Nitrate processes investigation for improved ecohydrological modeling at the catchment scale

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Abstract

Nitrate is one of the most important nutrients in predominantly agricultural catchments. Its excessive presence can result in serious negative impacts on water resources and ecosystems. This is currently a relevant topic in many countries. Many initiatives seek to reduce nitrate pollution of water bodies and are implemented at various legislation levels.

It is necessary to understand nitrate dynamics in water and soil related processes for targeted actions. For this, ecohydrological models can be used as approximations of reality to investigate natural processes and future activities for water quality improvement. Ecohydrological models simulate water and nutrient cycles in an integrated manner. For the simulation of management scenarios it is necessary that the model simulates the processes accurately.

The Treene catchment, in northern Germany, is predominantly agricultural and presents significant water quality problems caused by nitrate. This makes the catchment an appropriate study region for nitrate investigations targeting process understanding and further water quality improvement.

This thesis contributes to this subject by investigating first, the representation of nitrate processes in models through the analysis of temporal parameter sensitivity. This investigation (i) identifies the dominant model parameters, and processes, for each time step. The dominant temporally sensitive parameters are then used for calibrating a model. Thus, a new calibration procedure (ii) is developed to represent both discharge and nitrate loads accurately with the same parameter set. Distinct performance measures are selected to account for distinct parts of catchment hydrology and nitrate dynamics. This particular calibration approach leads to a model with more reliable results, which is important with regard to water quality improvement scenario applications. Furthermore, (iii) different Best Management Practices (BMPs) are implemented in the model to assess their efficiency in reducing nitrate loads at the catchment scale.

The dominant temporal nitrate parameters identified in the first step are related to nitrate transport with runoff components and to plant uptake processes. The multi-metric calibration procedure carried out afterwards resulted in a more reliable model run in all discharge and nitrate load phases, since it considers dynamics and magnitudes of discharge and nitrate loads in a balanced way. The simulation of BMPs indicated higher nitrate reductions by using BMPs containing fertilization reduction and buffer strips. The BMPs simulation results demonstrated the complexity of decision making facing possibly contrasting regulations that aim at economic development and environmental protection, respectively.

Finally, the methods proposed and tested in this thesis contribute to improve the representation of nitrate processes and their dynamics in models to obtain reliable simulation results to address ecohydrological challenges at the catchment scale. It is expected that the steps proposed here are applicable to other variables as well as to other catchments and ecohydrological models.

Zusammenfassung

Nitrat ist einer der wichtigsten Nährstoffe in landwirtschaftlich geprägten Einzugsgebieten. Seine übermäßige Präsenz kann zu erheblichen negativen Auswirkungen auf Wasserressourcen und Ökosysteme führen. Dies ist in vielen Ländern ein aktuelles und relevantes Thema. Verschiedene Initiativen mit dem Ziel, die Nitratbelastung der Gewässer zu verringern, werden auf unterschiedlichen gesetzlichen Ebenen umgesetzt.

Es ist notwendig, zunächst die Nitratdynamik in Wasser- und Bodenprozessen zu verstehen. Hierzu können ökohydrologische Modelle als Annäherungen an die Realität verwendet werden, um natürliche Prozesse und künftige Maßnahmen zur Verbesserung der Wasserqualität zu untersuchen. Ökohydrologische Modelle simulieren Wasser- und Nährstoffkreisläufe auf eine integrierte Art und Weise. Für die Simulation von Management-Szenarien ist es notwendig, dass das Modell die relevanten Prozesse zuverlässig abbildet.

Das Einzugsgebiet der Treene in Norddeutschland ist stark landwirtschaftlich geprägt und weist erhebliche durch Nitrat verursachte Wasserqualitätsprobleme auf. Dies macht das Einzugsgebiet zu einer geeigneten Beispielregion für Nitratuntersuchungen, die Prozessverständnis und eine Verbesserung der Wasserqualität zum Ziel haben.

Diese Doktorarbeit trägt zu diesem Thema bei, indem zunächst die Abbildung von Nitratprozessen in Modellen durch eine zeitliche Parametersensitivitätsanalyse untersucht wird. Dabei werden (i) die dominierenden Modellparameter und Prozesse für jeden Zeitschritt identifiziert. Die zeitlich dominanten sensitiven Parameter werden danach für die Modellkalibrierung verwendet. Somit wird (ii) ein neues Kalibrierverfahren entwickelt, das sowohl den Abfluss als auch Nitratfrachten genauer mit dem gleichen Parametersatz darstellt. Es werden verschiedene Gütemaßen ausgewählt, die verschiedene Teile der Einzugsgebietshydrologie und der Nitratdynamik berücksichtigen. Dieser besondere Kalibrierungsansatz führt zu einem Modell mit zuverlässigeren Ergebnissen, die im Hinblick auf die Analyse von Wasserqualitätsszenarien wichtig sind. Überdies werden (iii) verschiedene Best Management Practices (BMPs) im Model umgesetzt, um ihre Effizienz bei der Verringerung der Nitratbelastung auf Einzugsgebietsebene zu beurteilen.

Die zeitlich dominanten Nitratparameter, die im ersten Schritt identifiziert wurden, stehendurch die verschiedenen Abflusskomponenten und die Aufnahme durch die Pflanze im Zusammenhang mit dem Nitrattransport. Das sich anschließende multi-metrische Kalibrierungsverfahren führte zu einem zuverlässigeren Modelllauf in allen Abfluss- und Nitratfrachtphasen, da es die Dynamik und Höhe von Abfluss und Nitratfrachten in ausgewogener Weise berücksichtigt. Bei der Simulation der Managementszenarien zeigte sich,

dass besonders die Reduktion der Düngung und die Implementierung von Randstreifen zu einer starken Reduktion der Nitratbelastung führten. Die Ergebnisse der BMPs Simulationen zeigten die Komplexität der Entscheidungsfindung hinsichtlich möglicherweise gegensätzlicher Vorgaben, die sich aus den Zielen von wirtschaftlicher Entwicklung und Umweltschutz ableiteten.

Schließlich konnten die in dieser Doktorarbeit vorgeschlagenen und getesteten Methoden dazu beitragen, die Abbildung von Nitratprozessen und deren Dynamik in Modellen zu verbessern. So wurden zuverlässige Simulationsergebnisse für ökohydrologische Herausforderungen auf der Einzugsgebietskala erzielt. Es wird erwartet, dass die hier vorgeschlagenen Schritte ebenfalls für andere Variablen, andere Einzugsgebiete und andere ökohydrologischen Modelle anwendbar sind.

Resumo

O nitrato é um dos nutrientes mais importantes em bacias hidrográficas predominantemente agrícolas. Sua presença excessiva pode resultar em graves impactos negativos sobre os recursos hídricos e ecossistemas. Este é atualmente um tema relevante em muitos países. Muitas iniciativas visam reduzir a poluição por nitratos nos corpos d’água e são executadas em várias esferas jurídicas.

Para ações mais específicas é necessário, primeiramente, compreender a dinâmica do nitrato em processos relacionados com a água e o solo. Para isso, modelos ecohidrológicas podem ser usados como aproximações da realidade para investigar os processos naturais e sugerir atividades futuras de melhoria da qualidade da água. Modelos ecohidrológicas simulam ciclos de água e nutrientes de forma integrada. Para a simulação de cenários de gestão de recursos naturais é necessário que o modelo simule os processos com precisão.

A bacia hidrográfica do rio Treene, no norte da Alemanha, é predominante agrícola e apresenta significativos problemas de qualidade da água causados por nitrato. Esta realidade faz com que a bacia seja uma região apropriada para investigações relacionadas ao nitrato visando à compreensão de seus processos e a consequente melhoraria da qualidade da água.

Esta tese contribui com esta temática investigando, primeiramente, a representação de processos de nitrato em modelos através da análise da sensibilidade temporal de parâmetros. Este método (i) identifica os parâmetros de nitrato, e processos, dominantes no modelo para cada passo de tempo. Os parâmetros dominantes quanto à sensibilidade temporal são utilizados para a calibragem de um modelo. Assim, um novo procedimento de calibragem é desenvolvido (ii) para representar tanto vazão quanto carga de nitrato com maior precisão utilizando um mesmo conjunto de parâmetros. Distintas medidas de desempenho, que captam e avaliam partes distintas da hidrologia e da dinâmica de nitrato na bacia, são utilizadas. Esta particular abordagem de calibragem leva a um modelo com resultados mais confiáveis, o que é particularmente importante no que diz respeito a simulações de cenários para melhorar a qualidade da água. Além disso, diferentes Melhores Práticas de Manejo (BMPs) são simuladas no modelo para avaliar a sua eficiência na redução das cargas de nitrato na escala de bacia hidrográfica.

Os parâmetros de nitrato dominantes ao longo do tempo, identificados no primeiro passo, estão relacionados ao transporte de nitrato com componentes de escoamento e aos processos de consumo pelas plantas. A calibragem multimétrica realizada posteriormente resultou em um modelo mais fidedigno em todas as fases de vazão e de carga de nitrato, uma vez que considera as duas variáveis de forma equilibrada. Este modelo foi utilizado para simular BMPs

e os resultados mostraram grande redução de nitrato usando BMPs baseadas na redução de fertilizantes e na presença de faixas protetoras de vegetação permanente. Além disso, os resultados das simulações de BMPs demonstraram a complexidade na tomada de decisões considerando regulamentações possivelmente contrastantes que visam ao desenvolvimento econômico e à proteção do meio ambiente, respectivamente.

Finalmente, os métodos propostos e testados nesta tese contribuem para melhorar a representação dos processos de nitrato e sua dinâmica em modelos para obter resultados mais confiáveis para enfrentar os desafios ecohidrológicos na escala de bacia hidrográfica. Espera-se que os passos propostos aqui sejam aplicáveis a outras variáveis bem como outras bacias hidrográficas e modelos ecohidrológicas.

1 Introduction

1.1 Motivation

Agricultural activities can impact the water quality in river waters and groundwater negatively. The presence of nitrate in the water of predominantly agricultural catchments is one of the greatest elements leading to deterioration in their water quality (Colombo et al., 2015; Howden et al., 2011; Lam et al., 2012; Ruidisch et al., 2013). The increase in land use changes in the past decades and the intensification of agriculture practices lead to higher pressure on the environment in agricultural areas (Bouraoui and Grizzetti, 2014; Laurent and Ruelland, 2011).

In order to face the problems of nitrate surplus in water resources, different legal regulations were implemented in the European Union (EU). Firstly, the Nitrate Directive (Council Directive 91/676/EEC, 1991) was launched in 1991 and the Water Framework Directive (Directive 2000/60/EC, 2000) followed in 2000. Both legislations represent a great effort for an improvement of the water quality and the ecological status of all water bodies.

Investigation at the catchment scale based on both initiatives enables the assessment of effectiveness of these goals at this scale. Likewise, the catchment scale enables the investigation of complex and continuously interacting processes regarding nitrate. The water reaching the outlet of the catchment is an indicator of the processes occurring upstream. The water flow from headwaters to the outlet is affected by interactions of the water-soil-air system. This river water is characterized by a certain nutrient concentration. Nutrient time series provide information about the process dynamics related to water quality. The characteristics of the catchment can determine different reactions, relations and so different impacts to water quality. This is also true for the case of nitrate, which dynamics in environment include physical, chemical and biological processes and have highly complex interactions.

An understanding of nitrate processes and transport is still challenging (van der Laan et al., 2010). It is unclear how much nitrogen is present in the different chemical forms, where and when it is distributed and released to the river (Epelde et al., 2016; Ferrant et al., 2011; Howden et al., 2011). Likewise, the detection of the core challenge in understanding the nitrate process dynamics is unclear and difficult to determine. This is related to the small amount of general available nitrate measurement stations, also in comparison to discharge. Furthermore, nitrate is measured often in not daily, but only biweekly or monthly time steps.

Ecohydrological models are important tools for integrated investigation of hydrology, topography, soils, land cover elements and climate. They can also include human water demand systems, like ponds, irrigation systems and drainage tiles. The transformation and transport of substances is a key definer of ecohydrological models (Hesse et al., 2008). They are characterized by different complexities in the parameter number, space and time scale addressed and number of variables considered (Breuer et al., 2008; Hesse et al., 2008). Regarding this complexity, ecohydrological models can be empirical, conceptual or process-based.

The simulation of nitrate processes and dynamics in catchments with ecohydrological models is an important tool for a better understanding of transport and transformations processes (Hesse et al., 2008; Lam et al., 2010; Laurent and Ruelland, 2011; Rode et al., 2010). As an approximation of the real process dynamics, the representation of these dynamics in a model is highly difficult. There are high spatial and temporal variations in nitrate dynamics (van Griensven and Bauwens, 2003). The environmental complexity of nitrate process dynamics consequently makes the modeling approach complex, leading to uncertainties in the model simulations. Furthermore, Schmidt et al. (2008) reinforced the uncertainties regarding the representation of nitrate process dynamics by model simulations in larger catchments. The simplification and assumption of processes in the modeling approach also contributes to uncertainties (Pohlert et al., 2007). An understanding of process dynamics as well as possible and a good matching of simulated and measured nitrate data will be an important step for nitrate investigations. Thus, the water quality modeling activity becomes clearly important and model structure and processes need to be represented as correctly as possible for all these tasks (Kirchner, 2006, Clark et al., 2015).

There are different approaches and steps to investigate and further improve the process representation in models. Diagnostic model analyzes proposed by Gupta et al (2008) are very important to verify the reproduction of modeled processes in relation to real world observation. Model diagnostics are mostly applied to hydrologic models investigation (Gupta et al., 2008; Guse et al., 2014; Hrachowitz et al., 2014). However, a transfer to ecohydrologic modeling is also crucial and feasible. Diagnostic model analyzes seek to determine the accuracy of processes reproduction in the model (Gupta et al. 2008; Euser et al, 2013; Hrachowitz et al. 2014, Guse et al., 2016). Furthermore, the diagnostic analyzes are focused on the investigation of temporally resolved model behavior, which are related to the time steps of the corresponding processes (Guse et al., 2014; Herman et al., 2013; Reusser et al., 2009; Reusser and Zehe, 2011). As the processes representation in the model becomes more realistic, a higher consistency of modeling is achieved (Euser et al., 2013). Euser et al. (2013) proposed a framework to obtain both consistency and a better performance of the model but the idea of discussing hydrological consistency is still in its infancies and has not yet been solidly applied for water quality processes.

The Temporal Parameter Sensitivity Analysis (TEDPAS, Sieber and Uhlenbrook, 2005; Reusser et al., 2011; Guse et al., 2014) is one method belonging to the concept of model diagnostic analyzes. TEDPAS is based on temporally high resolution investigations of the model parameters dynamics. Thus, the method shows the dominant model parameters for each time step (Cloke et al., 2008; Guse et al., 2014; Reusser et al., 2011; Sieber and Uhlenbrook, 2005). This temporal resolution is the great difference to traditional sensitivity analyzis. The parameter with highest impact on the considered model output is given for the entire time series (Saltelli et al., 2000; van Griensven et al., 2006). Furthermore, since model parameters control processes within the model, temporal parameter sensitivity can be used as information for the diagnostic of process simulations.

Aside from overall model performance assessment, the diagnostic model analyzes aim to investigate the model structure (Gupta et al. 2008; Yilmaz et al., 2008). The improvement of process representation in models is usually assessed by model calibration and validation procedures. Model calibration is a crucial step for the use of simulated outcomes. The calibration approach seeks to approximate the model simulations to observations (Shafii et al., 2015; Wagener et al., 2001). Complex environmental conditions have to be considered in model calibration when comparing modeled and measured time series.

To account for the complexities of several processes, it is recommended to use different performance measures to evaluate the simulated processes in relation to observed data and thus to achieve plausible model simulations (Krause et al., 2005; Pokhrel et al., 2012; Guse et al., 2014, Pfannerstill et al., 2014a). A multi-metric calibration considers different performance measures to encompass distinct phases and/or conditions of the variable under investigation. Likewise, signature measures comprehend hydrologic aspects of the catchment and are a way to address specific hydrological components of a catchment (Yilmaz et al., 2008; Pokhrel et al., 2012, Pfannerstill et al., 2014b). It might also be worth applying signature measures to nitrate investigation, since nitrate also presents distinct temporal and spatial dynamics in the catchment.

Typical examples for hydrological signatures are different segments of the Flow Duration Curve (FDC, Vogel and Fennessey, 1994). It contains the runoff response of the catchment to rainfall and can be segmented to evaluate different phases of the hydrograph individually (Yilmaz et al., 2008; Pokhrel et al., 2012; Pfannerstill et al., 2014a). The FDC is a graphical representation of the relationship between discharge frequency and magnitude (Cheng et al., 2012). A calibration using FDC segments provides relevant information of catchment hydrology. However, signature measures are insensitive to events timing (Yilmaz et al., 2008). So, it is recommended combining both statistical performance metrics and signature measures to capture both dynamic and magnitude of the modeled output (Van Werkhoven et al., 2009). Pfannerstill et al. (2014a) split the FDC into five segments (5FDC) to enable a higher focus on very high and very low flow peaks. In their study, the five segments are evaluated separately by selecting the best runs of each segment as evaluated with a statistical performance metric. By intersecting these runs, the final best runs for discharge according to all segments of the FDC contain a good result for all discharge volumes.

In various studies (Bekele and Nicklow, 2007; Gupta et al., 1998; van Werkhoven et al., 2009; Vrugt et al., 2003), even with a multi-criteria calibration, just a unique output variable is considered, which, in the majority of the cases, is discharge. Different processes interact simultaneously in the catchment. An adjustment of one process by one single performance measure may lead to a worse performance in another. Since the water balance also affects nitrate processes, nitrate calibration also requires a multi-variable calibration of both discharge and nitrate. As for discharge, one or more performance measures need to be used to assess nitrate modeling performance (Santhi et al., 2001; van Griensven and Bauwens, 2003; Guse et al., 2015b; Jiang et al., 2015). Several statistical performance metrics can be used for the model evaluation. Each metric will present its benefits and drawbacks and needs to be chosen according the objectives and processes in the focus of research (Moriasi et al., 2007; Pfannerstill et al., 2014).

By achieving a good model run, its outputs are closer to the reality and so more reliable. A reliable model is crucial for the investigation of future scenarios regarding the impacts of climate, soil cover and land use changes on nitrate loads and concentrations (Bonton et al., 2011; Ferrant et al., 2013; Guse et al., 2015b). These investigations can improve the assessment and effectiveness of following recommendations for sustainable management options in the catchments. Likewise, River Basin Management Plans can profit from ecohydrological models once these models incorporate the perspective of an integrative approach of bio-physical and socio-economic systems (Collins and McGonigle, 2008; Garnier et al., 2014). Furthermore, in a broader perspective, the concept of Integrated Water Resources Management (IWRM, FAO, 2004; Jin et al., 2015; Mazvimavi et al., 2008; Qi and Altinakar, 2011) can be based on the results from an investigation of modeled process dynamics, and the applications of good calibrated models to assess scenarios for sustainable development.

1.1.1 The SWAT model

The Soil and Water Assessment Tool (SWAT, Arnold et al., 1998) is an appropriate ecohydrological model for the investigation of nitrate dynamics. It is a process-based, semi-distributed and continuous model and performs calculations firstly at a minor unit, the Hydrological Response Unit (HRU), then at sub-basin scale and afterwards aggregating values at the catchment scale. The SWAT model is open source, being adaptable to specific conditions of the study catchments. It is worldwide applied in distinct study areas for the investigation of water quantity and quality issues (Bieger et al., 2014; Fohrer et al., 2014; Francesconi et al., 2016; Memarian et al., 2013; Strauch et al., 2013). The SWAT model is suitable for nitrate process dynamics investigations since it allows the simulation of water and nutrient cycles in an integrated manner. It reproduces dynamic plant growing processes and several agricultural management activities. These activities consider, for example, tillage, seeding, grazing, harvesting and fertilization. Furthermore, the management activities can be implemented with spatial differentiation and their impact on water quality can be assessed. Based on these characteristics, SWAT can be applied to the simulation and investigation of scenarios regarding land use changes, alternative management implementation and climate change (Dechmi and Skhiri, 2013; Guse et al., 2015b; Lam et al., 2011; Laurent and Ruelland, 2011; Wagner et al., 2016).

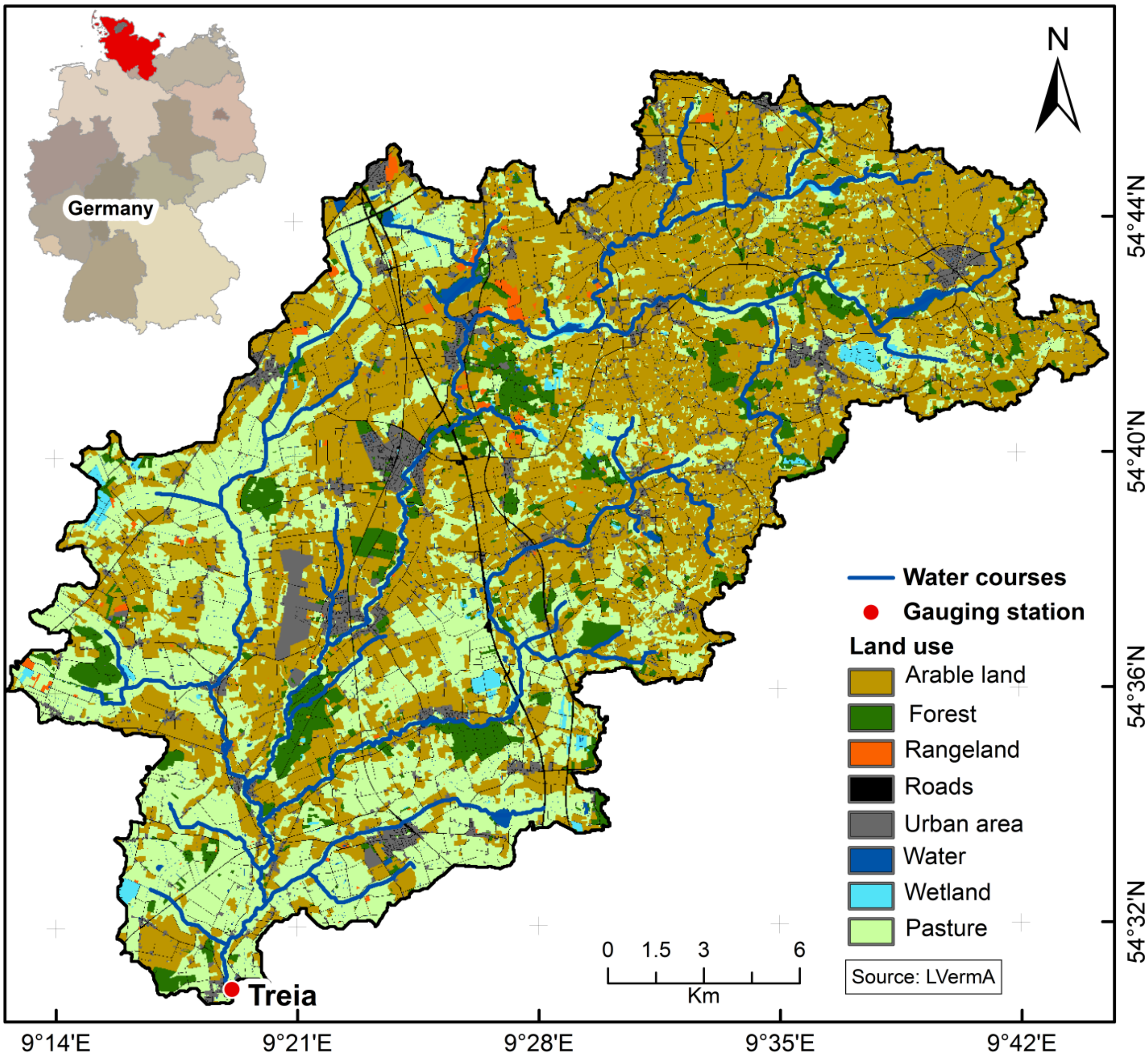
1.1.2 The Treene catchment

As study area for analyzing nitrate process dynamics with the SWAT model the Treene catchment was selected (Fig. 1.1). It is a lowland catchment in the State of Schleswig-Holstein, in northern Germany and near to the Danish border. The Treene catchment is a sub-catchment of the Eider River, which flows into the North Sea. The Treene catchment encompasses an area of approximately 481 km², with the outlet at the hydrological station Treia, at which point the river system is not influenced by tides. The altitude of the catchment does not exceed 80 meters above sea level, and the average rainfall in this region is 884 mm/year (station Schleswig, average value for the period 1981-2011). The Northeast of the catchment is characterized by hilly landscapes (Östliches Hügelland) with a slightly undulating terrain with smooth slopes and, in general, clay and sandy soils (Fig. 1.1). The south-west is covered with flatter areas and more sandy soils (Geest landscape) (Fig. 1.1).

Regarding soil coverage and soil use, the Treene catchment is predominantly agricultural, with crops and pasture areas covering approximately 80% of the catchment (LVermA, 2004) (Fig. 1.1). The high proportion of agriculture areas highlights the strong occurrence of dynamic plant growing processes. Likewise, the great crop variability is associated with a high input of nitrate in form of fertilizer. The fertilization occurs in different time periods since the crops have distinct requirements.

