median values from Tomich *et al.* (2016).

Treatment Strategy	***Capital Costs***	***Service Costs***	***Annualized Costs***
Reverse Osmosis	€713	€133	€135
Distillation	€827	€426	Not Reported
Ion Exchange	€1351	Not Reported	Not Reported
Avoidance Strategy	***Capital Costs***	***Service Costs***	***Annualized Costs***
Bottled Water	€0	€327	€327
Trucked Water	Not Reported	€817	€817
Drill Deeper Well	€21,500*	€52	€1,789
Drill New Well	€27,950**	€52	€2,322

* Assumes an increase in depth from 300 to 500 feet (~ 91 to 152 meters)

** Assumes a well dug to 300 feet (~ 91 meters)

With respect to treatment strategies, the annualized cost of €135 for a reverse osmosis system may be affordable for many households; however the capital costs of €713 may be a substantial financial burden for many. Given that no capital costs are needed to use bottled water as an alternative to tap water, this may be the most likely option for many households confronted with contaminated drinking water. And while the median annualized cost of €327 is relatively low, this cost will vary significantly depending on the local market. For example, the estimates from Tomich *et al.* (2016) for bottled water ranged from €163 to €1,084 per year, and in the case study where trucked water were compared for the same location and time, the cost of bottled water was ~ 33% higher than trucked.

In addition to the capital and service costs, none of these cost estimates consider the time, inconvenience, and additional related costs associated with having to acquire alternative sources of water on an ongoing basis. Finally, none of these estimates consider the costs that will be incurred if a household is simply unaware of a contamination issue, and are therefore consuming contaminated water. In this case, the cost to the consumer is potentially a serious impact on their health, particularly if the water is consumed by the young or health-impaired individuals who may be more susceptible to contaminated drinking water.

The impacts of the reduction in provisioning HES in the lower Vouga basin should also be considered with respect to future water availability and needs of the region. Climate change projections for Portugal predict an alteration in water availability, which may reduce water availability due to changes in precipitation and evapotranspiration (*e.g.* Nunes *et al.*, 2008); which raises the potential for a future need of these aquifers as a drinking water supply. In this case, given the current rates of nitrate pollution and the slow rate of natural nitrate decay, these aquifers may be substantially impaired as a future drinking water supply (*i.e.* a reduction in its HES 'option value'). In this case, the cost of current practices are simply being passed on to a future generation of water users.

8.3 Conclusion

The results of this section provide an estimate for how reduced rates of fertilizer inputs will affect crop yields, nitrate leaching, agricultural profitability. In general, the reduced rates of fertilization decrease the amount of leached nitrate substantially. However, this comes at the expense of a large drop in crop yield and profitability. Neither crop cultivation considered (corn or vineyards) appears to be are applying fertilizer at an economically inefficient rate, as increased fertilizer rates resulted in increase in profitability at all levels considered. These results also clearly indicate that in the lower Vouga basin there is a negative relationship between crop yield and nitrate export, which reveals that there is a discrepancy in the efficiency between different HRUs.

With respect to the two hypotheses proposed in this section:

> **Hypothesis 3a:** There are differences in the agricultural efficiency of the different HRUs in terms of crop yield vs. nitrate export, which could be used to assist in identifying further management options.

Hypothesis 3a is accepted, as there is a clear negative relationship between crop yields and nitrate export rates, and therefore relatively efficient and inefficient producing HRUs. Therefore, from a management perspective it may be beneficial to focus on either discouraging production in the inefficient areas, or implementing agricultural BMPs to mitigate their nitrate export rates.

> **Hypothesis 3b:** Fertilizer inputs could be reduced below current levels without substantially reducing crop yields and agricultural profits.

Hypothesis 3b is rejected, as the simulation of reduction in fertilization levels led to a large drop in crop yields and profitability in most cases. By contrast, the results from the vineyards indicate that these crops are being under-fertilized (in the SWAT model simulations), and that higher rates could be beneficial for increasing yields and profits. However, from a water quality standpoint, any further fertilization would only exacerbate the already high levels of groundwater nitrate pollution which are estimated to be occurring.