According to recent investigations, nitrate currently causes ecological problems by polluting surface and groundwater (Trepel et al., 2014). Daily sampling carried out within the IMPACT Project (Guse et al., 2015b) from 30/09/2010 until 02/10/2012 and the following daily samplings as part of this dissertation from 03/10/2012 until 10/10/2014 showed the water quality conditions at the catchment outlet Treia. The measurement campaign focused on nutrients and sediments to investigate temporal variances of water quality. The water samples were collected by an automatic stationary sampler, filtered in the laboratory and frozen for further analyzis in the laboratory. Filtration was carried out with cellulose acetate filter (0.45µm) to obtain sediments in suspension. Nutrient concentrations were provided by photometry and ion chromatography.

Furthermore, the measurements are necessary for the verification of the modeling approaches. The results of nitrate, ammonium, phosphate loads and also sediments are shown below for the entire period (Fig. 1.2). The results of the measurements emphasize the suitability of the Treene catchment for nitrate pollution investigation from agricultural activities affecting water quality.



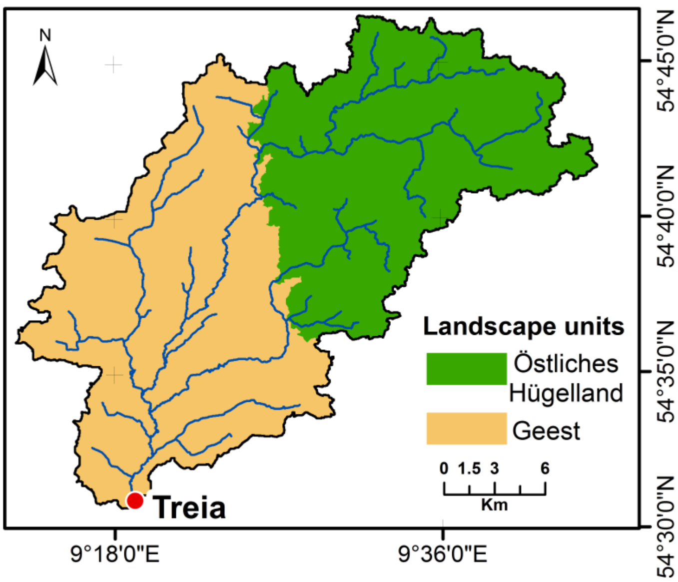


Figure 1.1: Treene catchment with, gauging station Treia, land uses and landscape units.

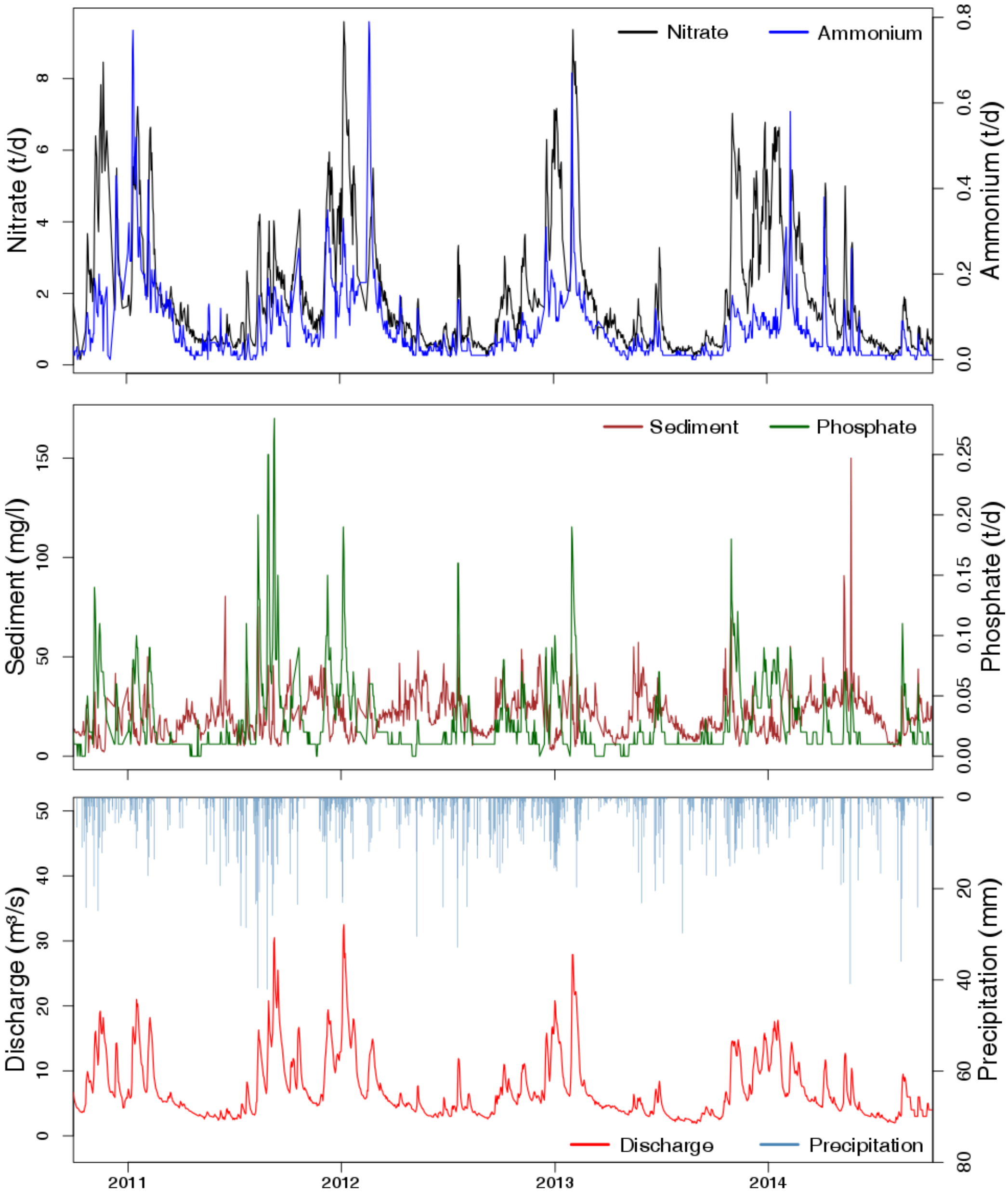


Figure 1.2: Measured nutrient loads and sediment at the Treene catchment outlet Treia.

1.2 Research questions and objectives

Since nitrate modeling can be an important tool for the processes investigation and the assessment of alternative management approaches in the catchments, it is crucial to understand how the nitrate process dynamics is controlled in the model at first. For this, the dominant model parameters, their temporal variations as well as their role in controlling the nitrate processes dynamics need to be analyzed. Within the complexity of water quality models, many parameters are included to simulate the nutrient cycles (Bailey and Ahmadi, 2014; Huang et al., 2009; Moriasi et al., 2013; Rode et al., 2007, 2010; Sincock et al., 2003). This complexity may hinder realistic estimations of these processes. Thus, the process representation of both water and nutrient cycles in the model need to be investigated to increase the understanding of the process dynamics. The following research questions emerged regarding the nitrate dynamics and processes representation in the model:

- *Is an ecohydrological model able to reproduce realistically temporal patterns of dominant model parameters for the complex nitrate cycle?*

Nitrate processes are highly variable in time in a catchment. A detection of these temporal variations is important for model behavior investigations and further processes understanding and improvement. This research question can be answered by the use of Temporal Dynamics of Parameter Sensitivity (TEDPAS, Reusser et al., 2011). It provides the sensitivity of each model parameter in a daily resolution. The method was up to now only applied to water quantity studies, but due to its general applicability, TEDPAS might also have the potential to be used for nitrate processes investigations. The temporal sensitivities can be linked to different processes occurring in the catchment in different times, giving insights about the most important nitrate process dynamics.

Once dominant nitrate parameters and so processes were identified in the model, it is possible to use this knowledge for an improved modeling. To investigate the catchment process simulations, a plausible calibration procedure is required which considers all different hydrological and nutrient conditions. As mentioned before, this approach approximates simulated to measured data (Moriasi et al., 2007; Pfannerstill et al., 2014; Rientjes et al., 2013). Furthermore, by investigating nitrate dynamics it is important to calibrate discharge as well, since a realistic reproduction of nitrate is based on an accurate representation of the hydrological conditions. Since nutrients are transported via discharge, measured and modeled time series of both discharge and nutrient need to match. Based on the importance of the calibration for model use and the relationship between nitrate and discharge, the second research question arose as follow:

- *How can river discharge and nitrate loads be jointly calibrated for ecohydrological modeling considering their interactions?*

This question can be answered by the development of a joined calibration method of discharge and nitrate loads. Following the state of the art in model calibration, both traditional statistic performance measures and signature measures need to be considered for both variables simultaneously. As a benefit of the flow and nitrate duration curves, a calibration approach should also take into account the different phases of discharge and nitrate in order to obtain a good performance for low and high periods. The importance of a good calibration for both the discharge and nitrate relies on the fact that hydrologic aspects are strongly related to the nitrate process dynamics (van Griensven and Bauwens, 2003).

With the simulation results provided by a calibrated and validated SWAT model, it is possible to proceed and use the model outcomes for further investigations of nitrate dynamics in the Treene catchment. As an actual issue, nitrate pollution of river water caused by agricultural activities and also land use changes can be investigated. The reduction of nitrate pollution in the river water is a demand of the WFD (Directive 2000/60/EC, 2000) and will contribute to achieve the goal of a better ecological status. With the use of a reliable model it is possible to simulate and assess management measures for this purpose. Also in this regard, it is almost impossible to investigate all alternative management measures with real field experiments. In this sense, the last research question focuses on the application of the SWAT model for the development and assessment of sustainable management options:

- *How effective is the implementation and simulation of different Best Management Practices (BMPs) for nitrate load reduction at the catchment scale?*

To answer this question, different BMPs for the Treene catchment were implemented in the SWAT model. The SWAT model allows the simulation of several BMPs for the evaluation of their effectiveness in nitrate reduction for different management practices and soil covering forms in the catchment. The BMPs are measures to reduce pollutant inputs to the environment (Cerro et al., 2014; Lam et al., 2011; Strauch et al., 2013). In agricultural areas these practices seek, for example, the reduction of nitrate pollution to groundwater and surface water. BMPs can be related to land use changes and to management practices modification. Agricultural activities in a catchment affect water quality and nitrate, in particular, has an important role as significant contributor to non-point pollution.

The investigation into the BMPs effectiveness can also enhance the comprehension of nitrate dynamics in the catchment, since certain BMPs can lead to higher reductions than others. The results of each BMP can affect different nitrate processes. Furthermore, BMPs simulation is an important tool for decision making. Possible scenarios of changes in land use or land practices can be helpful for future planning of resources, food production and nitrate pollution mitigation.

Finally, the three presented research questions frame a main line for the study to be carried out in logical succession, for improvements in nitrate simulations in ecohydrological modeling. The value of these steps relies on three connected aspects: the importance of model evaluation for improved processes simulations; the process understanding for better calibration; and finally also, an improved calibration procedure for more reliable model outcomes. So, the summary question and main objective is:

How to improve the representation of nitrate processes and their dynamics in models to obtain reliable simulation results to address ecohydrological challenges at the catchment scale?

This question can be taken in a broader context and the steps are theoretically transferable to other ecohydrological models and study areas. The Figure 1.3 gives an overview of the thesis structure.

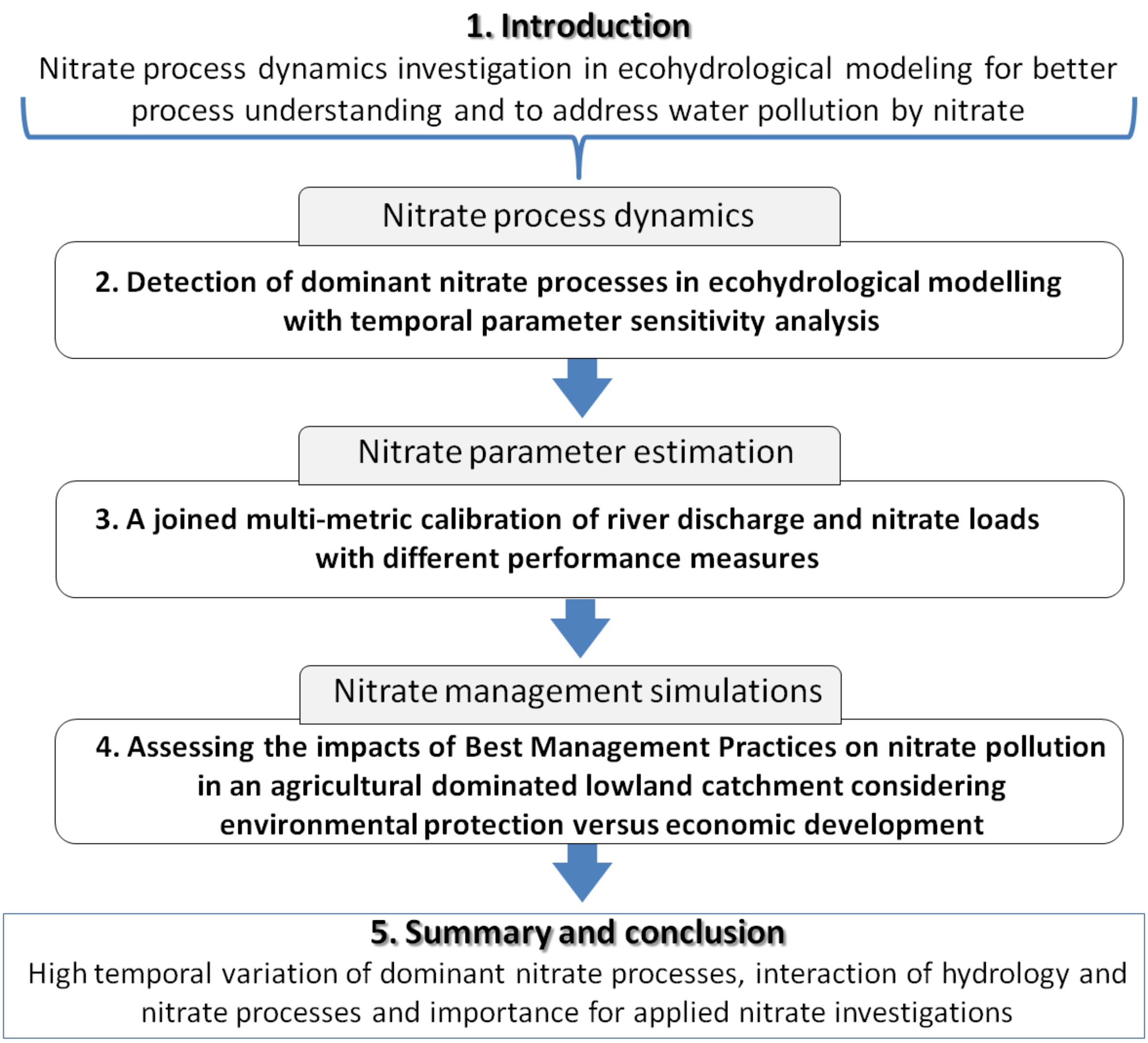


Figure 1.3: Thesis structure.

2 Detection of dominant nitrate processes in ecohydrological modelling with temporal parameter sensitivity analysis

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Abstract

River systems are impacted by nutrient inputs from the landscape. The transport of nitrate from agricultural areas into the river systems is related to numerous processes which occur simultaneously and influence each other permanently. Ecohydrological models aim to represent these complex nitrate processes. For reliable model results, it is essential to better understand the nitrate process dynamics in models.

This study aims to improve the understanding of nitrate process dynamics by using a temporal diagnostic model analysis. As diagnostic tool, a temporal parameter sensitivity analysis is applied on an ecohydrological model. With this method, phases of dominant model parameters are detected.

The results show that the sensitivity of different nitrate parameters varies temporally. These temporal dynamics in dominant parameters can be explained by temporal variations in nitrate transport and plant uptake processes. A better view on the dynamics of the temporal parameter sensitivity is obtained by analysing different modelled runoff components and nitrate pathways. Thus, a temporal parameter sensitivity analysis assists the interpretation of seasonal variations in dominant nitrate pathways.

2.1 Introduction

Catchments are characterized by a variety of processes, involving the environmental systems and human activities. Numerous processes occur simultaneously and influence the river water quality (Arheimer and Liden, 2000; Rode et al., 2010), which is highly affected by nutrient pollution coming from different diffuse and point sources of the surrounding landscape. Over the last decades, agricultural practices have adversely affected the environment, and thus the water quality (Lam et al., 2012; Laurent and Ruelland, 2011; Poor and McDonnell, 2007). A reduction of the nutrient pollution is thus a great challenge (Laurent and Ruelland, 2011) leading to studies of temporal and spatial patterns of nutrient pollutions.

To achieve these targets, ecohydrological modelling is an essential tool. In water quality modelling the complex interaction of all processes of the environment is integrated, including land management in addition to the hydrological cycle.

The nutrient concentration in river systems is highly affected by biochemical processes, fertilizer input, crop development and the nutrient transport along different pathways in soil and groundwater. Different studies analyse the pollution by nitrate and its growing presence in water bodies (e.g. Arheimer and Liden, 2000; Aubert et al., 2013; Gascuel-Odoux et al., 2010).

There are many studies showing the complexity of water quality model application. Within these complex water quality models, many parameters are included to simulate the nutrient cycles (Bailey and Ahmadi, 2014; Huang et al., 2009; Moriasi et al., 2013; Rode et al., 2010, 2007; Sincock et al., 2003; Wade et al., 2006). This complexity may hinder realistic estimations of these processes. Thus, the process representation of the modelling of water and nutrient cycles needs to be investigated to increase the understanding of the process dynamics.

For this, Gupta et al. (2008) proposed a diagnostic analysis of model behaviour. As contrasting to application studies, model diagnostic analyses are increasingly used to improve the relationship between real world processes and their implementations in hydrological models. With model diagnostic analyses, the model structure and the most relevant processes can be understood and compared with the dynamics in the catchment over time (Guse et al., 2014; Herman et al., 2013; Wagener et al., 2003).

A joined analysis of different aspects is a characteristic of diagnostic analysis to obtain an overall impression of the process dynamic in the model and in reality. The concept of model diagnostic analyses proposes to use several performance metrics to capture the different processes of the hydrograph (Gupta et al., 2008; Krause et al., 2005; Pfannerstill et al., 2014a; Pokhrel et al., 2012; Reusser et al., 2009; Wagener et al., 2003; Yilmaz et al., 2008). The diagnostic analyses are focused on temporally resolved analyses, which are related to the time step of the corresponding processes (Guse et al., 2014; Herman et al., 2013; Pfannerstill et al., 2014a; Reusser et al., 2011, 2009; Reusser and Zehe, 2011).

Reusser et al. (2011) and Wagener et al. (2003) mentioned that the dominant hydrological processes might vary temporally, e. g., between wet and dry periods. Thus, the dominating components of a hydrological model also change within the modelling period. To consider this, the discharge dynamics need to be investigated in a higher temporal resolution, which is adapted to the time scale of the related processes (Guse et al., 2014; Reusser et al., 2009; Reusser and Zehe, 2011).

One approach in this context is a temporal parameter sensitivity analysis which provides the sensitivity of each model parameter in a daily resolution. Thus, the temporal dynamic of parameter sensitivity (TEDPAS) shows the dominant model parameters for each time step (Cloke et al., 2008; Guse et al., 2014; Pfannerstill et al., 2015; Reusser et al., 2011; Sieber and Uhlenbrook, 2005). TEDPAS provides insights into the relevant model components and detects typical patterns of temporal dynamics. In this way, an improved understanding of the temporal dynamics of the model parameters is achieved.

While model diagnostic analyses are increasingly used in discharge studies, temporal diagnostic studies with TEDPAS for water quality variables are missing up to now. The water quality models can be an extension or an additional component of ecohydrological models. Therefore, they are more complex than comparable hydrological models and highly parameterized due to various processes and their interactions. Due to the capabilities of temporal parameter sensitivity analysis, we investigate its application for water quality process and the modelling of nitrate dynamics.

Thus, the goal of this study is to improve the understanding of nitrate process dynamics in an ecohydrological model with a temporal parameter sensitivity analysis. These results are combined with modelled runoff components and nitrate pathways to obtain additional information of the nitrate process dynamic.

2.2 Methods

The methodical approach of the analysis of the temporal dynamic of nitrate parameters is based on the temporal dynamic of parameter sensitivity (TEDPAS), which will be presented at first. In the following, the ecohydrological model SWAT and the included nitrate cycle is presented. The eight model SWAT parameters, which were used in the TEDPAS analysis, are explained in detail. Subsequently, the methodical approach of the discharge calibration as a basis for the nitrate analysis and an enhanced interpretation of the TEDPAS results by using different model outputs are described.

2.2.1 Temporal Dynamics of Parameter Sensitivity (TEDPAS)

Temporal Dynamics of Parameter Sensitivity (TEDPAS) is an analytic tool allowing the identification of dominant model parameters and components in a high temporal resolution with a parameter sensitivity analysis, as reported by Cloke et al. (2008), Guse et al. (2014), Pfannerstill et al. (2015), Reusser et al. (2011), and Sieber and Uhlenbrook (2005). In this study we understand TEDPAS as a method to identify dominant model parameters and components related to nitrate. With TEDPAS it is possible to observe the dominant parameters and thus processes within different periods.

This identification of dominant model components is related to a global sensitivity analysis that investigates and evaluates multiple locations in the whole physically possible parameter space (van Griensven et al., 2006). The sensitivity of the parameters is measured by using the first-order partial variance. This is realized by factor prioritization focused on the most relevant parameters, as proposed by Saltelli et al. (2006). Moreover, a partial variance-based method modifies the parameters simultaneously. Within this procedure, it investigates how the variance of these parameter modifications are related to the model output (Equation 1, from Reusser et al. [2011]). So, the first-order partial variance is defined as the variance caused by changes in one specific parameter divided by the total variance *V* over all model runs (Reusser et al., 2011).

Eq. (1):

$$V = \sum_{i} Vi + \sum_{i<j} Vij + \ldots + V1,2,3,\ldots,n$$

where *V* is the total variance, *Vi* the variance of parameter *θi* (first-order variance) and *Vij* the covariance of *θi* (second-order variance) and *θj* higher-order terms.

TEDPAS is an independent approach, and it can be used with any global sensitivity analysis method which is adequate for factor prioritization. In hydrological studies, the presence of nonlinearities demands specific analytics, and the Fourier Amplitude Sensitivity Test (FAST) is used because of its good performance in this case (Cukier et al., 1978, 1975, 1973). FAST has a high computational efficiency, achieving expected results with much fewer model runs in comparison to other methods, as for example the Sobol's method (Reusser et al., 2011; Saltelli and Bolado, 1998).

By definition, the first-order partial variance summed over all parameters cannot be higher than one, but due the interactions of the parameters it can be smaller. In this sense, the sensitivity observed, related to one parameter, is affected by the sensitivity of the others (Reusser et al., 2011).

The FAST methodology was applied using the R environment (R Core Team, 2013), specifically the algorithm implemented in the package FAST (Reusser, 2008). For each day of the time series, the sensitivity of the parameters is analysed in terms of the first-order partial variance. For further details, we refer to Reusser et al. (2011) for methodical details.

2.2.2 The ecohydrological model SWAT

The Soil and Water Assessment Tool (SWAT) (Arnold et al., 1998; Arnold and Fohrer, 2005) is an ecohydrological model which has been developed by the Department of Agriculture from United States (USDA). It is used world widely for continuous long-term model simulation of water, sediment and nutrients (Bieger et al., 2015; Du et al., 2013; Glavan et al., 2015; Guse et al., 2015b; Laurent and Ruelland, 2011; Strauch et al., 2013).

The SWAT model simulates cycles of water and nutrients in a daily resolution and takes the heterogeneity of the study area into account. In the SWAT model, subbasins are defined and it is possible to make the subdivision of the catchment into smaller units, the hydrological response units (HRU). The HRUs are grouped within the sub-basins based by the same combination of land use, soil and slope classes (Arnold et al., 1998). As the model is oriented to water quality and water balance in relation to agriculture, it includes a complex tool for land use and management, and it requires a high number of parameters to simulate the crop development during the year.

The simulation of hydrology processes in the SWAT model is separated into the land phase and the routing phase. Firstly, the water cycle is calculated at the land phase at a subbasin scale. The land phase is related to the total runoff and nutrients that flow into the main stream in each sub-basin. Afterwards the subbasins are connected and water continues to be modelled throughout the catchment. In the routing phase, the movement of water and nutrients through the drainage network of the catchment is considered.

Recognizing the complexity of subsurface processes and seeking to improve the modelling of groundwater processes, Pfannerstill et al. (2014b) developed a modification in the groundwater structure of SWAT model to enhance the nonlinear dynamics of groundwater processes. For this, the shallow aquifer was separated into a fast and a slow shallow aquifer. These modifications improve the simulation of the dynamics of the groundwater from one shallow aquifer to another and thus the dynamics of both shallow aquifers with the river channel and the deep aquifer. Likewise, it brought changes in the dynamics of subsurface water and leads to a better representation of low flow periods (Pfannerstill et al., 2015, 2014b).

2.2.3 Nitrate cycle in SWAT model

The nitrate cycle of the SWAT model is of special importance in this study. In the SWAT model, nitrate is modelled in the soil profile and in the shallow aquifer. Nitrate can be added to the soil by fertilizer, manure or residues application, bacterial attachment, mineralization and rain. In the opposite side, nitrate is removed from the soil by plant uptake, leaching, volatilization, denitrification and erosion. Withal, it can be transported in soil and groundwater.

The parameters used for the TEDPAS are presented in the Fig. 2.1 and Table 2.1. Fig. 2.1 shows the arrangement of the parameters according to their related processes. The majority of the parameters are related to processes occurring at surface and in the unsaturated soil zone. Nitrate input by rain and mineralization, nitrate losses via denitrification and plant uptake, and also nitrate transport by surface runoff and percolation take place in this zone. Likewise, there are two parameters related to the saturated zone, regarding to nitrate concentration in the aquifer.

Table 2.1: Nitrate parameters with boundaries values used for TEDPAS.

PARAMETER NAME	CODE	PROCESS	LOWER BOUND	UPPER BOUND	TYPE
Concentration of nitrogen in rainfall	RCN	Nutrient cycling	2	4	Range
Nitrate percolation coefficient	NPERCO	Nutrient cycling	0.01	1	Range
Denitrification exponential rate coefficient	CDN	Nutrient cycling	0	3	Range
Denitrification threshold water content	SDNCO	Nutrient cycling	1	1.1	Range
Rate factor for humus mineralization of active organic nitrogen	CMN	Nutrient cycling	0.0001	0.001	Range
Nitrogen uptake distribution parameter	N_UPDIS	Nutrient cycling	1	31	Range
Half-life of nitrate in fast shallow aquifer	HLIFE_NGW fsh	Groundwater	1	60	Range
Half-life of nitrate in slow shallow aquifer	HLIFE_NGW ssh	Groundwater	250	500	Range

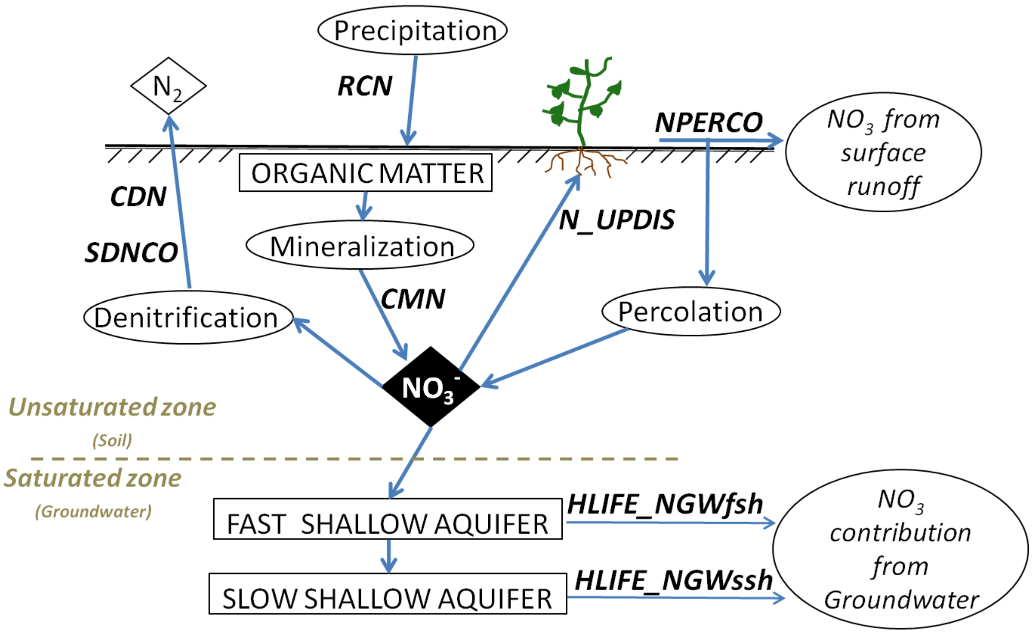

Figure 2.1: Flowchart of nitrate processes in SWAT and selected model parameters.

2.2.4 Nitrate parameters for TEDPAS

Eight parameters of the SWAT model which are related to the modelling of nitrate were selected for TEDPAS and explained as follows, based on Neitsch et al. (2011). The parameter ranges are shown in Table 2.1.

With the *concentration of nitrate in rainfall [mgN/l]* (RCN), the nitrate incorporated by the rainfall will be added to the 10 superior mm of the soil layer in the SWAT model (Eq. 1).

Eq. 1:

$$NO_{3rain} = 0.01 \; x \; RCN \; x \; R_{day}$$

where NO_{3rain} is nitrate added by rainfall (Kg N/ha) and R_{day} is the amount of precipitation on a given day (mm H_20).

The *Nitrate percolation coefficient* (NPERCO) controls the amount of nitrate removed from the surface layer in runoff relative to the amount removed via percolation (Eq. 2). Briefly, if NPERCO is close to zero, the nitrate concentration in runoff approaches zero, and if NPERCO is close to one, the surface runoff has the same concentration of nitrate as the percolate nitrate concentration. Thus, NPERCO regulates the distribution of nitrate between surface and soil (see Fig. 2.1).

Eq. 2:

$$NO3_{surf} = NPERCO \; x \; conc_{NO3,mobile} \; x \; Q_{surf}$$

$$NO3_{surf} = NPERCO \; x \; conc_{NO3,mobile} \; x \; Q_{lat,ly}$$

where $NO3_{surf}$ is the nitrate removed in surface runoff (Kg N/ha), $conc_{NO3,mobile}$ is the concentration of nitrate in the mobile water for the top 10 mm of soil (Kg N/mm H_2O), Q_{surf} is the generated surface runoff on the current day (mm H_20) and $Q_{lat,ly}$ is the water discharged from the layer by lateral flow (mm H_2O) considering the top 10 mm of soil.

The denitrification is controlled by the *denitrification exponential rate coefficient* (CDN). Briefly, the higher the value, the higher will be the loss of nitrate due to denitrification. Equation 3 shows that CDN is related to a temperature factor and to organic carbon presence. The relationship of CDN in the denitrification process leading to nitrate losses is also presented in Fig. 2.1.

Eq. 3:

$$N_{denit,ly} = NO3_{ly} \; x \; (1 - \exp\left[-CDN \; x \; \gamma_{tmp,ly} \; x \; orgC_{ly}\right])$$

where $N_{denit,ly}$ is the amount of nitrogen lost to denitrification (Kg N/ha), $NO3_{ly}$ is the amount of nitrate in layer *ly* (Kg N/ha), $orgC_{ly}$ is the amount of organic carbon in the layer (%).

The *denitrification threshold water content* (SDNCO) is the threshold value of *nutrient cycling water factor* for denitrification to occur. If the soil water content, considered as a fraction of field capacity, is ≥ SDNCO then anaerobic conditions are present and denitrification is modelled. The denitrification is also related with the *temperature factor* and *organic carbon* presence (Eq. 4). Moreover, Fig. 2.1 indicates the parameter relationship to the denitrification process.

Eq. 4:

$$N_{denit,ly} = NO3_{ly}\ x\ (1 - \exp[-\beta_{denit}\ x\ \gamma_{tmp,ly}\ x\ orgC_{ly}]) \quad \text{if } \gamma_{sw,ly} \geq SDNCO$$

$$N_{denit,ly} = 0.0 \quad \text{if } \gamma_{sw,ly} < SDNCO$$

where $N_{denit,ly}$ is the amount of nitrogen lost to denitrification (Kg N/ha), β_{denit} is the rate coefficient for denitrification [CDN].

The *rate factor for humus mineralization of active organic nitrogen* (CMN) calculates the mineralization of humus together with water and temperature factors of each soil layer. The mineralization is furthermore affected by the amount of nitrogen in the active organic pool (Eq. 5). Fig. 2.1 shows its relationship with the mineralization process, taking nitrogen originated from organic matter in soil into account and which will be stored as nitrate form.

Eq. 5:

$$N_{min,ly} = CMN\ x\ (\gamma_{tmp,ly}\ x\ \gamma_{sw,ly})^{1/2}\ x\ orgN_{act,ly}$$

where $N_{min,ly}$ is the nitrogen mineralized from the humus active organic nitrogen pool (Kg N/ha), $\gamma_{tmp,ly}$ is the nutrient cycling temperature factor for layer *ly*, $\gamma_{sw,ly}$ is the nutrient cycling water factor for layer *ly*, $orgN_{act,ly}$ is the amount of nitrogen in the active organic pool (Kg N/ha).

The *nitrogen uptake distribution parameter* (N_UPDIS) controls the depth distribution of nitrogen uptake and thus the maximum amount of nitrate removed from the upper layers. Lower layers in the root zone can compensate for lack of nitrate in the upper layers (Eq. 6).

Eq. 6:

$$N_{up,z} = \frac{N_{up}}{[1 - \exp(-N\_UPDIS)]}\, x \left[1 - \exp\left(-N\_UPDIS\ x\ \frac{z}{z_{root}}\right)\right]$$

where $N_{up,z}$ is the potential nitrogen uptake from the soil surface to depth z (Kg N/ha), N_{up} is the potential nitrogen uptake (kg N/ha), z is the depth from the soil surface (mm), and z_{root} is the depth of root development in the soil (mm).

The *half-life of nitrate in the shallow aquifer [in days]* (HLIFE_NGW) is related to the required time for the nitrate concentration in the shallow aquifer to fall half of its original value. The reduction is a net reduction of all processes that occur in the superficial aquifer. It is also related to the rate constant for removal of nitrate in the shallow aquifer (1/day).

As the $SWAT_{3S}$ model (Pfannerstill et al., 2014b) is used, the active shallow aquifer is separated into a fast and a slow shallow aquifer. With this situation, there are two HLIFE_NGW parameters, one for each shallow aquifer (see Fig. 2.1), and the general formula is as follow in Equation 7.

Eq.7:

$$HLIFE\_NGW = \frac{0.693}{k_{NO3}}$$

where k_{NO3} is the rate constant for removal of nitrate in the shallow aquifer (1/day).

2.2.5 Model set up and discharge calibration

The model set-up consists of a delineation of the catchment resulting in 108 sub-basins and 4524 HRUs for the total basin as presented in Guse et al. (2014). Three categories of slope for defining HRUs were chosen, which are: < 1.25%; from 1.25% to 3% and > 3%. For the definition of HRUs, land use classes whose areas in a subbasin are smaller than 5% and categories of soil less than 10% were reclassified to other classes in the SWAT model to reduce the number of HRUs.

The agricultural areas in the catchment were subdivided into five different crop rotations based on an actual distribution of the crops as presented in Guse et al. (2015b). The parameters for the soil and crop database were taken from a SWAT model study of Guse et al., (2014) and Fohrer et al. (2014).

All HRUs with activities of agriculture, pasture or rangeland areas, with a slope lower than 1.25% and a soil that have a high water table were assumed to contain subsurface tile drains. In this case, the parameters from the study of Kiesel et al. (2010) were applied.

In advance of the model diagnostic analysis for nitrate, the SWAT is calibrated for discharge. A period of six years (2000–2005) was selected for this study for the calibration of discharge and within this, a period of three years period was used as warm-up, so that the simulation was started in 1997.

The following parameters in Table 2.2 were used for the discharge calibration. The parameters of the new groundwater routine of $SWAT_{3S}$ model were selected according to Pfannerstill et al. (2014b).

Using the Latin Hypercube Sampling and the R-package FME (Soetaert and Petzoldt, 2010) as described in Pfannerstill et al. (2014a), combinations of the parameters were generated to cover the possible parameter space. These combinations were then applied in the model and a run was made. By using the Nash-Suctliffe efficiency (NSE) (Nash and Sutcliffe, 1970) and Percent bias (PBIAS) the model performance for each run was calculated.

Furthermore in order to calibrate the discharge volume the flow duration curve is used in a 5FDC methodological approach as proposed by Pfannerstill et al. (2014a). In this multi-metric evaluation methodology the flow duration curve is subdivided into five segments. Each segment is assessed individually with the ratio of root mean square error and standard deviation (RSR), seeking to a good performance in each segment resulting in an overall good performance. Based on the results from these measurements, a best model run with the overall best combination of all performance measures was selected.

Besides the calibration periods from 2000 to 2005 the period from 2006 to 2012 was used for the validation of the discharge simulation results.

Table 2.2: Parameters used for discharge calibration with value ranges and final values implemented in model.

PARAMETER NAME	CODE	PROCESS	TYPE	RANGE		FINAL VALUE
Baseflow alpha factor - fast shallow aquifer (1/day)	ALPHA_BF fsh	Groundwater	Range	0.1	1	0.554
Groundwater delay time - fast shallow aquifer (days)	GW_DELAY fsh	Groundwater	Range	2	30	11.466
Deep aquifer percolation fraction - fast shallow aquifer	RCHRG_DP fsh	Groundwater	Range	0.2	0.8	0.637
Baseflow alpha factor - slow shallow aquifer (1/day)	ALPHA_BF ssh	Groundwater	Range	0.001	0.1	0.005
Groundwater delay time - slow shallow aquifer (days)	GW_DELAY ssh	Groundwater	Range	10	35	32.033
Deep aquifer percolation fraction - slow shallow aquifer	RCHRG_DP ssh	Groundwater	Range	0.1	0.5	0.358
Initial SCS runoff curve number for moisture condition II	CN2	Surface runoff / soil water	Add	-5	15	3.834
Surface runoff lag coefficient	SURLAG	Surface runoff routing	Range	0.3	2	1.292
Threshold water level in shallow aquifer for base flow (mm H_2O)	REVAPMN	Groundwater	Range	8	20	15.499
Soil evaporation compensation factor	ESCO	Evapotranspiration	Range	0.7	1	0.898

2.2.6 Additional information from other SWAT model outputs

In order to consider the complexity of the nitrate processes, the interpretation of the TEDPAS outcomes are enhanced. In addition to the TEDPAS results for nitrate loads, other modelled outputs are analysed. Thus, two additional methodical approachesare included to intensify the temporal diagnostic analysis of the relationship between the nitrate processes and the temporal parameter sensitivities.

At first, the correlation between the time series of parameter sensitivity to different SWAT model outputs is investigated. The daily sensitivities of the eight model parameters are correlated to the modelled runoff components as well as to the nitrate transport along the different pathways. Thus, it can be investigated which parameters are highly related to a runoff component or a nitrate pathway.

In a second approach, the continuous daily time series of modelled outputs and parameter sensitivity are compared for highly correlated relationships. These correlations are shown to reinforce and visualize the behaviors of processes and modelled outputs, aiming to improve the detection of dominant nitrate processes.

2.3 Study area and data

2.3.1 Study area

The study area is the catchment of the river Treene (Fig. 2.2), a basin of 481 km² (hydrological station Treia at the catchment outlet). It is located in the lowlands of northern Germany, near the Danish border. The Treene catchment is a subbasin of the Eider River, which flows into the North Sea.

The altitude of the catchment does not exceed 80 metres above sea level, and the average rainfall is 884 mm/year (station Schleswig, 1981-2011). The Northeast is characterized by hilly areas (Östliches Hügelland) with a slightly undulating terrain with smooth slopes and, in general, clay and sandy soils. The south-west is covered with flatter areas and more sandy soils (Geest landscape, LANU, S-H, 2006).

The land use is predominantly agricultural (Fig. 2.2, LVERMA, 2004). 48% of the catchment is covered by agricultural area and 31% by pastures, representing together 79% of the land use. Only small areas are covered by forests (7%) or urban areas (10%). The strong interaction between surface and shallow aquifer results in a significant presence of tile drainages as an important characteristic in this agricultural lowland catchment (Fohrer et al., 2007; Kiesel et al., 2010).

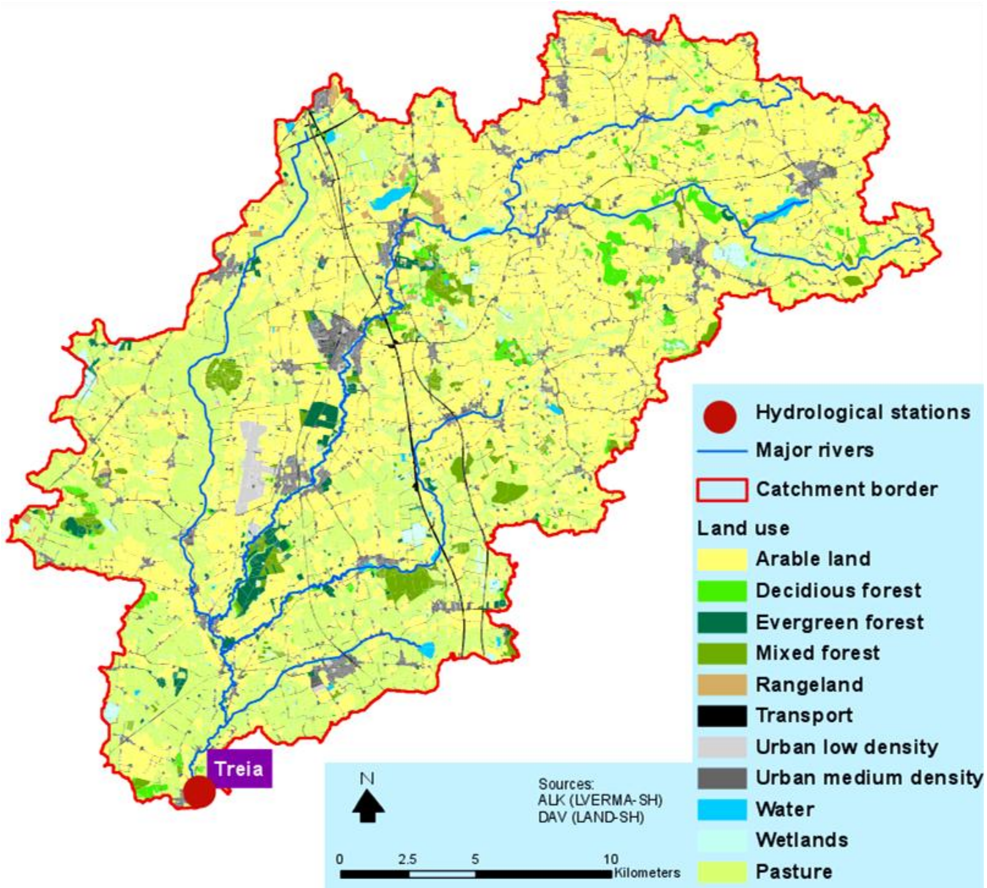

Figure 2.2: Treene catchment with outlet (Treia) and land use distribution (ad. from Guse et al., 2014).

2.3.2 Model input data

The principal input data for the model were provided by government agencies. Likewise, a digital elevation model with a resolution of 25x25m (LVERMA, 1995), together with a land use map (ALK, LVERMA, 2004) and a soil map with a spatial resolution of 1:200.000 ([BÜK 200], BGR, 1999) were provided. Information about point source inputs from sewage plants were obtained from the Landesamt Schleswig-Flensburg and implemented as monthly average values.

Fertilisers were the major input of nitrate in the SWAT model. The fertilizer application varies between the different crop rotations. Corn silage dominated crop rotations receive an annual average of 123 Kg N/ha and wheat dominated crop rotations receive an annual average of 207 Kg N/ha.

For climate time series, daily values for precipitation, minimum and maximum temperature, wind speed, relative humidity and solar radiation, were obtained from the German Weather Service (DWD) and interpolated by the Potsdam Institute for Climate Impact Research as described in Österle (2001) and Conradt et al. (2012).

The discharge data series from 2000 to 2013 at the catchment outlet in Treia is provided by the government agency for agriculture, environment and rural areas of the State of Schleswig-Holstein. Nutrient concentrations are available from a continuous measurement campaign at the station Treia (10/2010-12/2012) (Guse et al., 2015a), which is based on daily collections of water samples by an automatic stationary sampler. The mean nitrate concentration during our measurement campaign was 2.9 mg/l at the catchment outlet.

2.4 Results and discussion

2.4.1 Discharge modelling

In the discharge calibration, the best model was selected based on a performance evaluation with PBIAS, NSE and 5FDC as proposed by Pfannerstill et al. (2014a). The evaluation of this model run results in a satisfying performance for calibration and validation periods. The model parameters of this model run are shown in Table 2.2.

The visual inspection of the discharge for the calibration and validation periods (Fig. 2.3) shows a good matching of the observed (in blue) and the modelled (in red) discharge time series. Thus, it can be stated that the performance of the modelled discharge time series enables one to proceed with the evaluation of the nitrate modelling.

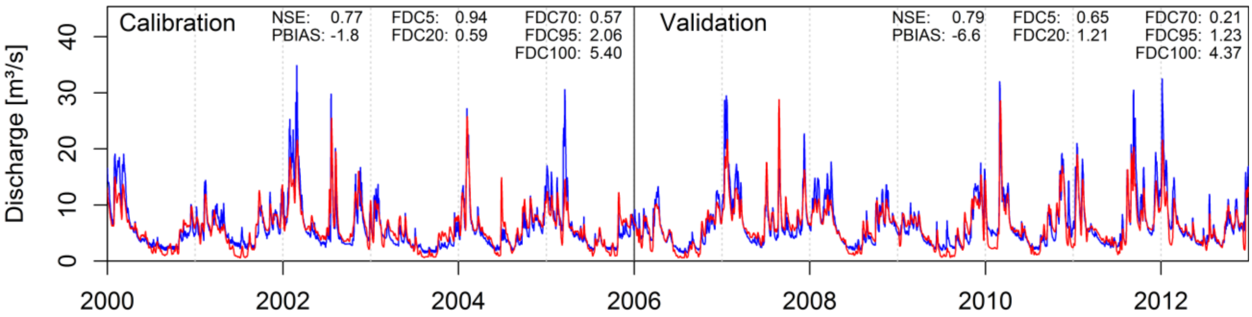

Figure 2.3: Measured (blue) and modelled (red) discharge series for calibration (2000-2005) and validation (2006-2012) periods at Treia station. NSE stands for the Nash-Sutcliffe Efficiency, PBIAS for the percent bias. The abbreviations FDC5, FDC20, FDC70, FDC95, and FDC100 represents the RSR (ratio of root mean square error [RMSE] and standard deviation) of five segments of the flow duration curve, namely the segments from 0-5%, 5-20%, 20-70%, 70-95% and 95-100% flow exceedances.

2.4.2 Temporal Parameters Sensitivity Analysis for nitrate

Regarding to the temporal dynamics of the model parameters, their sensitivity varies temporally between the eight parameters (Fig. 2.4). There are low and high sensitivities, as well as marked and not marked phases. The results from TEDPAS are described step-by-step for the eight parameters.

The concentration of nitrate in the rainfall (RCN) has a relevant sensitivity during almost the whole modelled period. One can still consider the response period after rainfall events. Further, there is a higher sensitivity in periods with a higher concentration of nitrate in water. So, RCN is continuously sensitive, but its most dominant phases are after periods with higher precipitation volumes in association with higher nitrate concentrations. This combination indicates a satisfactory representation of the process regarding the addition of nitrate to the soil. Consequently, there is a greater presence of nitrate in the river. In this way, the rainfall adds nitrate directly to the soil, and at the same time influences the amount of transported nitrate in the soil profile and via the runoff components.

A high sensitivity of the nitrate percolation coefficient (NPERCO), which regulates the transport of nitrate via surface runoff and percolation, is strongly related to rainfall events. These high sensitivities always appear after precipitation events. In addition, NPERCO is related to the nitrate removal within the soil.

The denitrification exponential rate coefficient parameter (CDN) and the denitrification threshold water content (SDNCO) have little sensitivity compared to other parameters without showing a typical dynamic. Its sensitivity behaves similarly to nitrate concentration in water and to the discharge. As proposed by Pohlert et al. (2005), the denitrification and leaching of nitrate processes are strongly related to water presence in soil, which may create a water competition under different conditions of wet soil and subsoil. Moreover, Anderson et al. (2015) presented the seasonality in the denitrification process regarding to nitrogen availability in periods during and after plants growing. So, SDNCO and consequently CDN are directly related to the denitrification process.

The rate factor for humus mineralization (CMN) is related to the nitrate concentration in water. The TEDPAS results present an increasing sensitivity of CMN in the coldest periods of year. Normally, after the harvest phase, at autumn, there will be more organic nitrogen available. In this period, coupled with water availability, the mineralization process can take place and add nitrate to soil. With more precipitation, the added nitrate is transported to the river.

A special feature was observed for the nitrogen uptake distribution parameter (N_UPDIS) with a short phase of very high sensitivity. This phase of high sensitivity occurs in spring during medium nitrate concentration in the river and low discharge conditions. This period is characterized by plant growing and thus a high demand for nitrate. Thus, a high sensitivity of N_UPDIS is related to low nitrate concentration near soil surface and in the root zone. This specific peak of high parameter sensitivity cannot be fully explained by the TEDPAS analysis and will be in the focus of further analysis as follows, in section 2.4.3.

The top of the soil interacts with surface runoff and influences the amount of nitrate available for transport in the surface runoff. The sensitivity peak of N_UPDIS does not overlap with a high sensitivity of NPERCO. This illustrates the relevance of nitrate uptake from deeper layers.

The half-life parameter of nitrate in the fast shallow aquifer (HLIFE_NGWfsh) presents a low sensitivity during almost the entire period. This behaviour represents of a greater susceptibility to other processes during the year. Thereby, the reduction of nitrate concentration in the shallow aquifer is related to surrounding processes with a nitrate demand.

The half-life parameter of nitrate in the slow shallow aquifer (HLIFE_NGWssh) is very sensitive during periods with lower concentration of nitrate and after rainfall events. A significant or lasting rainfall coinciding with a low concentration of nitrate in water results in an increasing sensitivity of this parameter. HLIFE_NGWssh has dominant phases in spring and summer periods. As in the case of HLIFE_NGWfsh, this pattern is affected by the relationship of the slow shallow aquifer with other processes with nitrate demand which reduces the nitrate concentration in the shallow aquifer.

The water flows into the second aquifer after infiltration or percolation and after passing through the fast shallow aquifer. Clearly the sensitivity arises strongly in spring and summer seasons in periods with crops development and fertilizer input. In these periods the plants are consuming nitrate, which leads to a lower nitrate concentration in the river.