9 Conclusions and Outlook

9.1 Summary of Findings

This research examined a range of topics concerning hydrologic ecosystem services (HES) in the Vouga basin, and their connection with land-cover/land-use. Specifically, the relationship between changes in forest and agricultural land-cover types, and associated changes in HES were examined using statistical and modeling approaches. In **Section 6**, the trends in streamflow quantity and yield in the Águeda watershed over a 75-yr period which coincided with large scale afforestation of *Pinus pinaster* and (later) *Eucalyptus globulus* were examined. Counter to the findings from meta-analysis studies of the effect of forest change on water availability (Bosch and Hewlett, 1982; Brown *et al.*, 2005; Farley *et al.*, 2005), this study did not detect statistically significant trends in streamflow. This supports the view of Andréassian (2004) that there are prerequisite climatic, pedological, and eco-physiological watershed conditions that are necessary to observe hydrologic impacts at the watershed scale, which are not present in the Águeda watershed. By contrast, the significant changes which were detected are related to baseflow, which correspond with different periods of afforestation, and may be attributable to the promotion of soil water repellency (SWR) under the mature pine and eucalypt stands.

Section 7 carried out an assessment of hydrologic and nitrate dynamics at the basin scale, using the SWAT model. This research indicated that there is a high degree of variability in nitrate export from the different parts of the basin, with the highest rates coming from the lower (agriculturally dominated portion) of the basin. The main flow pathways for nitrate export were found to be leaching from agricultural land-cover types, which consistently had the highest export for all land-use and pathways. These findings indicate that the water bodies at the highest risk of nitrate pollution in the Vouga basin are the groundwater aquifers. **Section 8** used the basin-scale SWAT model established in **section 7** to examine how reduced rates of fertilizer inputs would affect nitrate leaching, crop yields, and agricultural profitability in the lower Vouga basin. This research found that reduced rates of fertilization would reduce the amount of leached nitrate substantially, but that this would also lead to a large decrease in crop yield and profitability. A large difference in the inefficiency (*i.e.* crop production *vs.* nitrate export) between different HRUs was found, which could provide a focus for potential management action. This strongly indicates that such actions may be needed to reduce the negative impacts of this pollution on the value of the provisioning HES of these groundwater aquifers, and to avoid associated costs which are otherwise passed on to local water users (*e.g.* through higher water treatment costs).

9.2 Assessment of Modeling Methodology

This section provides a retrospective assessment of the modeling methodology used in this research, within the context of the SWAT modeling practices detailed in **Section 4.2.2** (SWAT Modeling "Best Practices Guide"). There were several overlapping goals for implementing these practices, including (1) compensating for limited data availability, (2) to represent the complex hydrogeological and anthropogenic conditions of the Vouga basin, and (3) an attempt to reduce model uncertainty.

One of the steps taken for goals #1 and #2 was the soil data modifications, in order to increase the soil data resolution with respect to the depth of the impervious layer within the soil profile. The effects of this modification can be seen in the basin scale behavior of the model (*c.f.* Section 7.4.4 and 7.45), which represents key hydrologic processes in the Vouga basin (*i.e.* lateral flows and low permeability in the middle and upper basin), which are unlikely to have been captured using the original soil data set. However, without further field data, these values cannot be validated against observed flow values.

The fertilization date modifications had a similar purpose of compensating for limited data, given that there was no field data available to indicate the actual date that fertilizer operations were conducted during the simulation years. This step may also help to represent real-world behavior of agricultural producers, as opposed to the base SWAT behavior (*i.e.* simultaneous fertilizer application basin-wide, even during wet conditions). Based on the comparison of the original and modified dates shown in Figure 15, this modification appears to have been beneficial in some cases to avoid unrealistically high nutrient export on some dates.

The model calibration methods related to 'Objective Function Selection', 'Pareto Parameter Set Selection', and 'Ensemble Model Predictions' were all implemented with the goal of reducing model uncertainty. Abbaspour *et al.* (2008) identifies three sources of uncertainty in eco-hydrological modeling; (1) model uncertainty, (2) input uncertainty, and (3) parameter uncertainty. The methods applied in this research were mostly an attempt at reducing the third source (*i.e.* parameter uncertainty). The results of the objective function selection and Pareto parameter set selection can be seen in Figure 17, which shows the selected parameters from the total cloud of potential parameter sets. This shows that the parameter sets were mostly selected from a relatively diverse range of the parameter front, which suggests that they represent somewhat different model processes. This should lead to a wider range of predictions to generate the ensemble prediction, and therefore more robust model predictions (*i.e.* the true value is more likely to fall within this range). However, this selection approach was not compared against a prediction from a single "best" parameter set, or predictions made using alternative objective functions, so it cannot be determined if the method used led to a better prediction than alternatives.

The result of the parameter set selection, in terms of range of predictions, can be seen in the ensemble streamflow and nitrate export plots (*c.f.* Fig. 18–21). These plots show that in some cases there were individual parameter-set predictions which show much worse representations of the observed streamflow or nitrate load than the ensemble prediction (and in some cases individual parameter sets were much better as well). This indicates that the ensemble modeling approach was successful as a strategy of "risk mitigation" to avoid the risk inherent in the selection of a single parameter set, which however comes at the expense of potentially discarding a single best performing parameter set.

With respect to non-parameter sources of uncertainty (*i.e.* model and input uncertainty), the approaches applied in this research will have less of an effect. The largest source of uncertainty in this model application is the lack of data available for model calibration and validation. There was a relatively limited amount of available streamflow or nitrate data available, which can't be compensated for by any modeling methods, but simply must be handled "as is". The lack of data was particularly acute in the lower basin, where the only gauge which was available (*i.e.* Requeixo) is of poor quality. In terms of water quality data, the lack of higher temporal measurements of nitrate is another major limitation in terms of input data, as the only available data was a single concentration value per month. Lastly, additional field data with respect to groundwater recharge and levels would have been very beneficial for validating the findings from **Section 8**, both in terms of the water and nitrate fluxes.

However, even if additional sub-surface flow and nitrate data was available, the SWAT model is not particularly well suited for simulating groundwater flows and aquifers. Without modification, the aquifers in SWAT are linked to their associated above-ground HRUs, and there is no complex simulation of below ground flows. In this respect, the recently updated version of SWAT model (*i.e.* SWAT+) may be very beneficial for this type of study, as the updated model has incorporated greater flexibility in defining aquifers and has facilitated linkage with a groundwater specific model (MODFLOW; Bieger *et al.*, 2017). Application of the SWAT+ model, in conjunction with observed data of groundwater flows and nitrate concentrations could provide a more detailed assessment of the lower Vouga basin groundwater nitrate dynamics than could be determined in this study.

Despite the model uncertainties from the this research, the overall findings of **Sections 7 and 8** still provide clear evidence of nitrate contamination of the lower basin aquifers. Even accounting for significant uncertainty, the magnitude of hydrologic and nitrate flows entering groundwater are unlikely to be in a range low enough to dismiss the overall conclusion that there is a high likelihood of contamination. Additionally, there is no reason to assume that any uncertainty would bias predictions solely to *lower* values, but could actually be an under-prediction. From a decision-making standpoint, the amount of certainty in predictions will depend upon the specific context, in particular if there is a potential cause for adverse environmental or health impacts (Guswa *et al.*, 2014). Therefore, despite the uncertainty of the findings, the outputs from this study could be of use in a local decision-making context as an indication of a general trend towards contamination, which should warrant further investigation.

9.3 Implications for Management and Further Research

By considering the inter-connections between the findings of the different components of the research, some wider conclusions can be drawn regarding land-use and HES in the Vouga basin. With respect to the connections between **Sections 6 and 7**, given the issues with nitrate pollution in the lower basin, the importance of the upper basin as a drinking water supply area is clear. Therefore, the lack of reductions in streamflow from the historical afforestation is beneficial, as it could have been anticipated to reduce water availability. However, this afforestation has also been seen to have resulted in a reduction in baseflow, and therefore water which is routed more quickly through the stream network than an area with high baseflow. This is undesirable from a water provisioning standpoint, which benefits from a gradual and steady supply of water, as opposed to larger amounts in quick flushes. This is particularly important in areas without large storage areas (*e.g.* reservoirs), when water is primarily sourced directly from river/streams (as in the Vouga). A further consideration for the upper basin water supplies in the Vouga basin is the connection between nitrate export and wildfires, as this region of Portugal experiences frequent large forest fires, which have been shown to lead to large post-fire flushes of nitrate exported in post-fire ash residues (Nunes *et al.*, 2017). This will also have large short-term effects on the drinking water supply, as the primary in-stream uptake points are located downstream of the most fire prone areas and will lead to higher water treatment costs to remove this contamination.

With respect to the connections between **Sections 6 and 8,** the findings of the fertilization scenarios exhibit the need for land-cover types/management practices which could offset the negative water quality impacts of the intensive agricultural activities. A range of different agricultural best-management practices (BMPs) are available to reduce rates of nitrogen export rates from landscapes (*e.g.* buffer zones or green strips near water bodies) and are a compulsory practice for farms to receive Common Agriculture Policy (CAP) direct payments, under the cross-compliance system for ‘Good agricultural and environmental conditions’ (European Commission, 2009). However, many of the widely used agricultural BMPs are primarily designed to reduce overland transport into surface water bodies but are less effective at reducing vertical nitrate movement through leaching. BMPs which help reduce the accumulation and movement of soluble nitrogen in the soil (*e.g.* avoiding over-irrigation, timing fertilizer application to plant demand, use of cover-crops) can assist in reducing rates of leaching, however, in cases where nitrate leaching is due to an existing accumulation within the soil profile, these BMPs may be of limited use. In this case, to reduce leaching rates over the long-term, substantial reductions in fertilizer inputs may be required.