In lowland catchments the shallow aquifer interacts more with the processes at the surface and in the upper soil zone. As a consequence, the nitrate processes in the shallow aquifer are also strongly affected by surface and soil processes.

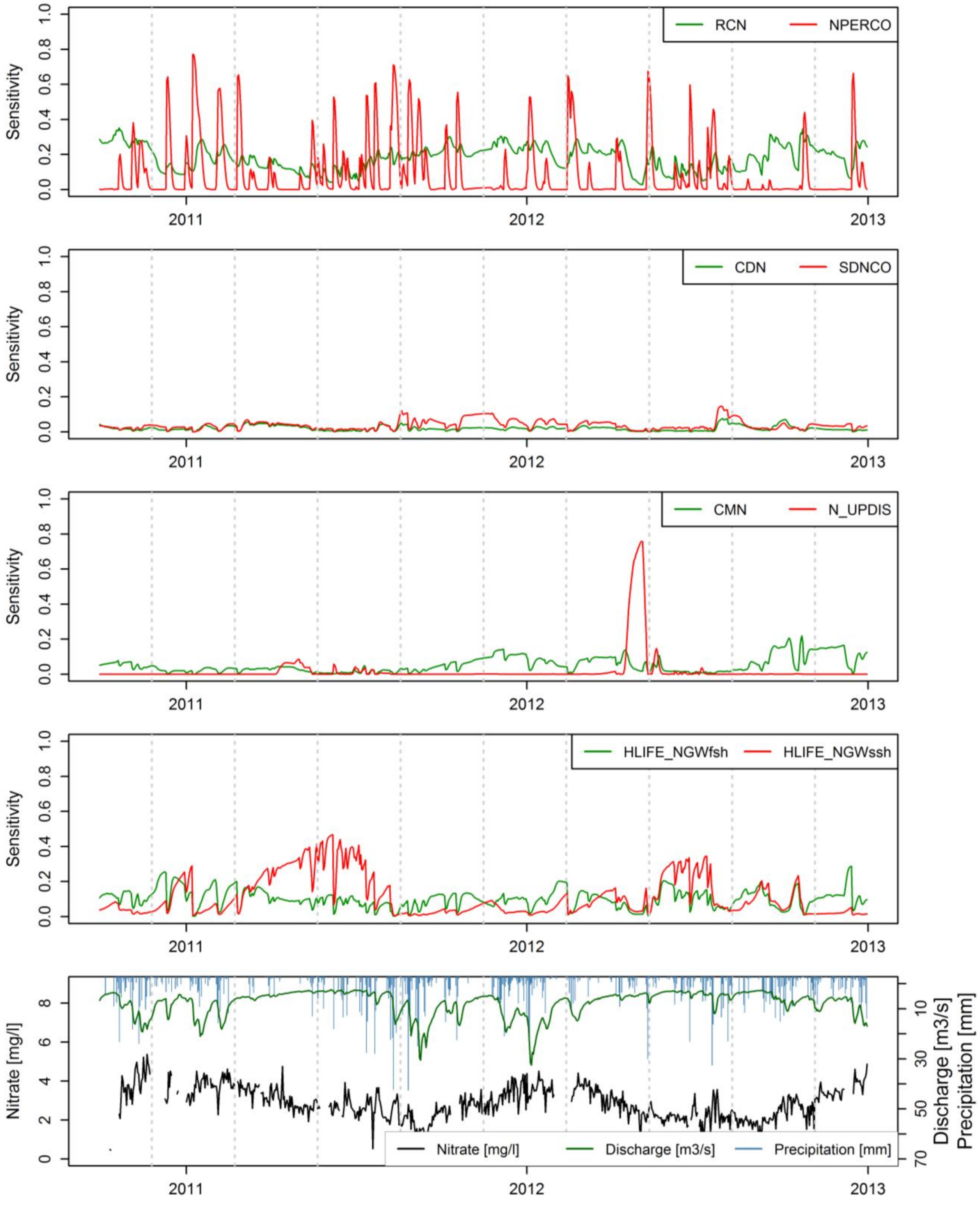

Figure 2.4: Temporal dynamics of the sensitivity of nitrate parameters for Treia hydrological station. The parameter sensitivity is shown as first-order partial variance.

2.4.3 Additional information from other SWAT model outputs

The TEDPAS results give insights into an improved understanding of the role of the nitrate parameters in the model and the nitrate process dynamic. Due to the complexity of nitrate processes in reality and in the model, further inspections are required to increase the understanding of the phases of high parameter sensitivity. For this, time series of other model outputs in addition to discharge were analysed and correlated to the time series of parameter sensitivity. For this, the modelled runoff components and nitrate pathways were analysed. Fig. 2.5 shows the correlation between the eight selected model parameters and different model outputs. The shades of blue represent a positive correlation and red indicate negative correlation.

The daily parameter sensitivity of RCN correlates with the daily time series of the runoff components and also with nitrate movement such as nitrate percolation and nitrate presence in tile drainages. These correlations reinforce the relationship of nitrate to modelled runoff components in the SWAT model. This parameter has a negative correlation with nitrate uptake by plants, which occurs independently from the rainfall event. Since the nitrate concentration in rainfall is a factor of the precipitation intensity, it is in particular relevant in phases of high precipitation. In these phases, also the runoff components are active.

The parameter NPERCO correlates with different runoff components (surface runoff, lateral flow, percolation) and nitrate transport pathways (nitrate in surface runoff, in lateral flow and nitrate percolated). As NPERCO controls the transport via surface runoff and the percolation, here the highest correlations were observed for these model outputs. In contrast, the correlation to tile flow and groundwater flow is low.

N_UPDIS and HLIFE_NGWssh present correlation with the nitrate concentration in crops (*NO3 in crop)*. The strong correlation of N_UPDIS demonstrates that active phases of N_UPDIS depend on the nitrate demand by crops. Thus, this analysis helps to explain the high sensitivity of N_UPDIS as shown in Fig. 2.4.

Furthermore, it is worth noting that both HLIFE_NGW parameters have a negative correlation with the other modelled outputs in the majority of the cases. In particular, HLIFE_NGWssh has a strong negative correlation with fast groundwater runoff and nitrate in tile drainages.

Thus, the correlation table clear shows that the correlation decreases from up to down. Considering that the parameters are ordered according to the vertical occurrence, it can be stated that the runoff components and nitrate pathways are higher positive correlated to the surface parameters such as RCN and NPERCO, while the correlation is negative for the nitrate parameters in the groundwater.

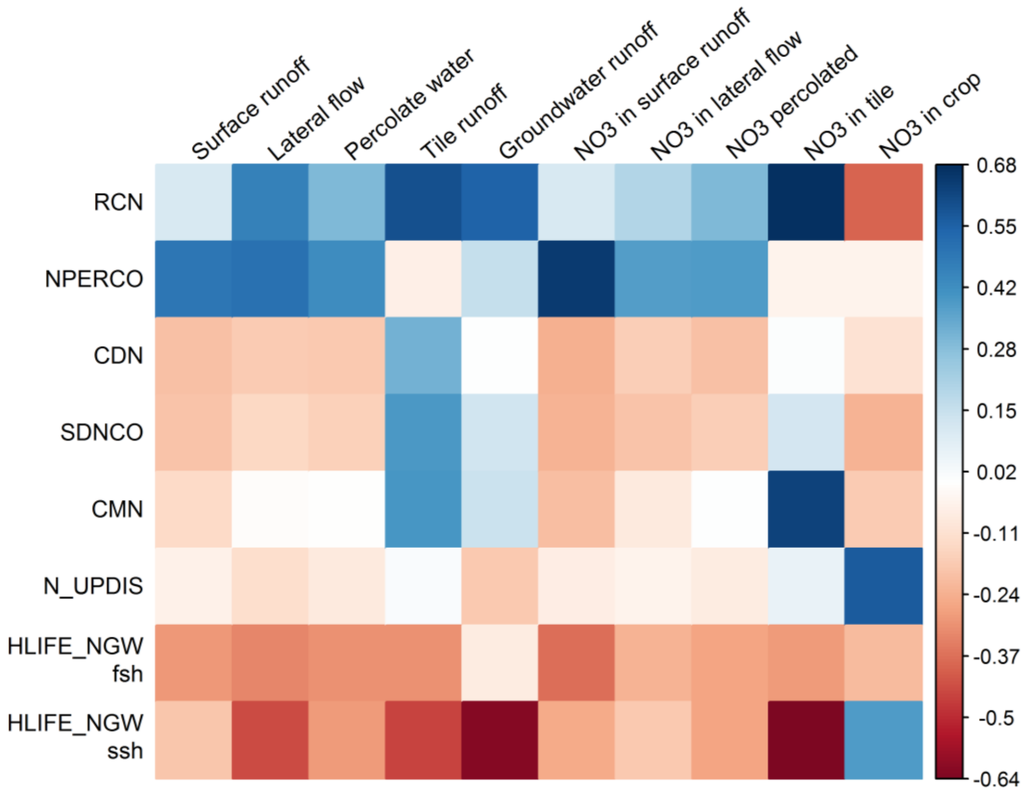

Figure 2.5: Correlation table between parameter sensitivities and SWAT modelled outputs. The shades of blue represent a positive correlation and red indicate negative correlation.

The results of the correlation plot were used to select nitrate related modelled outputs as continuous time series in relation to the daily parameter sensitivities. For this, the focus is exemplarily on the dominant model parameters NPERCO, HLIFE_GWssh and N_UPDIS (which is less sensitive, but shows short phases with high dominance), as well as RCN. Fig. 2.6 presents direct relations of the sensitivity of these parameters to the outputs of the SWAT model.

There is a clear coincidence of peaks of NPERCO sensitivity and the presence of nitrate in the surface runoff and lateral flow. Likewise, the NPERCO peaks match the peak of the percolated nitrate. This coincidence demonstrates that NPERCO works as expected and controls the amount of nitrate removed from the surface layer in surface runoff relative to the amount removed via percolation. NPERCO works as partitioning parameter of the nitrate transport on the surface and in the soil. The transport of nitrate is related to water presence and its movement, as also demonstrated the study of Glavan et al. (2015). Thus, the sensitivity of NPERCO expressed how it controls the nitrate processes dynamic.

N_UPDIS present a marked correlation with the *nitrate concentration in crops.* The dominant phases of N_UPDIS coincide with periods of increased nitrate uptake by plants in the root zone.

In these periods, crops are in development and consume nitrate. This sensitivity peak represents nitrate stress due to low nitrate concentrations in top of the soil in the phase of a high demand by plants. Then, the lower layers will compensate this lack, which results in a high sensitivity of the nitrate uptake parameter N_UPDIS.

HLIFE_NGWssh shows also a correlation with *nitrate concentration in crops.* Its dominant phases coincide with periods of increased nitrate uptake by plants. Likewise, during the crop development periods, there are strong phases with nitrate concentration decreasing in the slow shallow aquifer, which can be a consequence of the nitrate compensation in the soil upper layers in these periods. The impact of crop development on nitrate dynamics was highlighted by Laurent and Ruelland (2011) and Glavan et al. (2013b). This relationship was thus detected in the sensitivity behaviour of the parameters N_UPDIS and HLIFE_NGWssh.

As pointed out previously, a close interaction of groundwater with surface water is observed in lowland catchments. So, the TEDPAS results indicate a great activity from shallow groundwater as already shown in studies of Aubert et al., (2013), Lam et al. (2012) or Schmalz et al. (2008).

Furthermore, the nitrate transport through the tile drainages is analysed by observing the behavior of the nitrate concentration in drainage tiles (*NO3 Tile)* in relation to RCN. Drainage tiles modify the dynamics of water in the catchment and thus also the nutrient transport through soil (Jarvie et al., 2008; Schmalz et al., 2008). Thus, tile drainages may enhance the export of nitrate in humid phases.

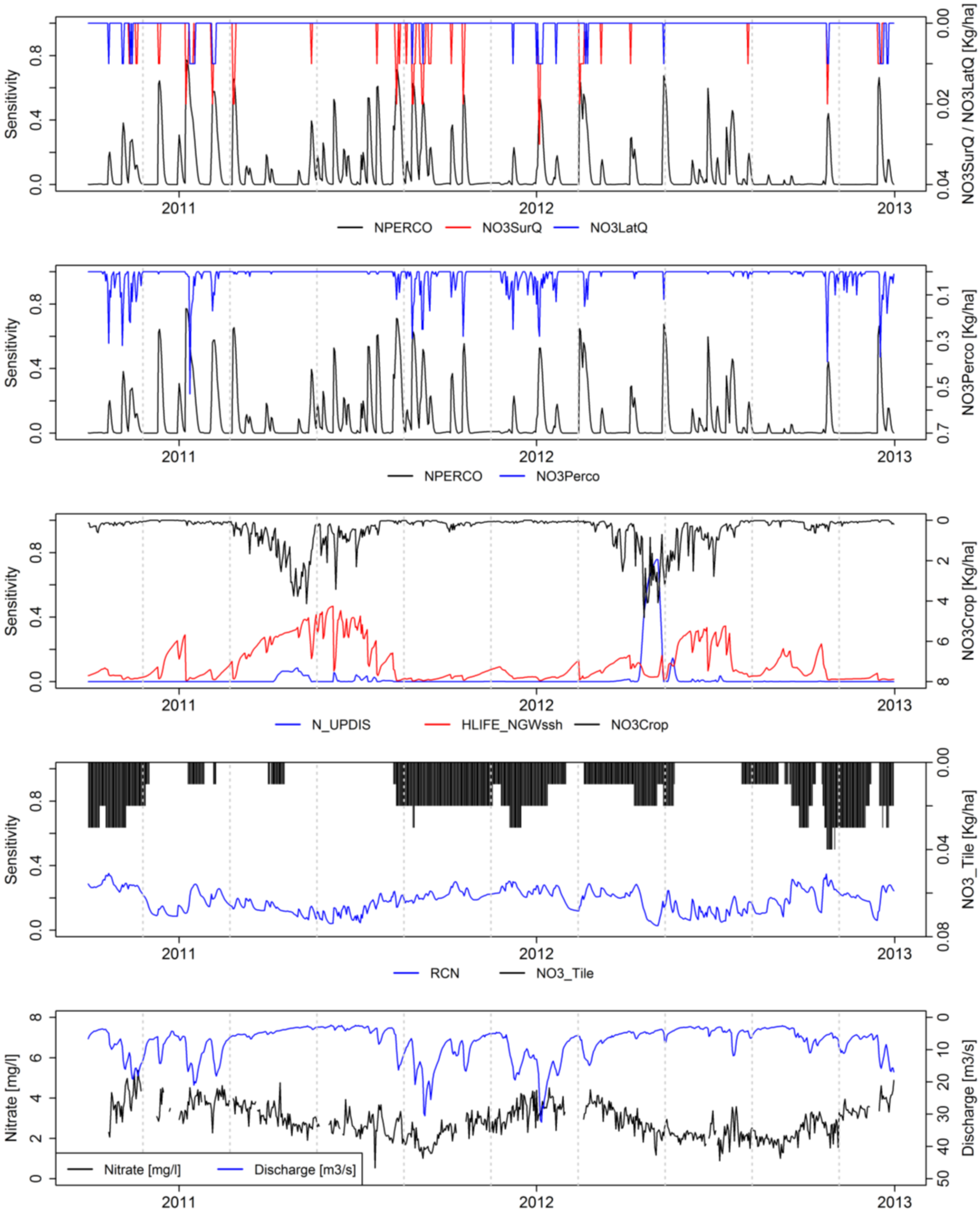

Figure 2.6: Nitrate related model outputs in relation to the parameter sensitivity.

2.5 Potential of TEDPAS to analyse and understand water quality model results

As demonstrated in this study, TEDPAS presents a high potential for a more accurate interpretation of water quality modelling. The temporal variations in the sensitivity of model parameters are pointed out and thus dominant nitrate processes are detected for each time step. In this way, the complex process structures within a model in terms of nitrate dynamics are disentangled.

Initially, Fig. 2.4 provides parameter dependent variations and dynamics of sensitivity during the modelling period. These temporal patterns are related with seasonal variations in the climatic conditions and in the land management. In a particular period of the year, different conditions of the environment increase or reduce the dynamics of nitrate in soil and water. So, TEDPAS detects the seasonality of sensitivity, indicating a higher or lower activity of a process in a certain period.

The temporal variability in the parameter sensitivity is strongly related to the water cycle which influences transport and transformations of nutrients. In the same way, temperature controls chemical transformation processes and thus influences the parameter sensitivity.

Spring and summer are the major periods of agricultural activities, with crop development phases and fertilization. This period of high agricultural activity is characterized by high nitrate transport dynamics in the soil profile, as shown in the dominance of the related nitrate parameters (see N_UPDIS in Fig. 2.4, regarding to nitrate uptake by plants).

Regardless of the time of year, NPERCO shows the dependence between the rain events, nitrate transport via surface runoff and nitrate leaching into the soil. The sensitivity of this parameter indicates the high solubility of the nitrate ion, since the sensitivity peaks indicate percolation and/or leaching.

Different intensities in nitrate dynamics were detected in periods of low crop growing, in autumn and winter. During the coldest periods of the year in times of high water availability in the soil, the temporal sensitivities variations of related parameters detects a low or no occurrence of the denitrification process. Moreover, this established climatic situation can still limit the gain of nitrate through the mineralization. This situation indicates a limitation for denitrification and mineralization activities brought by the colder conditions. Consequently, the reasons for high nitrate concentrations of the percolating water and measured in river water are expected to be dependent on other processes. These results from TEDPAS, regarding to denitrification and mineralization activities, meet the conclusions of empirical studies, with actual data and analysis, carried out by several authors regarding nitrate dynamics (e.g. Arheimer and Lidén, 2000; Aubert et al., 2013; Gascuel-Odoux et al., 2010; Poor and McDonnell, 2007).

In contrast to hydrological studies with TEDPAS as presented in Guse et al. (2014), Pfannerstill et al. (2015) or Reusser et al. (2011), the complex process integration for nitrate processes required an extended analysis. As the nitrate concentration in the river water is an integrated value of the hydrological conditions as well as of the nitrate processes in the catchment, the combination of all these processes are also combined in TEDPAS. However, not all model results of TEDPAS are clearly interpretable. To improve this, these results were further interpreted by including other modelled outputs than discharge.

As an extension of the classical TEDPAS approach, the time series of different model outputs were correlated to the parameter sensitivities. These correlations (Fig 2.5.) support a more substantial understanding between sensitivities and modelled nitrate processes. By it, one can note that the sensitivities of the parameters have indeed higher correlation with specific output information generated by the model and thus with related processes.

The relationship between model outputs and parameter sensitivities was further enhanced by showing the time series for highly correlated relations (Fig. 2.6). Even though that only a few selected figures were provided, the examples show the potential of these analyses. The matching of peaks of a nitrate pathway with a high sensitivity of a model parameter illustrates the controlling role of this parameter for the specific process. This analysis supports the previous assumptions regarding to nitrate transport and nitrate consumed by plant uptake.

In this way, a greater representation of a given process is detected, representing the dominance of the process for this given time. Thus, a focus on this process during this time periods might lead to a more accurate modelling. In certain periods, specific parameters are more active. An active parameter is of great significance for the representation of the process under investigation. In this sense, the applicability of TEDPAS as a tool for improvement of water quality modelling and assessment is emphasized.

2.6 Conclusion

In this study, the representation of complex nitrate dynamics in an ecohydrological model was investigated. To achieve this, a temporal parameter sensitivity analysis as an established model diagnostic tool in hydrological modelling, was applied to a model component for nitrate modelling for the first time.

The results present high variations in the temporal sensitivity between the eight investigated nitrate parameters. These sensitivities are related to the corresponding processes which control the nitrate dynamics.

There is a high sensitivity during all periods regarding to the processes of water and nitrate movement, from the top of soil throughout the profile and to aquifer and water course. Furthermore, the most outstanding dominant phases occur during crop development periods.

The diagnostic information was enhanced by correlating the parameter sensitivity with modelled runoff components and nitrate pathways.

Overall, a plausible relationship from model simulation and the environment can be noticed. Thus, we conclude that the detection of variations in the dominance of nitrate parameters is a useful tool to improve the understanding of dominant nitrate processes.

2.7 Acknowledgements

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3 A joined multi-metric calibration of river discharge and nitrate loads with different performance measures

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Abstract

Hydrological models are useful tools to investigate hydrology and water quality in catchments. The calibration of these models is a crucial step to adapt the model to the catchment conditions, allowing effective simulations of environmental processes. In the model calibration, different performance measures need to be considered to represent different hydrology and water quality conditions in combination.

This study presents a joined multi-metric calibration of discharge and nitrate loads simulated with the ecohydrological model SWAT. For this purpose, a calibration approach based on flow duration curves (FDC) is advanced by also considering nitrate duration curves (NDC). Five segments of FDCs and of NDCs are evaluated separately to consider the different phases of hydrograph and nitrograph. To consider both magnitude and dynamics in river discharge and nitrate loads, the Kling-Gupta Efficiency (KGE) is used additionally as a statistical performance metric to achieve a joined multi-variable calibration.

The results show that a separate assessment of five different magnitudes improves the calibrated nitrate loads. Subsequently, adequate model runs with good performance for different hydrological conditions both for discharge and nitrate are detected in a joined approach based on FDC, NDC, and KGE. In that manner, plausible results were obtained for discharge and nitrate loads in the same model run. Using a multi-metric performance approach, the simultaneous multi-variable calibration led to a balanced model result for all magnitudes of discharge and nitrate loads.

3.1 Introduction

Complex catchment models assessing hydrology and water quality are widely applied in hydrological and environmental research (e.g. Santhi et al., 2001; van Griensven and Bauwens, 2003; Guse et al., 2007; Tuppad et al., 2010; Bouraoui and Grizzetti, 2014; Cerro et al., 2014). These models seek greater understanding of processes occurring within the hydrological cycle, and how these processes affect nutrient pathways in the catchments and subsequently nutrient loads in the river. In this context, is challenging to adequately simulate and apprehend simultaneously discharge and nutrient loads in the same model simulation (Sincock et al., 2003; Rode et al., 2010; Moriasi et al., 2013; Bailey and Ahmadi, 2014).

Complex environmental conditions have to be considered in the model calibration when comparing modelled and measured time series. It is recommended to use different types of performance measures to evaluate the simulated processes and to achieve plausible model simulations (Krause et al., 2005; Pokhrel et al., 2012; Guse et al., 2014, Pfannerstill et al., 2014a). The main problem in using a single-metric approach is that each performance measure places emphasis on matching one aspect of the hydrograph and underestimates another, thus causing an imbalance situation in the hydrograph (Boyle et al., 2000; Pokhrel et al., 2012). In this way, it is necessary to utilize different performance measures to cover various hydrological situations of the model (e.g. Gupta et al., 1998; Krause et al., 2005; Bekele and Nicklow, 2007; Moriasi et al., 2007; Kollat et al., 2012; Pokhrel et al., 2012; Pfannerstill et al., 2014a). Different performance measures are adapted to a specific part of the hydro- or nitrograph, and have drawbacks in others. A multi-metric calibration considers different performance measures to represent distinct phases and/or conditions for discharge and/or nitrate. The term Performance Measures will be the used in this study to refer to the metrics assessing good-of-fitness in general. Performance measures are further distinguished between statistical performance metrics, e.g. Nash-Sutcliffe Efficiency (NSE, Nash and Sutcliffe, 1970), Kling-Gupta-Efficiency (KGE, Gupta et al., 2009), and signature measures, e.g. specific parts of the Flow Duration Curve (FDC, Vogel and Fennessey, 1994). Pfannerstill et al. (2014a) summarized these key aspects of several performance measures and pointed out the scope of each one. Typical statistical performance metrics used are the NSE (Nash and Sutcliffe, 1970; Santhi et al., 2001; Hesse et al., 2008; Kollat et al. 2012), *Percent Bias* (BPIAS) (Gupta et al., 1999; Zhang et al., 2011), *Root Mean Square Error* (RMSE) (Boyle et al., 2000; Madsen, 2000; Bekele and Nicklow, 2007; van Werkhoven et al., 2009) and the *Ratio of RMSE and standard deviation* (RSR) (Moriasi et al., 2007; 2013). The KGE (Gupta et al., 2009), as a statistical performance metric developed as a further development of the NSE index, considers bias, correlation and variability separately.

Signature measures comprehend hydrologic aspects of catchment hydrology and are a way to address specific hydrological components of a catchment system, like the overall water balance, and vertical and temporal water redistribution (Yilmaz et al., 2008; Pokhrel et al., 2012). In this context, every signature measure is statistically evaluated, seeking to maintain balance in the hydrograph. All the mentioned information can be extracted using the FDC, which shows how often the discharge of a given magnitude is equalled or exceeded (Vogel and

Fennessey, 1994; Yilmaz et al., 2008; Yokoo and Sivapalan, 2011; Cheng et al., 2012, Pfannerstill et al., 2014a, Guse et al., 2016). The FDC can be segmented to assess different phases of the hydrograph separately (Yilmaz et al., 2008; Pokhrel et al., 2012; Pfannerstill et al., 2014a). A separate calibration with a specific FDC segment provides relevant information such as the response of the catchment to precipitation (Yadav et al., 2007) or to long dry periods. However, Yilmaz et al. (2008) mentioned the insensitivity of signature measures to the timing of events. In this way, Van Werkhoven et al. (2009) recommended combining both statistical performance metrics and signature measures to capture both dynamic and magnitude of the modelled output.

The importance of simultaneous assessment of very low and very high magnitudes of discharge was also indicated in other studies (e.g. Dunn, 1999; van Griensven and Bauwens, 2003; Laaha and Blöschl, 2007, Guse et al., 2016). Pfannerstill et al. (2014a) splits the FDC into five segments (5FDC) to enable a higher focus on very high and very low flow peaks. In their study, the five segments are evaluated separately by selecting the best runs of each segment as evaluated with the RMSE. By intersecting these runs, the final best runs for discharge according to all segments contain a good result for all discharge volumes.

In several studies, even with a multi-criteria calibration, just one single output variable is considered, which is in the majority of the cases discharge. Since different processes interact in the catchment, an adjustment of one process may lead to a worse performance in another. The more parameters and so processes are considered, the more complex are the interactions which have to be taken into account in the calibration process (Gupta et al., 1999, Boyle et al., 2000; Bekele and Nicklow, 2007). Considering the importance of hydrology processes face nitrate processes, nitrate calibration requires a multi-variable calibration of both discharge and nitrate. In this way, as for discharge, one or more performance measures are used to assess the performance of nitrate modelling (Santhi et al., 2001; van Griensven and Bauwens, 2003; Guse et al., 2015b; Jiang et al., 2015).

A novel approach in water quality modelling is to transfer the method of a calibration with the FDC to modelled nitrate loads by constructing the Nitrate Duration Curve (NDC). The NDC may assist us in the investigation of different nitrate conditions in the model simulations. The works of EPA (2007, 2008) addressed the construction and use of duration curves to water quality assessment. However, to our knowledge, the nitrograph has up to now not been included in the model calibration of nitrate.

Thus, the main objective of this study is an overall joined multi-metric and multi-variable calibration considering discharge and nitrate loads using statistical performance metrics and signature measures. The aim is to represent all phases of the hydrograph and nitrograph adequately in the same model run. In the study, the multi-metric approach is considered using classical statistical performance metrics in combination with different segments of the flow and nitrate duration curves as signature measures for the two variables to be calibrated.

3.2 Methods and materials

A general overview of the novel model calibration method for discharge and nitrate loads is provided step-wisely in Figure 3.1. All steps are explained in the following subsections. In step 1, 6000 model runs were carried out with the ecohydrological model Soil and Water Assessment Tool (SWAT, Arnold et al, 1998) to provide discharge and nitrate load time series. A core point of this study is the FDC construction and its transfer to NDC (step 2). For the five different segments of FDC and NDC, separate RSR was calculated following by the calculation of a mean statistical value of the segments for discharge and nitrate loads (MeanFDC and MeanNDC, respectively). In step 3, the KGE, as a typical statistical performance metric was calculated. The step 4 refers to the estimation of a best model run in a multi-metric calibration separately for discharge and nitrate loads. Finally, step 5 shows the junction of the performance measures for discharge and nitrate loads to a combined approach for both variables. All these performance measures were calculated for each of the 6000 model runs.

In this way, discharge and nitrate loads are intended to be reproduced as appropriately as possible. The different statistical performance metrics and signature measures for both variables were selected to represent the dynamic and also different magnitudes of discharge and nitrate loads equally. To achieve this, a new multi-metric and multi-variable model calibration was presented.

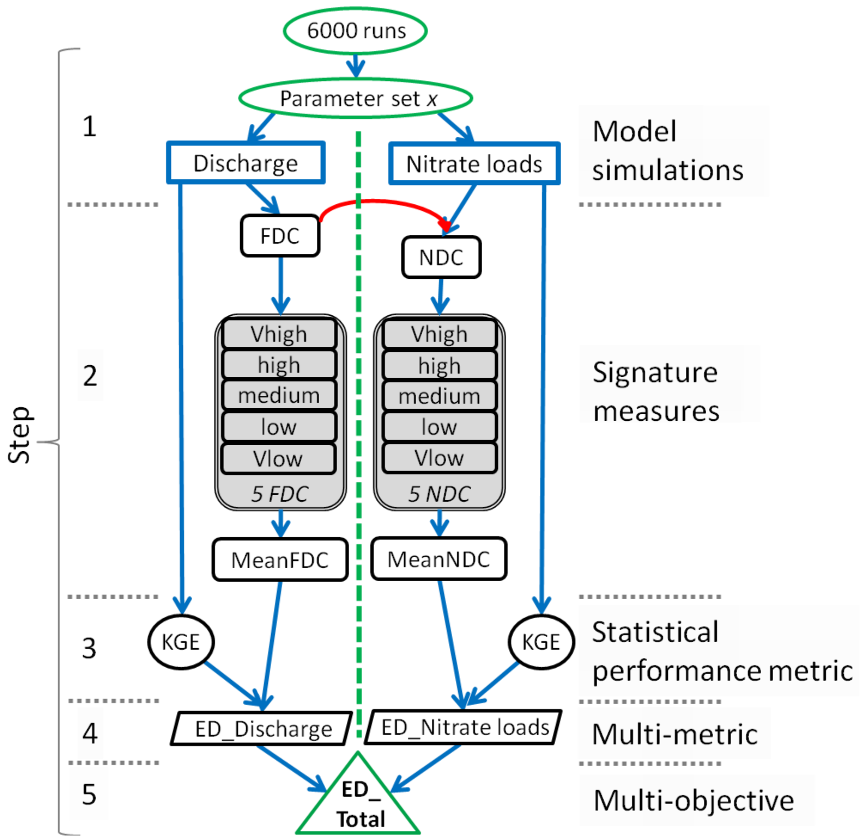

Figure 3.1: Methodological overview of the study.

3.2.1 SWAT model

The ecohydrological SWAT model (Arnold et al., 1998) was used in this study. It was already applied world widely for simulations of water, sediment and nutrient cycles in long-term daily resolution (Laurent and Ruelland, 2011; Du et al., 2013; Strauch et al., 2013; Guse et al., 2015b; Schmalz et al., 2015). Sub-basins are spatially defined and subdivided into smaller units, the hydrological response units (HRUs). The HRUs are based on the same land use, soil and slope classes and grouped within sub-basins.

The simulation of hydrological processes in the SWAT model is separated into land and routing (in water) phase. Firstly the water and nutrient cycles are calculated at the land phase in sub-basins. This phase is related to the total runoff and nutrients that flow into the main stream in each sub-basin. Afterwards the sub-basins are connected in the routing phase and water continues to be modelled throughout the catchment.

Since subsurface processes have a high complexity in lowlands, and seeking to improve the modelling of the nonlinearity dynamics of groundwater processes, Pfannerstill et al. (2014b) improved the groundwater structure of SWAT model by subdividing the shallow aquifer into a fast and a slow shallow aquifer. The modification improved the simulation of the groundwater dynamics and leads to a better representation of low flow periods (Pfannerstill et al., 2014b).

In the SWAT model, nitrate is modelled in the soil profile and in the shallow aquifer. According to Neitsch et al. (2011) nitrate can be added to the soil and removed from it in different ways. Furthermore, it can be transported in soil and groundwater. The majority of the nitrate parameters are related to processes occurring at the unsaturated soil zone. This is the case of nitrate input by rain and mineralization, nitrate losses via denitrification and plant uptake, and also nitrate transport by surface runoff and percolation. Likewise, there are parameters related to the saturated zone, regarding to nitrate concentration in the aquifer (see Haas et al. (2015) for an overview).

3.2.2 Simulation runs

For the multi-metric and multi-variable model calibration approach, 6000 model simulation runs were carried out with the SWAT model (see step 1 in Fig. 3.1). For this, 6000 parameter sets were generated by using the Latin Hypercube Sampling and the R-package FME (Soetaert and Petzoldt, 2010) in the R environment (R Core Team, 2013) as described in detailed in Pfannerstill et al. (2014a). This sampling method and number of parameter sets were chosen in order to capture the parameter space adequately.

Considering variations in precipitation and temperature in the modelling period between 2010 and 2014, the calibration period was chosen seeking to cover different climatic conditions across the whole period. The calibration period chosen for the simulation runs is composed of two parts, from September/2010-October/2011 (hydrological year 2011) and October/2012-October/2013. The time intervals from October/2012-October/2013 and October/2013-October/2014 were used as validation period.

The parameters shown in Table 3.1 were used for this calibration procedure. They were selected based on experiences with the new groundwater routine of $SWAT_{3S}$ model (see Pfannerstill et al., 2014a; Haas et al., 2015). Further description of the hydrologic and nitrate related parameters used in this study can be found in Neitsch et al. (2011), Guse et al. (2014) and Haas et al. (2015). The following analyses are based on the modelled discharge and nitrate load time series from the 6000 simulation runs.

Table 3.1: Parameter names and codes, and their minimum and maximum ranges as used for discharge and nitrate loads calibration:

	Parameter name	Code	Min	Max	Type
Hydrological processes	Initial SCS runoff curve number for moisture condition II	*CN2*	-10	10	Add
	Surface runoff lag coefficient	*SURLAG*	0.3	2.5	Range
	Soil evaporation compensation factor	*ESCO*	0.75	1	Range
	Plant uptake compensation factor	*EPCO*	0.3	0.9	Range
	Distance between two drain tubes or tiles (mm)	*SDRAIN*	15000	30000	Range
	Drain tile lag time (hrs)	*GDRAIN*	0.5	1.5	Range
	Multiplication factor to determine saturated hydraulic conductivity	*LATKSATF*	0.01	1.2	Range
	Groundwater delay time - fast shallow aquifer (days)	*GWDELAYfsh*	5	20	Range
	Deep aquifer percolation fraction - fast shallow aquifer	*RCHRGssh*	0.2	0.6	Range
	Baseflow alpha factor - slow shallow aquifer (1/day)	*ALPHABFssh*	0.001	0.08	Range
Nitrate processes	Concentration of nitrogen in rainfall	*RCN*	1.5	3	Range
	Nitrate percolation coefficient	*NPERCO*	0.6	1	Range
	Nitrogen uptake distribution parameter	*NUPDIS*	10	30	Range
	Rate factor for humus mineralization of active organic nitrogen	*CMN*	0.0003	0.003	Range
	Half-life of nitrate in shallow aquifer (days)	*HLIFESH*	5	250	Range
	Half-life of nitrate in deep aquifer (days)	*HLIFEDP*	350	800	Range
	Initial concentration of nitrate in deep aquifer (mg N/l or ppm)	*DEEPSTN*	30	60	Range

3.2.3 Multi-metric model calibration

The multi-metric model calibration involved initially the selection of signature measures and statistical performance metrics (see steps 2-3 in Fig. 3.1). The FDC represents the distribution of cumulative frequencies of river discharge magnitudes. It is a graphical representation of the relationship between discharge magnitudes and the percentage of time that this discharge is equalled or exceeded (Smakhtin, 2001). Displaying the total discharge ranges of a river from extreme low flows to flood events, all discharge magnitudes are highlighted in the FDC (Smakhtin, 2001; Laaha and Blöschl, 2007; Yilmaz et al., 2008; Pfannerstill et al., 2014a). Moreover, low flow may strongly influence the water quality too, in particular in lowland catchments (Schmalz et al., 2008).

In this study the FDC was used for the model calibration and its concept was transferred for the first time in model calibration to represent different magnitudes of nitrate loads, enabling the investigation of nitrate loads conditions in the same manner as discharge (step 2 in Fig. 3.1).

As shown in Pfannerstill et al. (2014a), the FDC was sectioned into five segments concerning distinct signature measures. The segments are based on the exceedance of very high flows (0-5%, Vhigh_Q), high flows (5-20%, high_Q), medium flows (20-70%, mid_Q), low flows (70-95%, low_Q) and very low flows (95-100%, Vlow_Q). Likewise, the NDC was sectioned into these five segments (5NDC), with the same intervals and also denominated Vhigh_NO3, high_NO3, mid_NO3, low_NO3 and Vlow_NO3, respectively. The higher detail in the segmentation of NDC will help to investigate in a balanced way the very low and very high phases of nitrate loads. With the 5FDC and 5NDC the same units for discharge and nitrate loads were generated.

The RSR was estimated for each of the five segments, for all 6000 model simulations seeking the best run. The RSR is a statistical performance metric related to the RMSE, but standardized via calculation of the ratio of RMSE and standard deviation of the measured data (Moriasi et al., 2007). The use of RSR is a difference to the methodology presented by Pfannerstill et al. (2014a), who used the RMSE. The RSR values of the different segments are better comparable than the RMSE which is higher for higher absolute values due to the quadratic term in its equation. The RSR was calculated separately for all five FDC and NDC segments for every run derived from the 6000 parameter sets.

After the calculation of the RSR for the five segments for each run, the mean of the RSR values for the five FDC segments was calculated for each model run and designed as MeanFDC, summarizing the performance in all segments. The RSR mean for the five NDC segments was also calculated for all runs (denoted as MeanNDC). The MeanFDC and MeanNDC were used in a following step, for the joint approach of multi-metric calibration. The KGE was applied as statistical performance metric (Gupta et al., 2009; step 3 in Fig. 3.1). The KGE is based on a decomposition of the NSE index into its three fundamental criteria, namely bias, correlation and variability, seeking a better model performance, since the three components are equally considered (Equation 1). To calculate the KGE, the Euclidean distance (ED) is calculated from the ideal point for all points. The three criteria (bias, correlation and variability) are distinguished in a direct tri-dimensional balanced evaluation. Subsequently, the point which has the shortest distance between optimal and ideal point is selected (Gupta et al., 2009). The optimal value for KGE is 1. For more details of the KGE applicability see Gupta et al. (2009).

Eq. 1:

$$KGE = 1 - \sqrt{(r-1)^2 + (\alpha-1)^2 + (\beta-1)^2}$$

with:

r = linear correlation between simulated and measured value x;

α = relative variability in the simulated and measured values *x* (standard deviation);

$\beta = \mu s / \mu o$ = bias (ratio between the mean simulated and mean observed variable).

In this study, the KGE for discharge (named as KGE_Q), for nitrate loads (named as KGE_NO3) and the KGE generated from the mean of KGE_Q and KGE_NO3 (named as KGE_Q_NO3) were calculated as statistical performance metrics.

3.2.4 Combined multi-metric calibration with KGE and 5FDC/5NDC

As a last step, a combined multi-metric calibration was carried out using the KGE as dynamic statistical performance metric and the MeanFDC and the MeanNDC as signature measures. This led to a selection of the best model runs based on ED between KGE and MeanFDC for discharge, and the KGE and MeanNDC for nitrate loads, respectively to their optimum value (shown in step 4 in Fig. 3.1).

The aim was to minimize the Euclidean distance to the optimum value of its performance measure in the same model run (KGE=1 and MeanFDC/MeanNDC=0, respectively). The ED seeks the best possible value for the run with minor distance from simulated to measured values regarding the mentioned performance measures. The ED for discharge (ED_Q), considering the KGE_Q and MeanFDC, and the ED for nitrate loads (ED_NO3), considering KGE_NO3 and MeanNDC, were firstly calculated separately.

3.2.5 Best runs selection of multi-variable model calibration

To summarize our approach for both variables, the multi-variable calibration consisted of a joint calibration of discharge and nitrate loads. The separate calculation of different statistical performance metrics and signature measures was followed by the combined evaluation. The goal was to select one model run which covers adequately both variables in all their magnitudes.

For this, the results of ED_Q and ED_NO3 were summed (Equation 2) and called ED_Total. Likewise, 6000 ED_Total values were generated for the final selection of the best model run (representing step 5 in Fig. 3.1).

Eq. 2:

$$ED_{Total} = ED_Q + ED_{NO3}$$

where ED_Q represents the Euclidean distance for discharge, ED_{NO3} represents the Euclidean distance for nitrate loads and ED_{Total} is the summed Euclidean distance.

Since different best runs could be observed according several performance measures for 5FDC, 5NDC, MeanNDC/MeanFDC, KGE and for ED, the best model simulations were selected to compare the results of different performance measures with the best run as selected with the proposed approach in this study. The presentation of these best models according to different performance measures, separately for discharge and nitrate loads, and of the joint metric ED_Total allowed a comparison under which hydrological conditions a specific performance measure leads to a good or poor performance. An overview of the used performance measures is given in Table 3.2, presenting statistical performance metrics and signature measures for discharge and nitrate loads and their application scope.

The novel performance measure ED_Total was compared with typical statistical performance metrics. For this, KGE_Q was selected as representative best run for a classical discharge calibration without considering nitrate, whilst KGE_Q_NO3 shows the best run for a joined calibration of discharge and nitrate loads using a classical approach with a statistical performance metric. In this analysis, discharge and nitrate load time series as well as FDC and NDC were constructed for the best runs according to these three performance measures and compared with the measured ones.

Table 3.2: Performance measures used in the study and application scope:

Performance Measure	**Name**	**Scope**
RSR	Ratio of root mean square error and standard deviation	Total time series
KGE_Q	Kling-Gupta Efficiency for discharge	Total discharge time series
KGE_NO3	Kling-Gupta Efficiency for nitrate loads	Total nitrate loads time series
KGE_Q_NO3	Kling-Gupta Efficiency Mean for discharge and nitrate loads	Total discharge and nitrate load series
Vhigh_Q	RSR of Very high flows	0-5% of flow exceedance
high_Q	RSR of high flows	5-20% of flow exceedance
mid_Q	RSR of medium flows	20-70% of flow exceedance
low_Q	RSR of low flows	70-95% of flow exceedance
Vlow_Q	RSR of very low flows	95-100¨% of flow exceedance
Vhigh_NO3	RSR of very high nitrate loads	0-5% of nitrate load exceedance
high_NO3	RSR of high nitrate loads	5-20% of nitrate load exceedance
mid_NO3	RSR of medium nitrate loads	20-70% of nitrate load exceedance
low_NO3	RSR of low nitrate loads	70-95% of nitrate load exceedance
Vlow_NO3	RSR of very low nitrate loads	95-100¨% of nitrate load exceedance
MeanFDC	Mean of RSR value for the five FDC segments	-
MeanNDC	Mean of RSR value for the five NDC segments	-
ED_Q	Euclidean Distance for discharge between optimal values for KGE_Q(1) and MeanFDC(0)	-
ED_NO3	Euclidean Distance for nitrate loads between optimal values for KGE_NO3 (1) and MeanNDC (0)	-
ED_Total	The sum of best ED_Q and best ED_NO3	-

3.3 Study area and model input data

To test the multi-metric and multi-variable calibration approach, the catchment of the river Treene was selected as study catchment. The Treene catchment is a lowland catchment (maximal altitude of 80 m.a.s.l.) of 481 km² (hydrological station Treia at the catchment outlet) located in northern Germany, near the Danish border. The land use in the catchment is predominantly agricultural, with only small areas covered by forests or urban areas. Agriculture has an important role regarding pollutants coming from manures and fertilizers applied to crops and pastures. Guse et al. (2015b) and Haas et al. (2015) emphasised the important role of nitrate in the catchment.

Another important characteristic of the study area as lowland catchment is the strong interaction between surface water and shallow aquifer, which leads in a significant presence of tile drainages (Fohrer et al., 2007; Kiesel et al., 2010, Pfannerstill et al., 2015) affecting water and nutrient dynamics. Further details about the study area are given in former studies (Guse et al., 2015a, b; Haas et al., 2015).

The major input data used for model simulations were provided by government agencies. They provided the digital elevation model with a resolution of 25 x 25 meters (LVermA, 1995), a land use map (ALK, LVermA, 2004) and a soil map with a spatial resolution of 1:200.000 (BÜK 200, BGR, 1999). The data regarding point source inputs from sewage plants were obtained from the State Bureau Schleswig-Flensburg and implemented as monthly average values. Regarding climate time series, daily values for precipitation, temperature (minimum and maximum), wind speed, relative humidity, and solar radiation were obtained from the German Weather Service (DWD) and the Potsdam Institute for Climate Impact Research. The discharge data series from 2010 to 2014 at the catchment outlet in Treia was provided by the Agency for Coastal Defence, National Park and Marine Conservation of Schleswig-Holstein (LKN-SH). The nutrient concentrations are available from our own continuous measurement campaign at the station Treia (30/09/2010-10/10/2014), based on daily mixed water sample collection by an automatic stationary sampler.

The SWAT model set-up for the Treene catchment consisted of the catchment delineation resulting in 108 sub-basins and in 4524 HRUs as presented in Guse et al. (2014) and Haas et al. (2015). The agricultural areas in the catchment were subdivided into five crop rotations to give a realistic spatial distribution (Kühling, 2011; Guse et al., 2015b). Also soil information is adapted to the region, based on previous studies from Dietrich (2010), Guse et al. (2014) and Kühling (2011). For further details of the SWAT model set-up for the Treene River, we refer to Haas et al. (2015).

3.4 Results

3.4.1 Comparison of model performance for different performance measures

Considering the model simulations with the 6000 parameter sets, Table 3.3 shows the distribution of performance measures in quantiles. The quality of the model performance varies between the different performance measures and between discharge and nitrate loads. For discharge, 75% of the runs have a performance for the KGE >= 0.84. For nitrate loads, on the other hand, the 75% quartile is >= 0.66 which is a lower value, but shows also the good performance in terms of KGE.

The signature measures distribution varies between the segments, displaying the need for separating the segments in the model calibration. In regard to discharge, the segments for very high (Vhigh), high, and mid flows generally perform well. In contrast, low and in particular very low (Vlow) flows show a worse performance. For MeanFDC, it is remarkable that the second quartile already reaches higher RSR values, driven by the poor performance of the majority of the model runs in low and Vlow segments. Similarly, the ED for discharge presents a high increase up to the first quartile.

For nitrate loads, the evaluation of the calculated performance measures is more complex. Here, both Vhigh and Vlow flows have a poor performance in the majority of the model results. Thus, it is required to consider the extreme nitrate loads separately. In contrast to discharge, the very low values are overall better represented in the case of nitrate. MeanFDC and MeanNDC are in the same order of magnitude. The increase of the RSR in ED_Total illustrates the difficulty to find parameter combinations, i.e. model simulations, which are able to represent both variables simultaneously.

Table 3.3: Distribution of the performance measures for the 6000 parameter sets:

Variable	**Q**								**NO3-N loads**								**ED_ Total**
Quantile	**KGE**	**Vhigh**	**high**	**mid**	**low**	**Vlow**	**Mean FDC**	**ED**	**KGE**	**Vhigh**	**high**	**mid**	**low**	**Vlow**	**Mean NDC**	**ED**	
		(RSR)								**(RSR)**							
0%	0.56	0.34	0.10	0.07	0.11	0.32	0.34	0.35	0.40	0.30	0.27	0.07	0.08	0.33	0.46	0.47	1.58
25%	0.84	0.61	0.24	0.37	1.14	3.96	1.30	1.30	0.66	1.04	0.45	0.42	0.71	0.91	0.96	0.99	3.11
50%	0.88	0.65	0.38	0.51	1.98	6.64	2.02	2.02	0.72	1.69	0.57	0.76	1.44	1.73	1.30	1.33	3.48
75%	0.90	0.72	0.61	0.69	3.06	8.58	2.69	2.70	0.78	2.33	0.76	1.16	2.67	3.13	1.82	1.85	3.87
100%	0.93	1.57	1.88	1.30	5.55	12.12	4.29	4.31	0.90	4.59	1.72	2.36	8.94	11.10	4.42	4.44	6.92

3.4.2 Selection of the best model runs for discharge and nitrate calibration

The best model runs according to the different performance measures shown in Table 3.2 are presented in Table 3.4. The best runs vary for the different performance measures. The best runs for discharge do not necessarily have a good performance for nitrate loads. For example, considering a good KGE for discharge (0.93), the KGE for nitrate loads is also plausible (0.70), but this model run does not have a good performance in terms of low and very low values.

The FDC segments values in Table 3.4 illustrate the trade-off between different signature measures. The best run for Vhigh_Q has a poor performance for Vlow_Q. Furthermore, also the RSR values for the NDC segments are worse. By looking on the best run for the very low nitrate loads segment (Vlow_NO3, RSR=0.33), the very high (Vhigh_NO3) and middle (mid_NO3) segments of the NDC in this model run are not satisfying.

Likewise, the best values of ED for discharge (ED_Q) will result in worse performance of nitrate loads (ED_NO3) and other way round. Still, observing all the best runs for MeanNDC, the values of MeanFDC are much worse. In contrast to selecting the best model runs with all other performance measures, the best model run for ED_Total serves good performance in discharge and nitrate loads at the same time. This means that all five segments of FDC and NDC present relative low RSR values and the KGE indices are also plausible for both variables. Compared to the other selected model runs (in Table 3.4), this model run leads to the overall best results of all performance measures.

By considering the KGE_Q_NO3 as a classic statistical performance metric comprising discharge and nitrate loads, the best run represents simultaneously both variables in a good way. However, the run shows inadequacies in the low and Vlow segments for both variables.