An alternative, or complimentary, step to the implementation of agricultural BMPs could involve partial land-cover changes, in the form of an expansion of the forested land-cover types examined in **Section 6** into the agricultural lowlands. While forested land-cover would not directly address the issue of leaching in existing agricultural land, it could be considered as an alternative in areas which are at greatest risk of nitrate leaching, simply by increasing the amount of area which does not receive nitrogen fertilizer inputs. Fast growing tree species (such as *Eucalyptus globulus*) would also be expected to consume large amounts of sub-surface water in the lower basin, given the deeply developed soils and good growing conditions present there. This could also reduce rates of percolation to groundwater, and therefore nitrate leaching. However, this benefit may be somewhat offset by the climate characteristics of the region, given that the period of greatest soil moisture (winter) is out of phase with the peak growing season (summer).

Regardless, the replacement of intensive agricultural land-use with forested land-cover would be expected to have water quality benefits, and the selection of species which have both HES benefits and economic benefits could be explored. Plantations of *Eucalyptus globulus* are already extensive in the Vouga basin, which are grown primarily for the production of paper pulp, and therefore the local market/economic system is already in place for these wood products. However, the profitability of this land-use would presumably be substantially lower than is received by intensive agricultural production. This reduction in profitability could potentially be offset through incentives provided to the land-owner, to reflect the value of the HES protection this would provide.

This need to consider the environmental impacts in tandem with wider economic considerations is also clear from the findings of **Section 8**, and the potentially large negative HES valuation impacts of the *status quo* land-use system. Improving the protection of HES in the Vouga basin will require more integration of environmental impacts assessments with the application of economic methods and a consideration of societal well-being (Roebeling *et al.*, 2016). Such an approach is in-line with Portugal's commitments under the EU Water Framework Directive (WFD), which mandates the restoration of Europe's water bodies to "good ecological status" by 2027, and states the need to *"Take account of the principle of full recovery of the costs of water services, including environmental and resource costs and in accordance with the "polluter/user pays principle""*.

This means that ultimately the agricultural producers are responsible for the reduction in water quality being incurred by nitrate leaching from intensive agricultural activities, and in theory that a payment for compensation of damages could be sought. In practice, it would be very difficult to quantify non-point source of groundwater pollution with a level of precision which would be needed to directly attribute specific agricultural activities to a contaminated water supply, which receives input from myriad sources. Such a system would be very difficult to implement in manner which is equitable, and in practice, a more feasible approach is to incentivize land-managers to reduce their negative impacts. This could take the form of a 'Payment for Ecosystem Services' (PES) scheme being established by a relevant water authority, in which agricultural producers are compensated for taking actions which reduce nitrate leaching. This compensation could help to offset the reductions in profitability shown in **Section 8**, where lower rates of fertilization lead to markedly reduced profits per area of cultivation (*c.f.* Figures 32 and 36).

The effective implementation of such measures would require an improvement in the management in the Vouga basin, which has been impeded both by the inherent complexity of the basin, as well as the complexity of multiple planning frameworks which have not always been well-coordinated or focused on local concerns at appropriate scales (Fidelis and Roebeling, 2014). One step which is needed for improved management would be the development of a more comprehensive understanding of how different land uses in the Vouga basin are impacting HES, in particular with respect to groundwater supplies in the lower basin. The current study indicates there is ample reason for concern regarding nitrate leaching, however it does not provide nearly enough detail to be actionable from a management standpoint.

To expand upon the current study, the application of a groundwater specific hydrologic model could be carried out, in order to simulate the surface to sub-surface flows in a more detailed manner. SWAT has only a relatively simplified representation of groundwater, and is therefore not the most appropriate tool for examining interaction between surface flows and multi-layered aquifers. Such a study would require a more comprehensive collection of key explanatory variables, particularly at critical points for water resource management within the basin (*i.e.* the Pateira de Fermentelos, groundwater recharge areas). In addition to a more detailed groundwater modeling study, further socio-economic assessment would be beneficial as well. In particular, a survey of current groundwater extraction points (including the extraction depth to identify the specific aquifer) would help better define current groundwater use patterns. This could be paired with an assessment of the costs of different groundwater treatment/pollution avoidance methods which are being implemented, to move towards a comprehensive assessment of the costs of groundwater pollution in the Vouga basin.

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