Table 3.4: Performance measures for the best model runs from the 6000 parameter sets, regarding discharge (Q) and nitrate loads (NO3-N loads). For KGE, the best value is 1 and for the other performance measures it is 0.

run	*Best for*	Q								NO3-N loads								KGE_ Q_ NO3	ED_ Total
		KGE	Vhigh	high	mid	low	Vlow	Mean FDC	ED	KGE	Vhigh	high	Mid	low	Vlow	Mean NDC	ED		
88	*KGE_Q*	**0.93**	0.58	0.27	0.14	0.37	0.49	0.37	0.38	0.70	1.30	0.42	1.10	4.68	5.44	2.59	2.61	0.82	2.98
1601	*Vhigh_Q*	0.87	**0.34**	0.58	0.90	1.15	4.08	1.41	1.42	0.74	1.81	0.55	1.11	2.55	3.30	1.86	1.88	0.81	3.30
2764	*high_Q*	0.89	0.71	**0.10**	0.13	0.66	3.92	1.10	1.11	0.68	1.67	0.47	0.95	4.96	7.56	3.12	3.14	0.79	4.25
190	*mid_Q*	0.91	0.76	0.19	**0.07**	0.36	2.72	0.82	0.83	0.70	2.37	0.67	0.14	1.35	2.70	1.45	1.48	0.81	2.30
40	*low_Q*	0.87	0.64	0.77	0.25	**0.11**	0.37	0.43	0.45	0.75	1.26	0.43	0.85	3.18	4.49	2.04	2.06	0.81	2.51
347	*Vlow_Q*	0.88	0.80	0.15	0.34	0.75	**0.32**	0.47	0.49	0.65	1.87	0.47	1.20	5.33	5.46	2.87	2.89	0.77	3.37
5790	*MeanFDC*	0.93	0.54	0.35	0.11	0.29	0.43	**0.34**	0.35	0.66	0.90	0.60	1.41	5.41	6.26	2.92	2.94	0.80	3.29
4563	*ED_Q*	0.92	0.54	0.34	0.26	0.12	0.45	0.34	**0.35**	0.66	1.36	0.47	1.42	5.19	6.11	2.91	2.93	0.79	3.28
5587	*KGE_NO3*	0.75	0.75	1.08	0.74	4.04	10.19	3.36	3.37	**0.90**	0.84	0.36	0.62	0.85	0.98	0.73	0.74	0.83	4.11
1222	*Vhigh_NO3*	0.91	0.57	0.27	0.45	2.24	7.39	2.18	2.19	0.69	**0.30**	0.69	1.50	2.52	2.12	1.42	1.46	0.80	3.64
843	*high_NO3*	0.86	0.62	0.71	0.36	2.25	7.05	2.20	2.20	0.88	1.00	**0.27**	0.27	0.18	0.99	0.54	0.55	0.87	2.76
1708	*mid_NO3*	0.91	0.66	0.34	0.52	1.47	5.96	1.79	1.79	0.68	2.69	0.82	**0.07**	0.19	1.00	0.95	1.01	0.80	2.80
1187	*low_NO3*	0.75	0.81	1.17	0.50	3.22	8.75	2.89	2.90	0.74	0.90	0.91	0.81	**0.08**	0.58	0.66	0.71	0.75	3.61
2517	*vlow_NO3*	0.85	0.60	0.55	0.72	3.51	9.40	2.96	2.96	0.78	1.66	0.53	1.06	0.50	**0.33**	0.82	0.85	0.82	3.81
2412	*MeanNDC*	0.81	0.67	0.88	0.51	3.10	8.55	2.74	2.75	0.88	0.53	0.44	0.49	0.41	0.43	**0.46**	0.47	0.85	3.22
2412	*ED_NO3*	0.81	0.67	0.88	0.51	3.10	8.55	2.74	2.75	0.88	0.53	0.44	0.49	0.41	0.43	0.46	**0.47**	0.85	3.22
2814	*KGE_Q_ NO3*	0.91	0.60	0.50	0.22	0.54	2.31	0.83	0.84	0.86	0.89	0.33	0.42	1.27	2.45	1.07	1.08	**0.89**	1.92
5735	*ED_Total*	0.78	0.71	1.17	0.48	0.84	0.69	0.78	0.81	0.87	0.69	0.40	0.41	0.29	2.04	0.77	0.78	0.83	**1.58**

3.4.3 Flow and Nitrate Duration Curve

Figure 3.2 shows the 5FDC (left column) and 5NDC (right column) obtained from the best runs regarding different performance measures in the calibration period. In order to clearly present the differences to the measured FDC and NDC, respectively, the duration curves are presented in form of the deviations between modelled and measured FDC and NDC. A positive value means here a higher value in the modelled time series.

Figure 3.2 shows that the best run for each segment presents a good agreement in its own segment and is not so appropriate for the others. For example, the best model run for Vhigh_Q shows a good performance for very high flows but a worse performance in the mid flow segment (Fig. 3.2, subplot A). The best run for Vlow_Q performs well from mid flows to very low flows, but overestimates high flows. All these model runs show a similar performance in terms of the NDC (Fig. 3.2B), with an increasing underestimation towards very high flows and an overestimation from mid flows to very low flows. In the case of MeanFDC (Fig. 3.2C, D), the best run shows a good performance for discharge in all segments, but not for nitrate loads.

The best runs for the five segments of NDC do not result in a good run for discharge (Fig. 3.2E). As for discharge, the best run for each segment of NDC is worse for the other segments in the case of nitrate loads (Fig. 3.2F). The best model run for Vhigh_NO3 shows a good performance, but it gets worse from the high segment and only improves slightly in the end for low nitrate loads. Conversely, the best run for Vlow_NO3 presents a good performance in the very low segment.

The fourth row is related to the MeanNDC and KGE_NO3, showing a good performance for nitrate loads but not for discharge (Fig. 3.2G). The subplot H shows a good and similar performance of the best runs for MeanNDC and KGE_NO3. The very high, and also the end of high until the second half of mid segments present greater differences in relation to measured curves.

The last row presents the runs ED_Q, ED_NO3 and ED_Total. Considering discharge (Fig. 3.2I), the ED_Total model run presents higher differences at very high and high flows in comparison to ED_Q and ED_NO3. However, these two last mentioned runs are not suitable for nitrate loads (Fig. 3.2J). The best run for ED_NO3 presents visually a plausible run for discharge in almost all periods, but the extremes of the curve are far from observed values. In this way, although the run ED_Q is visually better than the run ED_Total for discharge, and also the ED_NO3 is better than ED_Total for nitrate loads, the run ED_Total is at once plausible for both variables.

There is a general underestimation of the modelled discharge and nitrate loads in the Vhigh phase both for discharge and nitrate loads and for all best runs. However, going in the direction of low flows, there is greater agreement between measured and modelled values. The selected best run presents this mentioned behaviour too, but is more balanced in the distribution of the performance measures in all phases.

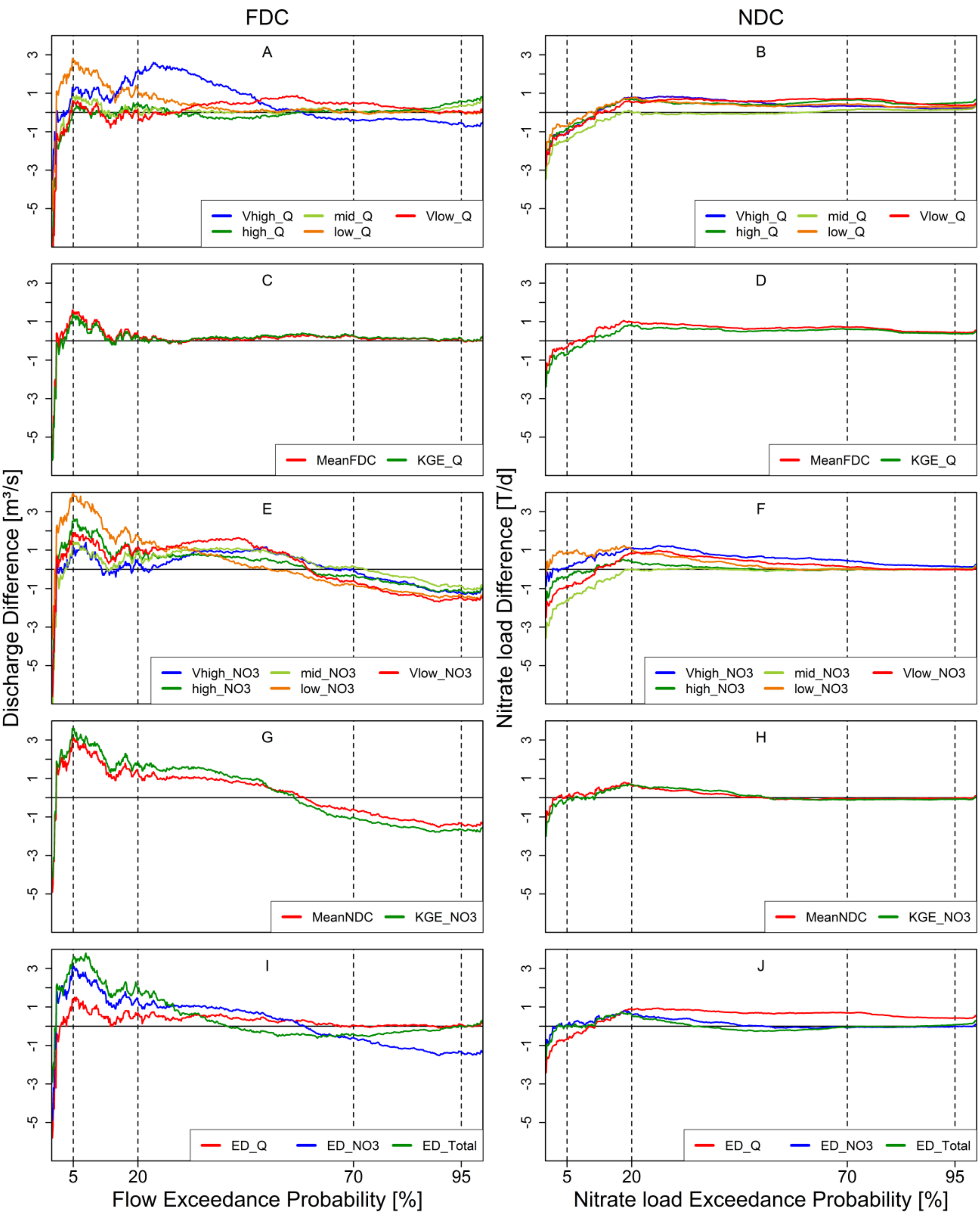

Figure 3.2: Differences between simulated and measured Flow Duration Curve (FDC, left column) and Nitrate Duration Curve (NDC, right column) for the best runs according different performance measures in the calibration period.

3.4.4 Best model run from the novel method and best runs from classical approaches

The selected parameter combination from ED_Total is compared with the best model runs according to KGE_Q and KGE_Q_NO3. As can be observed above (Table 3.4), discharge achieves a good simulation performance for these three runs. For this reason, ED_Total is compared with KGE_Q and KGE_Q_NO3 for the best runs according to all selected performance measures, which are depicted as bar plots (Fig. 3.3). Firstly, at left, are presented the three best runs when exclusively considering the traditional statistical performance metrics KGE (KGE_Q, KGE_NO3 and KGE_Q_NO3). For each of these runs, the KGE_Q, KGE_Q_NO3 and ED_Total values indicate a good simulation performance. The signature measures derived from FDC and NDC and also the ED values are presented on the right side (Fig. 3.3). KGE_Q particularly provides not so good results for nitrate loads, while KGE_Q_NO3 presents a worse performance in the Vlow_Q segment and thereby on the ED_Q. The ED_Total is more consistent for both variables leading to the best performance compared to KGE_Q and KGE_Q_NO3. Thus, the ED_Total run preserves lower RSR values in all five segments resulting in the best performance in the joined assessment.

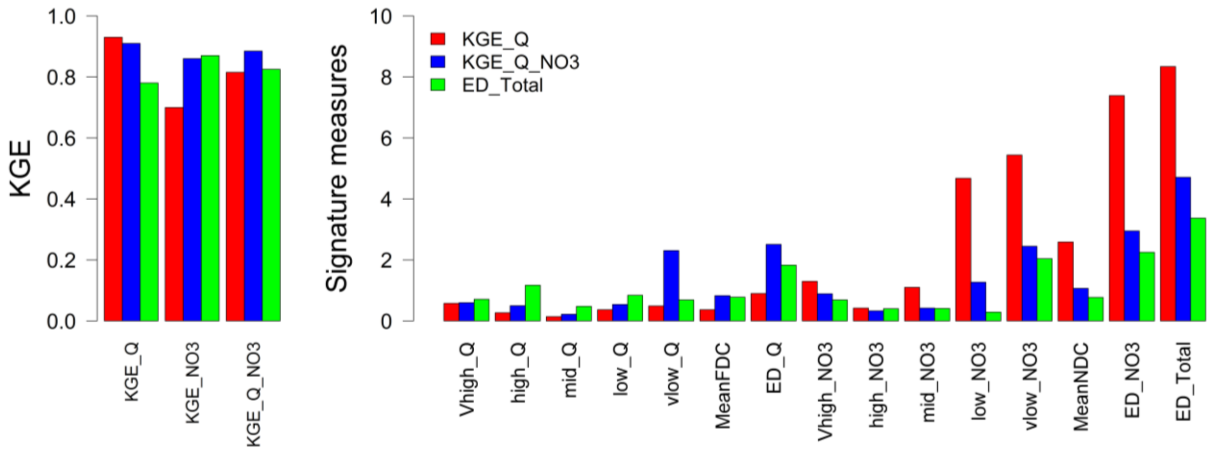

Figure 3.3: Comparison of best model runs for ED_Total, KGE_Q and KGE_Q_NO3.

3.4.5 Calibrated and validated discharge and nitrate loads

The results of this joint approach for the calibration period indicate a plausible simulation of the discharge and nitrate loads by the SWAT model. Table 3.5 shows that the KGE is good for discharge (0.78) and for nitrate loads (0.87), based on Moriasi et al. (2007). The performance measures of 5FDC and 5NDC segments for this period show a good matching between modelled and observed discharge and nitrate loads. Likewise, the visual inspection of ED_Total in Figures 3.2, 3.4 and 3.5 confirm the good performance of the selected best model run.

Table 3.5: Discharge and nitrate loads performance measures for calibration and validation periods for the best run implemented in the SWAT model.

Variable/Period \ Performance	KGE	Vhigh	high	mid	low	Vlow	Mean	ED
Discharge/Calibration	0.78	0.70	0.69	0.37	0.87	0.68	0.66	0.85
Discharge/Validation	0.94	0.30	0.18	0.23	0.66	0.97	0.47	1.08
Nitrate load/Calibration	0.87	0.71	0.32	0.33	0.48	2.02	0.77	0.90
Nitrate load/Validation	0.83	0.64	0.54	0.12	1.26	1.72	0.86	0.84

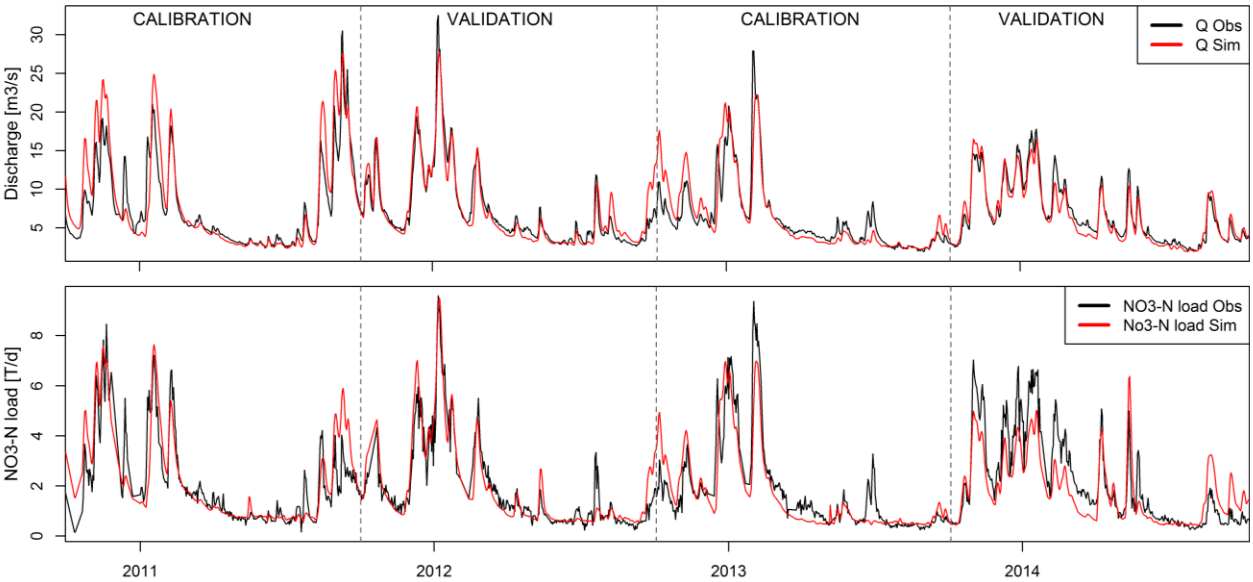

Figure 3.4: Discharge (top) and nitrate load time series (bottom) of the best model run defined by ED_Total for calibration and validation periods at Treia gauging.

For the validation period, the performance measures for discharge and nitrate load are also good. Discharge is particularly good with a KGE of 0.94 (Table 3.5). The performance for nitrate loads is also good in this period (0.83). In terms of 5FDC and 5NDC performances, the discharge has a slight improvement resulting in a better MeanFDC. Only the RSR value for the very low segment decreases. The MeanNDC is slightly higher in the validation period due to a lower performance in the high and low segments.

The visual inspection in Figure 3.4 permits to note that the simulated discharge and nitrate loads curve present good performances. The discharge presents a very good agreement between simulated and measured discharge. The nitrate loads curve presents more deficiencies related to some peaks in relation to measured values. Also the 5FDC and 5NDC in Figure 3.5 show a good agreement for the duration curves and dynamic behaviour in the validation period.

In this way, the model run supported by the KGE and the five segments of FDC and NDC evaluated by RSR together with the visual observation shows a plausible balanced performance for validation. Thus, the best run (ED_Total) as selected in the calibration and applied in the SWAT model simulates discharge and nitrate loads in a satisfactory manner also in the validation.

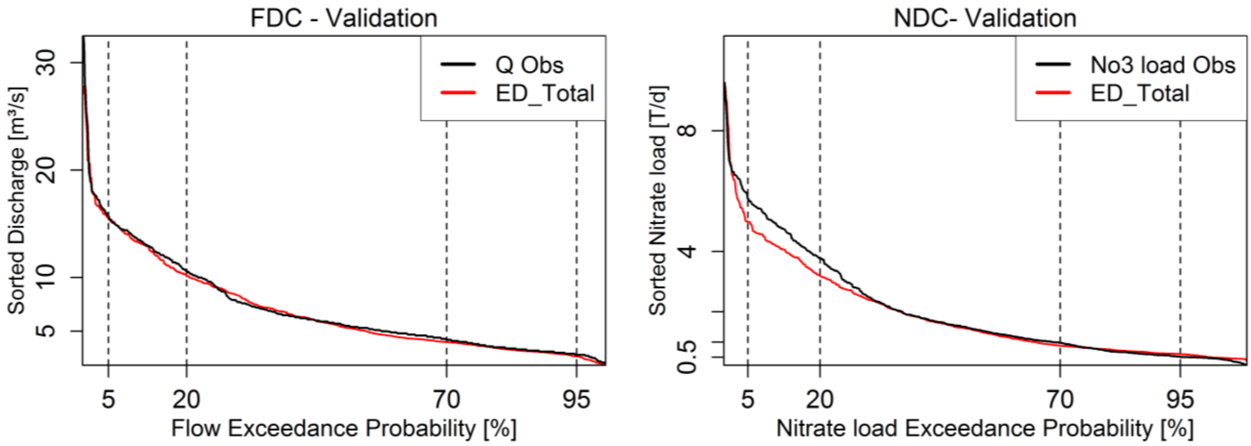

Figure 3.5: Flow and nitrate duration curves for the best run defined by ED_Total of the validation period.

3.5 Discussion

3.5.1 The transfer of 5FDC to 5NDC in model calibration

In this study, the 5FDC model calibration (Pfannerstill et al., 2014a) is transferred for the first time to nitrate loads (5NDC). In this way, the construction of nitrate duration curves and the separate calculation of an RSR for the five segments differ from other studies assessing water quality model calibrations only with statistical performance metrics. Thus, the presented multi-metric and multi-variable calibration approach permits a detailed investigation of different nitrate load magnitudes in addition to different discharge magnitudes resulting in a simultaneous assessment of discharge and nitrate load magnitudes. The 5FDC approach developed by Pfannerstill et al. (2014a) demonstrated the benefits of a more segmented, and consequently a more detailed assessment of the flow duration curve to obtain an overall good model performance. Likewise, the construction of 5NDC and thus a detailed investigation of the different magnitudes of nitrate loads are important in the same degree as shown in this study.

The calculation of the RSR for each of the five segments of FDC leads to a balanced consideration of discharge magnitudes in the model calibration. By assessing the RSR of the 5NDC individually, good model results are obtained along the magnitudes of modelled nitrate loads. A simultaneously good model simulation for discharge and nitrate loads is achieved by combining 5FDC and 5NDC together with statistical performance metrics.

Assessing the 5NDC may assist the investigations of nitrate loads related to precipitation events and catchment responses, and ongoing contribution of nitrate loads in periods without precipitation in a same way as highlighted for the FDC (Yilmaz et al., 2008, Cheng et al., 2012, Pokhrel et al., 2012, Yaeger et al., 2012). In regard to extreme conditions, for example, peaks of nutrient loads after precipitation and the behaviour of these loads in periods without precipitation are important issues. Smakhtin (2001) also mentioned the importance of low-flow studies regarding river ecosystem management, which emphasizes the water quality issue and further assessments. Thus, the joined calibration of 5FDC and 5NDC can be a tool to enhance water quality assessment, since it investigates different discharge and nutrient conditions in the catchment and in different seasons. It enhances the possibility of detailed calibration of modelled nitrate loads by assessing individually the different magnitudes for discharge and nitrate loads.

3.5.2 Trade-off between different performance measures and selection of the best run

The trade-off between optimum values of different statistical performance metrics and signature measures shows the difficulty to achieve an overall good model run and reinforce the need for a multi-metric calibration (Gupta et al., 1998; Van Werkhoven et al., 2009; Vrugt et al. 2003; Pokhrel et al. 2012). Considering the KGE, a high number of model runs shows good simulation results. However, analysing the signature measures displays a different result. When considering signature measures based on FDC and NDC jointly, less model runs provide a good performance. Thus, the importance of achieving the purpose of well distributed model simulations by using this approach with different performance measures is highlighted.

The selection of the best model run points out that different best runs can be selected according different performance measures. Beven (2006), Choi and Beven (2007) and Pechlivanidis et al. (2011) discussed the equifinality of model simulations, in which different parameter sets can lead to good model simulations. Madsen (2000) also mentioned the normally non-occurrence of a unique model covering all the targets of the investigation. Model uniqueness (Doherty and Johnston, 2003; Moore and Doherty, 2006, Yeh et al., 2015) aims at obtaining a unique best model simulation according to a specific goal, and the developed approach is singular in this sense, by considering a jointly balanced calibration with statistical performance metrics and signature measures. Based on Sincock et al. (2003) the present study is a way for a unique model search, since it uses a multi-metric calibration which considers more extensive data information. In this way, as observed in the present study, if details of dynamics and processes are examined, less model runs will be suitable.

In this approach, the results show that each performance measure has its strengths and weaknesses, which could be demonstrated in Figure 3.2. The KGE is used to evaluate the discharge and nitrate load dynamics, while 5FDC/5NDC signature measures are selected for a greater coverage and detailed consideration of different magnitudes of discharge and nitrate loads. The five segments of FDC and NDC allow an individual assessment of each phase of the hydrograph and nitrograph by the RSR values.

Following on the separated calculations for discharge (KGE_Q, MeanFDC and ED_Q) and for nitrate loads (KGE_NO3, MeanNDC and ED_NO3), the ED_Total is provided as overall balanced performance measure. By minimizing its value, the best ED_Total model run shows a balanced result of different statistical performance metrics and signature measures leading to an overall good calibration.

The comparison of the best model simulations according KGE_Q, KGE_Q_NO3 with the run ED_Total also demonstrates the before mentioned trends. ED_Total run show good KGE values for both variables, but they are not as good as the values of KGE_Q and KGE_Q_NO3. However, even though discharge is generally good simulated by the cited two model runs, KGE_Q shows a poor simulation of nitrate loads and KGE_Q_NO3 does not present the same performance quality in all segments for discharge and nitrate loads. Thus, the selection of this multi-metric method based on the ED_Total for a simultaneous multi-variable calibration proves to be a way to obtain a balanced modelled time series of both discharge and nitrate loads by considering the 5FDC/5NDC approach together with KGE as a classical statistical performance metric.

The presented methodical approach leads to a model run that has a good performance in all segments and for all performance measures considered. Furthermore, the comparison of the different performance measures clearly demonstrates the weakest points of each selected model run. Thus, the strength and weaknesses of each performance measure are demonstrated.

3.5.3 Calibrated and validated discharge and nitrate loads

As observed in Table 3.5 and in Figures 3.2 to 3.5, a plausible jointly multi-variable calibration approach is achieved. The performance measures for discharge and nitrate loads in the simulations are good during calibration and validation periods. There is a balance in terms of performance measures and also a good simulation by visually inspecting both the periods and variables.

Observing the five FDC/NDC segments in Figures 3.2 and 3.5, the low and Vlow phases present a good simulation of discharge and nitrate loads. This can be explained by the use of the modified $SWAT_{3S}$ model (Pfannerstill et al., 2014b), with the development of a modification in the groundwater structure of the model. The FDC of the validation period shows a decrease in the simulation quality only in the very low phase in comparison to calibration period. With the NDC, the results are worse in validation period for two segments, namely the high and low phases.

By a visual inspection of the discharge and nitrate curves, it is notable that the deficiencies in some peak events for nitrate loads need to be reviewed more thoroughly, since this phase is very important in water quality studies. Normally, higher uncertainties may arise in the nitrate simulations in comparison to discharge, due yearly variability in crops, fertilizer application timings and rates, extreme precipitation or drought events, and also a combination of some of these. Such exceptional events, if not covered by the model simulations, lead to uncertainties. The studies of Hesse et al. (2008) and Glavan et al. (2011), for example, support these susceptible influences on nitrate processes. Also the study of Williams et al. (2015) showed the complexity arising with drain tiles presence in catchment simulations, which could be the case of our study area since it presents many tiles.

According to Bekele and Nicklow (2007), the calibration of a SWAT model as a semi-distributed model with huge amount of different parameters is complex, principally when considering two variables simultaneously. Beyond that, a multi-variable calibration makes the task more difficult since there are different parameters, and so many interdependent processes (Gupta et al., 1999). Furthermore, parallel to hydrology simulation, a good nitrate simulation in water quality modelling is important for improvement of the nutrient processes understanding. In this case study, the ecohydrological model SWAT can represent both hydrological and nutrient processes satisfactorily with the proposed multi-variable and multi-metric calibration.

3.6 Conclusion

This joint multi-metric and multi-variable calibration procedure for discharge and nitrate loads is based on the use of the KGE and the 5FDC as well as a new idea, the 5NDC approach. To test this calibration method, the ecohydrological model SWAT is used in the Treene river catchment. In this context, the following major results can be pointed out:

The 5FDC concept for model calibration is transferred for the first time to nitrate (5NDC).

The 5NDC enhances the possibility of detailed investigation of nitrate loads by assessing individually their different magnitudes. A balanced model run regarding statistical performance metrics and signature measures is selected.

The results of this joint multi-metric and multi-variable calibration approach are plausible with objective consideration of the best model simulation. The selected model is able to simulate simultaneously in a balanced form both discharge and nitrate loads for all magnitudes.

Likewise, this model calibration method is, in general, applicable in all catchments and should be further tested in other catchments and with other ecohydrological models. The presented method contributes to achieve higher confidence in the selection of good model runs within the model calibration as a basis for future applications of models in environmental and water quality studies.

3.7 Acknowledgements

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4 Assessing the impacts of Best Management Practices on nitrate pollution in an agricultural dominated lowland catchment considering environmental protection versus economic development

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Abstract

Water quality is strongly affected by nitrate inputs in agricultural catchments. Alternative practices aim to mitigate the impacts derived from agricultural activities and to improve water quality. Best Management Practices (BMPs) apprehend this intention and are worldwide used to reduce nitrate pollution in rural areas. Management activities are influenced by contrasting governmental policies like the Water Framework Directive (WFD) and the Renewable Energy Sources Act (EEG). Their distinct goals can hamper an integrated sustainable development. Both need to be considered in the actual conjuncture in rural areas and a way is due Integrated Water Resources Management (IWRM). Ecohydrological models like the SWAT model are important tools for land cover and land use changes investigation and the assessment of BMPs implementation effects on water quality.

Thus, in this study, different BMPs were implemented in the SWAT model for the Treene catchment investigating their efficiency in terms of nitrate loads reduction and implementation costs at the catchment scale. Buffer strip, fertilization reduction, alternative crops and also the end of pipe solutions were considered as BMPs. The practices correspond to the catchment conditions and are based on small and mid areal changes. Furthermore, the BMPs were evaluated from the perspective of ecologic and economic policies. The results evidenced different responses of the BMPs at the catchment scale. The critical periods were addressed by the most BMPs and there is a great nitrate reduction potential for a combination of BMPs. Furthermore, spatial and temporal scales showed importance in BMP investigations for better approaches. The discussion about efficiency showed the complexity of costs stipulation and the relation with arable land and yield losses. Furthermore, as the government policies can be

divergent an integrated approach considering all the involved actors is important and seeks a sustainable development.

4.1 Introduction

Water quality is strongly affected by land cover and land use. In this aspect, agriculture has been greatly responsible for water quality degradation over the last decades (Aouissi et al., 2014; Glavan et al., 2013b; Lam et al., 2011; Laurent and Ruelland, 2011; Ruidisch et al., 2013; Strauch et al., 2013). The assessment of agricultural activities contribution to pollution is complex due to the generation of nonpoint pollution sources (León et al., 2000; Liu et al., 2013; Mostaghimi et al., 1997; O'Shea and Wade, 2009). In this regard, studying pollution from agriculture requires elaborated approaches and is still a challenge (Behera and Panda, 2006; Liu et al., 2013; Tuppad et al., 2010; Ullrich and Volk, 2009).

River catchments are naturally bounded spatial units, in which complex interacting processes occur, influencing rivers water and converge at the outlet. Due the integrated value of discharge, one can use the catchment water courses (and, more specifically outlets) as monitoring points of ecological conditions (hydrology, biology and chemistry) in the catchment. Lowland catchments have attributes which uniquely influence the natural processes. They are characterized by flat topography, high subsurface water table and so a greater, faster interaction of surface and ground water (Hesse et al., 2008; Kiesel et al., 2010; Schmalz et al., 2007). These properties also influence nutrient dynamics (Lam et al., 2011; Schmalz et al., 2007; Wriedt and Rode, 2006). Commonly drainages tiles are implemented in lowland arable lands to better control moisture conditions (Kiesel et al., 2010). Therefore, drainages are an extra challenge for water quality investigation in agricultural areas since they affect and modify natural dynamics of water and nutrients in soil (Fang et al., 2012; Jaynes, 2013).

Nitrate is one of the most abundant pollutants in water of rural areas, coming specifically from chemical and organic fertilization for crops (Almasri and Kaluarachchi, 2007; Beaudoin et al., 2005; Bonton et al., 2011; Garnier et al., 2014). It is an important nutrient for plants, vital for their growth and development (Kunrath et al., 2015; Saiz-Fernández et al., 2015). However, an excessive presence of nitrate in soil and water leads to environmental and human health problems (Anderson et al., 2014; Arheimer and Liden, 2000; Askegaard et al., 2011; Bonton et al., 2011; Bouraoui and Grizzetti, 2008; Ferrant et al., 2013).

Faced with the problem of large nitrate contamination of water resources, many policies were developed. These initiatives are organized in different governmental levels. Inside the Europe Union (EU) the Nitrate Directive from 1991 (Council Directive 91/676/EEC, 1991) regulated the amounts and periods for nitrate application under fertilization or manure form. Later, in a broader spectrum but also considering nitrate, the Water Framework Directive (WFD, (Directive 2000/60/EC, 2000) enters into force. It attempted to achieve a good ecological and chemical status for all water bodies by the year 2015. Despite the initiatives, Germany did not achieve the expected results until 2015. In April 2016 Germany was sued by the European Commission by the lack of initiatives for nitrate pollution reduction according to the WFD. The report of the German federal state Schleswig-Holstein in 2014 showed that many water bodies did not achieved a good ecological status. Inside the state, the predominantly agricultural catchment of the river Treene is an example for the problem of nitrate pollution.

In Germany, in parallel with the WFD the Renewable Energy Sources Act (EEG, Federal Ministry for Economic Affairs and Energy, 2014) was delivered. The legislation is in accordance with the EU policy for Renewable Energy Directive (Directive 2009/28/EC, 2009) and establishes higher utilization of renewable energies in the country and regulates their uses. It creates incentives for increased utilization of bioenergy crops. This perspective may lead to a greater pressure on the environment, resulting in negative impacts due higher fertilization rates or monocultures, for example.

Thus, on the one side there is a policy seeking a return to a good ecological status of water resources, and on the other side, a policy which indirectly stimulates on land use intensification. This situation creates in the last years a conflict of goals between two spheres, the economic development and environmental protection. This dichotomy between ecology and economy creates a detachment between two important concerns that need to be considered and managed.

With such a diverse presence of interests for land uses, that strongly affect water quality, there is a need of approaches to prevent or reduce environment pollution. The subject of water quality and nonpoint pollution sources has led to many studies and attempted solutions; one of these are the Best Management Practices – BMPs (Arabi et al., 2006a; Chaubey et al., 2010; Chen et al., 2015; Mostaghimi et al., 1997; Qi and Altinakar, 2011). The implementation of BMPs is an approach with actions for control and reduce the sources of sediments and nutrients degrading water quality in relation to current activities (Cerro et al., 2014; Laurent and Ruelland, 2011; Strauch et al., 2013; Tuppad et al., 2010). The BMP approach can provide management alternatives to achieve better ecological conditions keeping the agricultural activities. Thus, they are measures that look for several prevention or mitigation forms of negative impact to the environment, reconciling economic development and environmental protection.

An Integrated Water Resources Management (IWRM) is a modern helpful instrument in land use planning used in the context of water quality improvement at catchment scale (Giri and

Nejadhashemi, 2014; Hu et al., 2014; Qi and Altinakar, 2011). The concept of IWRM was developed in an international level by the United Nations (FAO, 2004) in the last years. The BMPs are closely linked to IWRM since they are related to mitigation or conservation practices, and involve different actors across different sectors of society. In this way, as a tool for cooperative approach for water quality issues, IWRM is also a foundation in the WFD implementation (Panagopoulos et al., 2011). So, as both WFD and EEG are currently operative, it is needed to assess their effects on the environment, here specifically the water quality in regard of nitrate, in an integrated way.

Water quality models are important tools for the investigation of environmental processes, principally in the catchment scale (Bärlund et al., 2007; Cerro et al., 2014; Panagopoulos et al., 2011; Strauch et al., 2013). In this way, complex ecohydrological models are of great importance in studies regarding the understanding of nutrient dynamics (Haas et al., 2015), pollution mitigation and future scenarios (Cerro et al., 2014; Guse et al., 2015b; Ullrich and Volk, 2009). Thus, models addressing water quantity and quality are widely used to simulate BMPs for environment pollution minimization and investigation of better natural resources use.

In order to obtain reliable scenario simulations, an accurate representation of the discharge and the nutrient dynamics is required. This is based on a good understanding of these processes both in the catchments and in models (Gupta et al., 2009). To achieve this, it is required to identify the driving elements of nutrient dynamics and the controlling factors in models such as demonstrated by (Haas et al., 2015) in deriving the dominant model parameters to nitrate loads. A good reproduction of the nutrient dynamics can be considered by evaluating models using different contrasting performance measures capturing different parts of magnitude and dynamics in nutrients as proposed recently in Haas et al. (2016) using a method developed by (Pfannerstill et al., 2014a).

The Soil and Water Assessment Tool (SWAT, Arnold et al., 1998) has been applied for a wide range of environmental conditions across the globe to predict flow, sediment and nutrient loads from catchments of various sizes (Aouissi et al., 2014; Bieger et al., 2014; Cerro et al., 2014; Haas et al., 2016; Niraula et al., 2013; Strauch et al., 2013; Ullrich and Volk, 2009). Likewise, numerous studies have used the SWAT model to evaluate the impact of BMPs on water quality at catchment scale (Arabi et al., 2006a; Bracmort et al., 2006; Cerro et al., 2014; Dechmi and Skhiri, 2013; Glavan et al., 2013a, 2011; Lam et al., 2011; Laurent and Ruelland, 2011; Panagopoulos et al., 2011; Tuppad et al., 2010). The SWAT model proved to be a good ecohydrological tool for the investigation and assessment of these management practices and nitrate dynamics, as was also shown for nitrate (Haas et al., 2015).

In this way, by applying the SWAT model the results in potential reduction of nitrate pollution for different initiatives (BMPs) can be investigated. Even small land use and cover changes in the catchment need to be investigated for assess the BMPs effects, since this is sometimes the possibility for the farmers. The assessment can be done according to different land use trajectories and interests, as the dual situation on ecology and economy created by distinct policies in different institutional levels. These contexts of actual and possible scenarios investigation in water quality is the basement of IWRM actions at catchment scale.

Likewise, the nutrient dynamics occurring under different agricultural activities can be investigated with model simulations. For this, it is also required to represent the discharge and nitrate conditions at the catchment under study. Following, based on this introduction, the main objectives of this study are:

To assess to which extent regional adapted agricultural BMPs, with small and medium- change proportions, lead to a reduction on the nitrate pollution at the catchment scale;

To evaluate the nitrate reduction and the costs of agricultural BMPs jointly in the context of two government policies having contrasting goals;

Based on these main objectives, the approach also aims to discuss the contribution possibilities of BMPs to the IWRM. Likewise, the approach can contribute to improve the understanding of nitrate dynamics and water quality regarding agricultural catchments.

4.2 Materials and methods

The study is based on the following approach in Figure 4.1. At first, an ecohydrological model is set-up and calibrated for a lowland catchment. Following on this, individual BMPs are implemented in the model and their impacts on nutrients are investigated using model simulations. The results of model simulations are assessed based on two contrasting criteria, i.e. nitrate loads reduction and costs of implementation. Furthermore, all simulated BMPs are evaluated face to two different realities, namely ecology and economy, and their contributions for integrated watershed management programs.

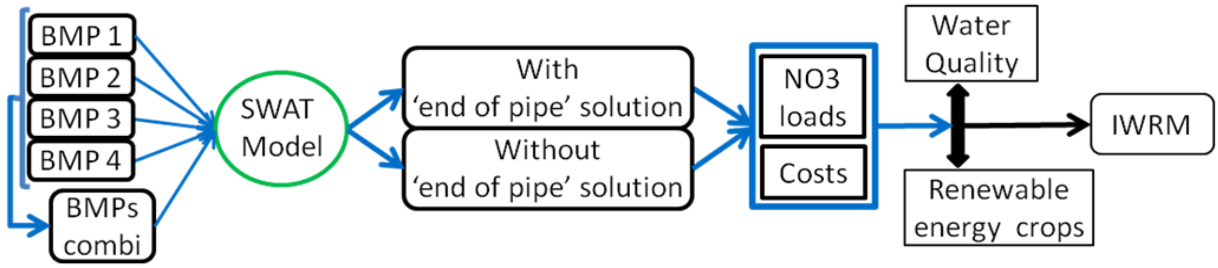

Figure 4.1: Flowchart of study approach.

4.2.1 Study area

The study was carried out in the catchment of the river Treene (Fig. 4.2), which has a size of 481 km² (hydrological station Treia at the catchment outlet). The catchment can be viewed as a medium to large catchment and is located in the lowlands of northern Germany, near the Danish border, with altitudes only up to 80 meters (m) above sea level. The average rainfall for the catchment is about 884 mm/year (station Schleswig, 1981-2011). The northeast of the catchment is characterized by a slightly undulating terrain with smooth slopes and, in general, clay and sandy soils. This is part of the geomorphologic unit Östliche Hügelland. The south-west part presents flatter areas and more sandy soils (LLUR-SH, 2006), as part of the Geest unit.

The land use in the catchment is predominantly agricultural (Fig. 4.2, LVermA, 2004). About 48% is covered by agricultural areas and 31% by pastures. Only a small part of the catchment is covered by forests (7%) or urban areas (10%). As an important issue in the catchment, the nitrate loads at Treia presented a daily mean of 2 tons (t/d) from the measured data for the period of 9/2010-10/2014. Winter period (including fall and winter) presented around 3 t/d nitrate loads while summer period (comprising spring and summer) presented around 1 t/d.

The strong interaction between surface and shallow aquifer in a lowland catchment results in a significant presence of tile drainages (Kiesel et al., 2010; Schmalz and Fohrer, 2009). Further details about the study area are given in former studies (Guse et al., 2014; Haas et al., 2015).

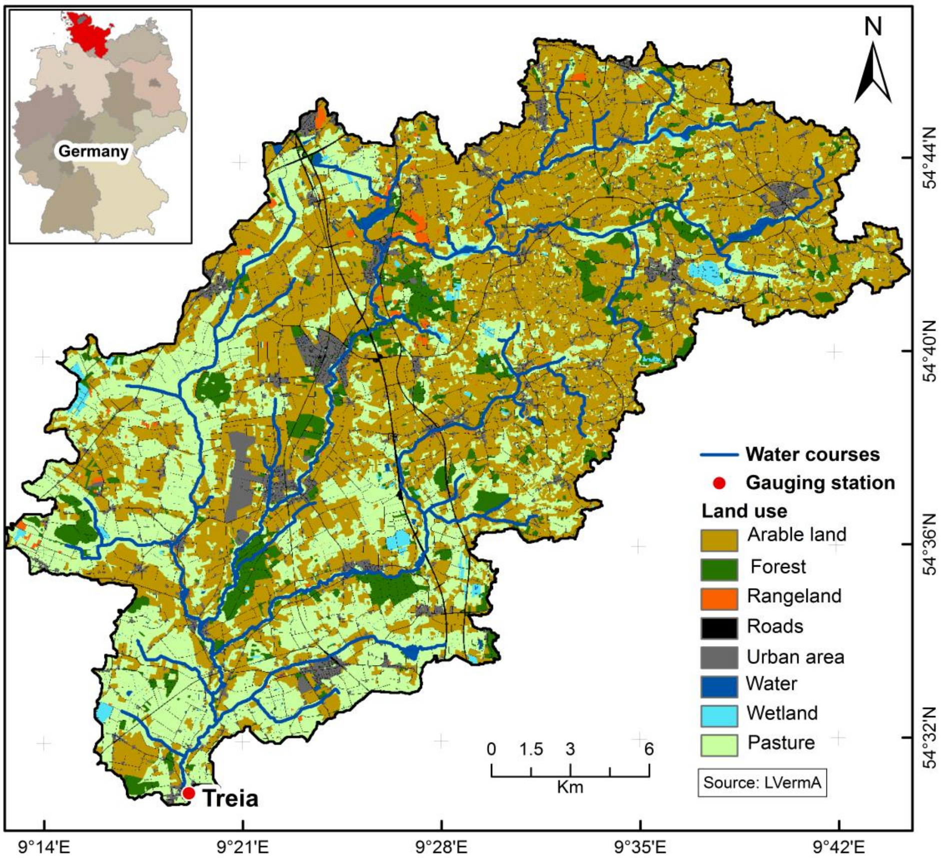

Figure 4.2: Treene catchment with land cover and land uses.

4.2.2 SWAT model

The ecohydrological model SWAT (Arnold et al., 1998) is based on watershed and continuous-time scale operations. It is a physically-based and semi-distributed model which simulates hydrological and nutrient cycles in a daily time resolution. As model input climatic variables are required such as daily precipitation, maximum/minimum air temperature, solar radiation, wind speed and relative humidity. An important ability of the SWAT model is the simulation of different land management processes using different crop rotations and allowing a dynamic update of land use information (Guse et al., 2015b; Pai and Saraswat, 2011; Wagner et al., 2016).

The spatial differentiation of the SWAT model is firstly based on the catchment division into sub-basins. Further, Hydrologic Response Units (HRUs) are derived, which are homogenous in land use, soils and slope areas. The processes are simulated initially for each HRU and after aggregated for the sub-basin simulation. The water from the different flow paths are summarized for each sub basin and connected to the reach. Although not being spatially located, the HRUs apprehend specific features of the catchment that are important in the processes characterization. Thus, there is valid considering them as analysis units.

To improve the process dynamics in lowland catchments, Pfannerstill et al. (2014b) modified the groundwater structure of the SWAT model to enhance nonlinear dynamics of groundwater processes ($SWAT_{3S}$). For this, the shallow aquifer was separated into a fast and a slow shallow aquifer. These modifications improve the simulation of the groundwater dynamics from one shallow aquifer to another, and thus, the dynamics with the river channel and the deep aquifer, as shown in (Pfannerstill et al., 2014b).

Nutrient simulation is also an important point of the SWAT model and was successively realized with $SWAT_{3S}$ (Haas et al., 2016). Nitrate is modeled in the soil profile and in the shallow aquifer. In these spaces, the model simulates a complete nitrate cycle and takes changes in the chemistry of the cycle into account, including processes summarized under mineralization, decomposition and immobilization. Furthermore, nitrate transport processes occur in soil and groundwater. Haas et al. (2015) investigated the nitrate dynamics in the SWAT model using the temporal dynamics of parameter sensitivity (TEDPAS, Guse et al., 2014; Reusser et al., 2011). The study showed the high temporal variability of the parameter sensitivity associated to nitrate transport on surface, shallow and groundwater runoff and also to the plant uptake periods.

Agricultural activities are also included intensively in the SWAT model. This includes dynamics regarding since soil characteristics, seeding, tillage, fertilization from plant growing, grazing and harvesting. With the Land Use Update (LUP) tool is it possible to make updates in the distribution of land uses in each HRU during the model simulations. This enables the considerations of changes in land uses over the simulated years in the model (Guse et al., 2015b). Given the mentioned characteristics, the SWAT model is suitable for the simulation and assessment of approaches like BMPs. It simulates the agricultural activities and the interchanges of plants with soil-water-air system. The SWAT model allows assessing the impact of fertilization reduction on crop yields and crop growth as well as on hydrological variables such as actual evapotranspiration or surface runoff. Furthermore, it can be assessed how much nitrate is stored in the soil as a comparable value between scenarios. In this way, the model has been word widely applied for studies regarding alternative management and land uses (Arabi et al., 2006a; Chiang et al., 2012; Jiang et al., 2014; Lam et al., 2011; Laurent and Ruelland, 2011; Strauch et al., 2013).

4.2.3 Model setup and data input

The SWAT model set up for the Treene catchment was based on the earlier studies of Guse et al. (2014) and Haas et al. (2016, 2015). It consisted of the catchment delineation in 108 sub-basins and in 4524 HRUs. The agricultural areas subdivision was made into different crop rotations based on an actual distribution of the crops, based on Guse et al. (2015b) and Kühling (2011). For further details of the SWAT model set-up for the Treene catchment, we refer to Haas et al. (2015).

Regarding the baseline crop rotations and management practices, six real agricultural activities were implemented in the SWAT model, as proposed in Guse et al. (2015b). They are based on silage corn and winter wheat monocultures, pasture areas as well as on 3-year crop rotations (silage corn-winter pasture-winter pasture, silage corn-silage corn-rye and winter wheat-winter barley-rape). The yearly elemental nitrogen average applied to each crop (in KgN/ha), also including the contribution of manure, is shown in Table 4.1. The applied fertilizer rates are distributed in time within the crop growth period. Furthermore, fertilizer quantities are in accordance to the current guidelines for fertilization of the state of Schleswig-Holstein (Landwirtschaftskammer Schleswig Holstein, 2011).

Table 4.1: Average nitrogen (N) applied to each crop at the Treene catchment.

Crop	N applied (kg/ha/year)
Silage corn	180
Winter wheat	225
Winter barley	170
Rye	160
Rape	200
Pasture (organic soils)	100
Pasture (mineral soils)	180

Major data input for the SWAT model set up is obtained by governmental agencies, like topography (Digital elevation model – 25x25m, (LVermA, 1995), soil information (1:200.000, (BGR, 1999) and land use (25x25m, (LVermA, 2004). Daily values of precipitation, temperature (min. and max.), wind speed and relative humidity for four climate stations are used as available from the German Weather Service (DWD) for the modeling period. Daily values of solar radiation are provided from DWD and interpolated by Potsdam Institute for Climate Impact Research (PIK). Likewise, the information for the land use updates as considered in the simulations were taken from statistical data (Statistikamt Nord), namely spatial distribution of land use in the years 2007 and 2010 (see for details on this approach: (Guse et al., 2015a, 2015b).

4.2.4 Model calibration and validation

The SWAT model was calibrated and validated based on the previous study of (Haas et al., 2016). A joint multi-metric and multi-variable calibration approach for discharge and nitrate loads was carried out. The procedure was based on classical statistical performance metrics (KGE, Kling-Gupta efficiency, Gupta et al., 2009) and on signature measures (flow and nitrate duration curves – FDC and NDC). The duration curves are divided in five segments and their evaluation consists on the separated assessment of all five segments with the RSR index (Ratio of RMSE [Root Mean Square Error] and standard deviation). This approach resulted in the joint and broad consideration of the dynamics and magnitudes of discharge and nitrate.

The discharge data series from 2010 to 2014 at the catchment outlet in Treia used for calibration and validation was provided by the Agency for Coastal Defense, National Park and Marine Conservation of Schleswig-Holstein (LKN-SH). The nutrient concentrations are available from our own continuous measurement campaign at the station Treia (30/09/2010-10/10/2014), based on daily mixed water sample collection by an automatic stationary sampler. In this way, based on the nitrate data availability, the period for calibration and validation were constituted of two time series. The calibration apprehends the period from September/2010-October/2011 and October/2012-October/2013. The period from October/2011-October/2012 and October/2013-October/2014 was used for validate the simulation results. Both the calibration and validation periods contained one year with more and one year with less precipitation. Considering climatic variations in precipitation and temperatures between 2010 and 2014, the calibration procedure covers different conditions across the whole time period to have plausible results for the BMPs simulation.

4.2.5 Best Management Practices

Best Management Practices (BMPs) can be a useful strategy to mitigate nonpoint source pollution resulting from agricultural activities (Arabi et al., 2006b, 2004; Bouraoui and Grizzetti, 2014; Laurent and Ruelland, 2011). They have been widely used for the abatement of diffuse pollution through sediment and nutrient transport reductions (Jiang et al., 2014; Laurent and Ruelland, 2011; Parajuli et al., 2008). BMPs investigation can also assist the assessment of critical source areas within a catchment, as pointed by (Mostaghimi et al., 1997) and (Giri and Nejadhashemi, 2014).

Several spatial particularities will influence differently the benefits of each BMP to water quality and will also influence their economic costs. The geographical situation of the study area, the land use intensiveness and the BMP age after implementation are strong influencing factors (Borin et al., 2005; Syversen, 2005). Giri and Nejadhashemi (2014) discussed the importance of BMP placement, timing, and selection procedures for their performance after implementation. Besides, the choice of BMP location should be based on local particularities, like critical zones with high pollution, soil types and slopes. Thus, it is important to have data of the spatial differences in the catchment and operate suitably on each area. In this way, the spatial scale affects the results. The BMP location can be directly at the arable land or it can be implemented afterwards, beneath the field or in the riverine. Fertilization management, e.g., is a BMP direct at field while buffer strips and end of pipe solutions are BMPs located beneath the field (Holsten et al., 2012a; Krause Camilo, 2016; Woli et al., 2010).

There are studies based on field measurements before and after BMP implementation showing different approaches and the effectiveness in different pollutant reduction (Borin et al., 2010; Jia et al., 2014; Lemke et al., 2011; Williams et al., 2015). However, this type of study requires extensive monitoring, accounting for a long time. Moreover, few of them could be inserted in the normal farm dynamics. In this way, the major studies available are based on model simulations (Bossa et al., 2012; Cerro et al., 2014; Lam et al., 2011; Strauch et al., 2013). This is also the case of this study, and the BMPs implemented in the modeled catchment were represented in the SWAT model by altering corresponding management operations and parameters (Arabi et al., 2008, 2006a; Ullrich and Volk, 2009). So, the assessment of simulated nitrate loads after BMPs implementation in the actual land use in the Treene catchment was made. A comparison of model predictions for these practices enabled the impacts determination of each BMP on nutrient loads at the outlet. The chosen BMPs are based on regional reality and previous studies from (Holsten et al., 2012a).

4.2.5.1 BMPs configuration, implementation and assessment

The calibrated SWAT model was used to assess the impacts of BMPs on nitrate loads in the catchment. The BMPs as described below were firstly implemented separately in the SWAT model and simulated individually. The BMPs were considered in a way that they take realistic situations into account by avoiding scenarios with exaggerated and unrealistic changes. This can help us to investigate the impacts of such management practices in a tangible reality, in a short time scale and to use them potentially in the practice.

The efficiency of each BMP regarding nitrate loads reduction and costs was afterwards assessed and compared with the others. The assessment was based on the difference between the current simulation values and the values after BMPs implementation. These comparisons were based on temporal differences such as seasonality, the spatial scale and by the use of the nitrate duration curve (NDC, Haas et al., 2016). The NDC represents the relationship between nitrate loads magnitudes and the percentage of time that this load is equaled or exceeded. A 5% exceedance probability, for example, means that these load values are only exceedance in five percent of the overall values. Hereby, high loads are represented, related to high precipitations and higher runoff events. In this way, the NDC is helpful for the investigation of different nitrate load magnitudes. So, the different BMPs simulated in the SWAT model are described successively as follows:

- *Buffer strip (BS)*

Buffer strips are important measures which are not directly coupled with the agricultural activity. In a buffer zone, flow from a crop area passes through the buffer strip acting as filter of sediments and nutrients between crop fields and water courses. The effectiveness of a buffer strip depends on many factors, including the vegetation type, soil type, flow velocity, and slope (Parajuli et al., 2008; Sahu and Gu, 2009; Syversen, 2005). The strip width is also one of the most important characteristics and is often related to the vegetal composition of the strip (Borin et al., 2005; Borin and Bigon, 2002; Parajuli et al., 2008; Syversen, 2005). The relationship between these mentioned different factors and the BSs targets become clear. For example, Leeds-Harrison et al. (1999), Borin and Bigon (2002) and Borin et al. (2005) assessed the buffer strips effectiveness regarding nitrate removal.

The SWAT model allows implementing BSs in the catchment at the edge of the field and can be defined in every HRU (Arabi et al., 2008; Parajuli et al., 2008). Based on different studies that considered nitrate in their scope (Bärlund et al., 2007; Laurent and Ruelland, 2011; Syversen, 2005; Ullrich and Volk, 2009) we assessed the effects of four realistic variations of BS widths for evaluate the best results on nitrate loads reduction, namely 1.5 m (BS1.5), 3 m (BS3), 5 m (BS5) and 6 m (BS6). The widths are controlled in SWAT by changing the model parameter FILTERW (Neitsch et al., 2011). The parameter controls the trapping efficiency of nutrients and sediment. The BSs were applied to all HRUs with agriculture and pasture activities.

- *Pasture Land Increase (PLI)*

This procedure consisted in the conversion of crop areas to permanent pasture. For this increase, areas with monoculture of silage corn and winter wheat in the catchment were equally reduced considering two scenarios: less 10% (PLI10) and 20% (PLI20) areas both for silage corn and winter wheat. These areas are converted into pasture. The rates were chosen according to expected changes in the catchment in a short and middle time scale. To simulate this situation, the crop rotations in the SWAT model were edited in the management operations, together with related activities (tillage, seeding and fertilization) and the curve number to consider the different surface runoff attributes.

- *Less silage corn monoculture for biogas (RYC)*

Rye is used as alternative for biogas production. It has similar yields potential, but needs less fertilization compared to silage corn and is better for the soil, since comprehends greater crop rotation. The crop rotation uses rye, silage corn and grass, which can still be used for the biogas production, in a 2-year system. Rye is sown at fall and harvested in spring. The nitrogen fertilization rate for rye in this BMP is 100 KgN/ha/year. Afterwards follows normal silage corn cultivation as in the other rotations. In the second year, after harvesting and kill the silage corn, there is a cultivation of grasses. It covers the soil during winter and can be harvested before sowing new crop in the next year.

The new rotation was implemented in the SWAT model as substitute for silage corn monoculture in 50% of the areas, considering this an average for the silage corn areas used for biogas production in the last years in the state Schleswig-Holstein (Claus, 2013).

- *Fertilization Reduction (FR)*

This BMP is one of the most often implemented practices and are used in several studies pointing out the benefits of these practices (Chiang et al., 2012; Jiang et al., 2014; Lam et al., 2011). Based on previous simulations of FR as BMP, the effects of two different fertilization reduction rates in the catchment regarding nitrate loads were assessed: a reduction of 15% (FR15) and of 30% (FR30). Fertilizer reductions can be directly implemented in the management operations in the SWAT model. All BMPs are summarized in Table 4.2 showing the abbreviations which will be used in the following chapters.

Table 4.2: BMPs names and codes:

BMP NAME	CODE
Buffer strip 1.5 m	BS1.5
Buffer strip 3 m	BS3
Buffer strip 5 m	BS5
Buffer strip 6 m	BS6
Fertilization reduction 15%	FR15
Fertilization reduction 30%	FR30
Pasture areas increase 10%	PLI10
Pasture areas increase 20%	PLI20
Alternative crop rotation	RYC

- *Combination of the best BMP results*

A combined approach of the different BMPs was implemented and simulated in the SWAT model. All the combinations of the above mentioned practices were simulated to investigate the nitrate loads reduction in the catchment.

- *End of pipe approach (EP)*

The end of pipe approach is a BMP type also placed beneath agricultural fields. It seeks to retain pollutants carried out with water from the crop fields. The practices implemented on the fields act in a certain area and time, and the EP acts, downwards, after the cropland area. The EP were already applied in several studies in different countries and have high potential for nitrate retention (Addy et al., 2016; Holsten et al., 2012a; Jaynes et al., 2008; Krause Camilo, 2016; Schipper et al., 2010; Woli et al., 2010). The major reduction of this BMP is related to denitrification processes reducing nitrate concentrations reaching the water course in surface and sub-surface runoff. In this way, as Schipper et al. (2010) and Holsten et al. (2012a) showed, different systems like walls, beds, boxes, graves and filters are implemented for the nitrate retention. The systems are mainly based on tree mulch, woodchips and sawdust (Holsten et al., 2012a; Krause Camilo, 2016; Schipper et al., 2010; Schmidt and Clark, 2012). Nevertheless, according to the studies of Woli et al. (2010) and David et al. (2015), for example, side effects of end-of-pipe approach need to be better investigated.

Different from the other BMPs in this study, the end of pipe approach was applied as a theoretical tool. For this study the reduction rates obtained by Pfannerstill et al. (2016) in the sub-catchment of the Treene catchment were subtracted from the nitrate loads reduction simulated with the SWAT model. They concluded that a nitrate reduction of 35% for spring, 14% for fall and 5% for winter is expected for this area, even if many other studies presented higher reductions. These obtained values were applied to all BMPs simulated in the model as a combination form. The structure considered was a simple bioreactor bed in a dig with woodchips. The dimensions of woodchip filled area are: 20 m long, 1 m deep filled and 1.2 m width.

4.2.6 BMP costs

In addition to the nitrate reduction, also the costs of BMPs need to be evaluated for an overall BMP assessment as addressed by Arabi et al. (2006a), Lam et al. (2011) and Panagopoulos et al. (2012, 2011). The costs evaluation considered the implementation/installation costs for BSs, FR and EP, the yields loss in less area for BS and also the contribution margin for land use changes (PLI and RYC). The contribution margin is the result from difference between market revenue and total variable costs. This value reflects the profitability of a crop and is mostly used for the evaluation of a possible crop implementation (KTBL, 2016). Thus, a positive value means a lucrative crop. However, in case of pasture areas, for example, the contribution margin can be low or negative since the pasture yield will be used to feed livestock or generate biogas, which increase the profits.

The costs for BMP maintenance are generally necessary for repairs and/or for monitoring. They are only discussed afterwards since they represent a part or the same as the costs for implementation. Moreover, the maintenance costs are very variable in time and for each farm condition.

The costs for the BMPs implementation and contribution margins were based on the data available at Association for Technology and Structures in Agriculture (KTBL, 2016) for the years 2012/13 and on the Agricultural Chamber of the state Schleswig-Holstein (LKSH, 2016) for the years 2015/16. These sources address relevant fixed and variable costs as seeding, fertilizers, insurance, interests, machinery, fuel and labor for each activity. The costs are given in Euros per hectare (€/ha) for a better comparative. The EP costs are given in Euros per structure (€/structure) and the calculations also considered variables taken into account by Schipper et al. (2010), Pfannerstill et al. (2016) and regional machinery rings (Maschinenring Laufen e.V., 2015; Maschinenring Mittelholstein, 2016). These costs calculated for the BMPs are general reference values, once many variables can suffer alterations in the short term and have particular differences in each farm, as emphasized by Lam et al. (2011).

Besides the direct costs of BMPs implementation, another cost issue related is the less income from the changes in soil use and from arable land loss. The income loss in areas affected by BMPs implementation was evaluated. The area occupied by BMPs implementation (ha) or the yields losses due fertilization reduction (t/ha) were multiplied by the mean actual crops productivity (t/ha). The result was then multiplied by the actual crops market prices (€/t/ha). The evaluation was based on current market prices for cereals, silage corn and pastures, which are an average of the months Mai and June 2016 (LKSH, 2016). These values are not constant since yields can vary in a year through different factors like climatic conditions and also the crop seed variety.

Following, the less income was related to the BMPs implementation costs. The initial implementation costs were added or subtracted from the costs regarding income losses. This costs variation is further named as *Costs_Total* (in €/ha) for including the revenue losses.

Furthermore, the effectiveness of the BMPs implementation was also assessed in relation to their costs and the nitrate loads reduction. The areas in the catchment (ha) that received BMPs were firstly multiplied by *Costs_Total* of each practice. For BMP combinations the costs were summed before. After, the cost obtained for each BMP was divided by the yearly reduced nitrate loads in the simulations (t). This resulted in the effectiveness value (BMP_efficiency) and the best results are lower values. The approach is similar to Panagopoulos et al. (2011). The equation is like follow (equation 1):

Eq. 1:

$$BMP\_efficiency = \frac{Costs\_Total}{loads\ reduction} \quad (1)$$

However, we believe that the term ‘cost-effectiveness’ is very subjective and complex. Such an evaluation requires a deeper and broader discussion of regional, national and international economic conjunctures. A discussion of products prices and interests of involved actors is needed, given the globalization of processes and dynamics of raw materials and wares. In this way, we refer the effectiveness for the catchment by the minimization of the relation costs/nitrate loads reduction.

4.2.7 Crop yields simulation

The consideration of simulated crop yields for BMPs assessment improves the accuracy of plant uptake of nutrients modeling and of water dynamics related to plants (Jiang et al., 2014). Furthermore, as one objective of this study is the investigation of fertilization reduction impacts on nitrate pollution abatement, the crop yields estimations by the SWAT model should be as realistic as possible. The plant parameters in the SWAT model were checked. The silage corn radiation-use efficiency and leaf area index were manually optimized to reach higher yields.

In this way, crop yields simulation was considered acceptable in the case of differences between measured and simulated mean annual yield within a range of ± 10% (Hu et al., 2007). The simulated yields were compared with actual annual averaged crop yields, based on data from the Statistical Agency for Hamburg and Schleswig-Holstein (Statistikamt Nord, 2015).

4.2.8 Dichotomy between ecology and economy

Face the policies of EU and Germany regarding water protection and renewable energies incentives a dichotomy between ecology and economy may arise. The WFD goal represents efforts including restrictions of intensive land use. Since the objectives are difficult to achieve, the second phase of the WFD is running, from year 2016 to 2021.

In contrast, at least on a first sight, the EEG can lead to an intensification of resources exploitation (Franko et al., 2015). The EEG commences defending a sustainable development (paragraph I). However, brings also the purpose of renewable energies use by a mean of 40-45% in the year 2025. Today this rate is about 25% in Germany (AEE, 2016; BMWi, 2016). In the state of Schleswig- Holstein biogas is presently strong alternative energy. In 2013, the biogas fraction of electricity generated from renewable energy sources was 22.5% (AEE, 2016). (Franko et al., 2015) also brought information and highlighted the importance of biogas production for Germany.

These two policies are well present, influencing decision makers like governments and farmers. In this sense, regarding nitrate loads, the WFD seeks the reduction, but the consequences of the EEG could be a greater nitrate entrance. In this context, the brought up BMPs were discussed under the deliberation of the two policies, considering the aspects that can be conflicting or not for each policy towards their goals.

4.2.9 The Integrated Water Resources Management (IWRM) approach

Several studies in the last years and different countries evidenced the useful approach of IWRM (Gandolfi et al., 2014; Giri and Nejadhashemi, 2014; Hu et al., 2014; Qi and Altinakar, 2011). The foundation of IWRM is joint activities for an effective planning and management of water quality and sustainability. The benefits will be a balanced approach and apprehension of all actors.

Since water quality degradation caused by nitrogen can be partly attributed to agricultural activities, the issue is very important for catchments with this reality. According to (Qi and Altinakar, 2011), IWRM approaches effectively linking agricultural land use planning will include BMPs, resulting in environment protection and economic development for long-term. Furthermore, effective BMPs implementation strategies can only be achieved with simultaneous consideration of environmental, economic and social aspects (Giri and Nejadhashemi, 2014) and with an extensive social participation (Carr, 2015). In this way, the present study addressed the IWRM approach inside the implementation of BMPs and the actual scenario signalized earlier between WFD and EEG policies. They have distinct objectives and a constant dialog, mediation, is needed for both coexist.

4.3 Results and discussion

4.3.1 SWAT model simulations: discharge, nitrate loads and crop yields

The results of the Treene catchment were considered at the gauging station Treia. Discharge simulation of the SWAT model presented good results in terms of visual inspection and the calculation of performance measures. All performance measures of the joint evaluation approach with performance metrics and signature measures as presented in (Haas et al., 2016) provided good results. The 5FDC/NDC segments evaluation showed a plausible simulation. Likewise, both performance metrics (KGE, NSE and PBIAS) and visual inspection showed a plausible simulation (Tab. 4.3, Fig. 4.3). Thus, the SWAT model is able to simulate the nitrate loads in this study in a lowland catchment.

Table 4.3: Performance of the SWAT model for calibration and validation periods. The best value for RSR and PBIAS is 0 and for KGE and NSE is the best value 1 (see (Haas et al., 2016).

PERIOD	***VARIABLE***	***PERFORMANCE MEASURE***							
		RSR Vhigh	***RSR high***	***RSR mid***	***RSR low***	***RSR Vlow***	***PBIAS***	***NSE***	***KGE***
Calibration	***Q***	*0.53*	*0.34*	*0.41*	*0.58*	*0.58*	*4.5*	*0.86*	*0.91*
	NO3-N	*1.39*	*0.26*	*0.33*	*0.55*	*2.06*	*-8.0*	*0.79*	*0.81*
Validation	***Q***	*0.41*	*0.41*	*0.22*	*0.38*	*0.35*	*-3.5*	*0.92*	*0.89*
	NO3-N	*0.77*	*0.7*	*0.21*	*2.32*	*2.54*	*-9.4*	*0.78*	*0.8*

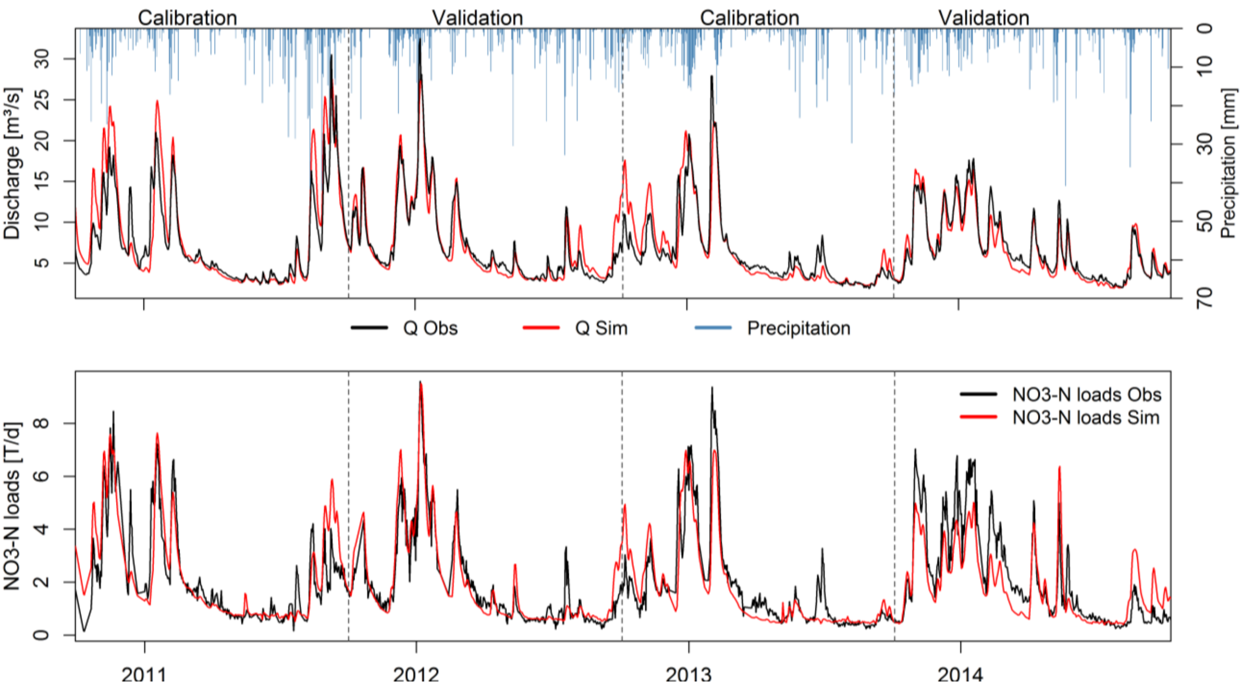

Figure 4.3: Discharge and nitrate loads curves for the calibration and validation periods.

The simulated crop yields of the SWAT model and the actual averaged crop yields (Statistikamt Nord, 2015) are shown in the Table 4.4 for the period from 2007 to 2014. The simulated crop yields remained within the stipulated bound by Hu et al. (2007). Silage corn presented highest difference in comparison to actual yields, followed by pasture. The comparison between simulated and measured yields demonstrated the plausibility of SWAT model simulations. This also indicated a realistic plant growth processes in the model, including nitrate transformations and plant uptake.

Table 4.4: Actual and simulated mean yearly crop yields (T/ha):

Crop	Yields (T/ha)		Variation (%)
	Observed (Statistik Nord, 2010-2014)	Simulated (SWAT model)	
Silage corn	38.9	35.5	-8.8
Rape	4.1	4.2	1.5
Rye	7.1	7.1	0.6
Winter barley	8.2	8.3	1.1
Pasture	8.1	8.5	4.9
Winter wheat	8.8	8.7	-0.5

4.3.2 Spatial and temporal analysis of nitrate leaching

Analyzing discharge components is also important in investigating nitrate dynamics. For the Treene catchment, the modeled components showed that about 61% of the water reaching the river via groundwater runoff. Further, 28% is transported by tile drainages and surface runoff contributes to discharge about 11%. These results emphasize the importance of nitrate transport in groundwater and drainages in the study area and are in coincidence with the study of Pfannerstill et al. (2015, 2014b).

Arable lands showed the greatest contribution of nitrate to the river in the catchment. Based on model simulations, agriculture and pasture areas contributed with 73% of the nitrate loads, which is equivalent to an average of 56000 t nitrate per year. So, a spatial variation based on land use could be observed, since arable land and pasture areas showed higher contribution of nitrate to water pollution in absolute values. Likewise, the pressure of agricultural activities on water quality in the catchment became clear. This behavior showing the strength of diffuse pollution from agriculture is well known from previous studies (Bouraoui and Grizzetti, 2008; Lam et al., 2011; Laurent and Ruelland, 2011; Naramngam and Tong, 2013). Furthermore, the study of Makareviciute (2015) in the Treene catchment investigated the ecological status of rivers based on phytoplankton as indicators. The approach suggested a better ecological status in a sub-basin predominantly covered with pasture.

A pronounced temporal distribution of nitrate leaching was also detected for the simulated time series. Higher load rates were registered during the winter period. Nitrate loads in winter represented 70% of the total loads (Fig. 4.4). The winter period showed 50% of the days with precipitation, with a mean of 3 mm/day. The summer, already presented 38% of precipitation days, with a mean of 2 mm/day. In winter, there is a smaller amount of plant uptake due lower plant growing processes, leading to more soil exposed to erosion. The higher precipitation in this period lead to more nitrate leached to the river. Seasonal patterns were also demonstrated by Arheimer and Liden (2000), Lam et al. (2012) and Guse et al. (2015b). Thus, the results indicated the requirement of greater nitrate loads reduction in winter. The relevance of temporal distribution together with soil cover during winter periods is emphasized.

4.3.3 Simulations of BMPs

The impacts of BMPs implementation are varied, as observable in the literature (Chaubey et al., 2010; Lam et al., 2011; Laurent and Ruelland, 2011; Liu et al., 2013). In a general way the implementation of BMPs presented reductions on nitrate loads at the catchment outlet Treia. The results are presented in a yearly period. In the following, the BMPs are analyzed separately.

The nitrate loads reductions simulated with BSs were significant at the catchment outlet. They showed different responses in loads reduction according to the width (Fig. 4.4). The BS1.5 indicated 3.9% nitrate loads retention per year. Doubling up the width to BS3, nitrate loads were reduced by 5.4%, while BS5 led to a reduction of 8% and BS6 to 9.3% of nitrate loads at the outlet (Fig. 4.4).

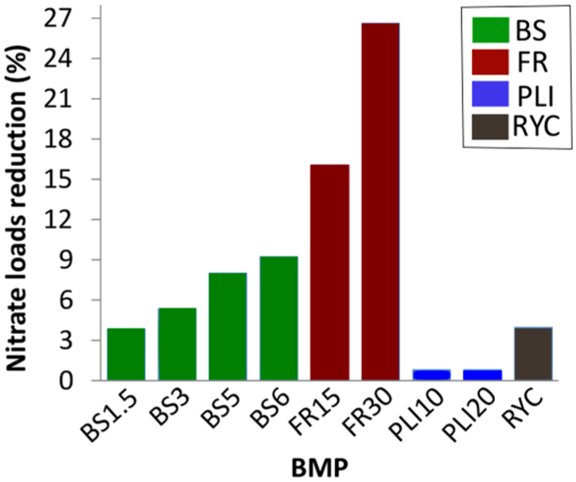

Figure 4.4: Nitrate loads reduction of the BMPs implemented in the SWAT model.

The relationship between nitrate reductions and the different BSs widths is not linear. By doubling BSs area the nitrate reduction was not doubled. Thus, considering the area required for BS implementation and nitrate loads reduction, wider BS would not necessarily be the most efficient. The field study carried out by Syversen (2005) demonstrated such a possibility by obtaining the result of a 5 m width BS being more efficient per square meter as a BS with 10 m width. However, BS6 showed higher nitrate loads reduction in absolute values.

Furthermore, the study area present higher water movements in deeper groundwater flow and by drainage tiles, which not interact so much with the BSs. According to Leeds-Harrison et al. (1999) and Ranalli and Macalady (2010), BSs will normally be more effective in surface and shallow groundwater runoff due interactions from vegetation with nutrients at the root zone, which is important for nutrient retention and plant uptake.

More specified, Figure 4.5 shows the difference between the original five segments of NDC (5NDC, Haas et al., 2016) and the 5NDC of the simulated BMPs. The curves were generated for winter and summer periods. The 5NDC method shows the effectiveness of nitrate loads reduction in different exceedance probability phases.

The highest reduction effect for the BSs was clearly at the very high and high phases for both seasonal periods, with nitrate loads exceedance probability of 5% and until 20% (Fig. 4.5-A,B). There is a higher reduction in the winter period (Fig. 4.5-A) until the low phase (loads exceedance probability of 70%). This represents longer effectiveness of BSs during the studied period. Possibly a greater presence of water in the environment explains this behavior. In summer, the reductions are effective in the phase with nitrate loads exceedance probability of 5% (Fig. 4.5-B), related to high load peaks.

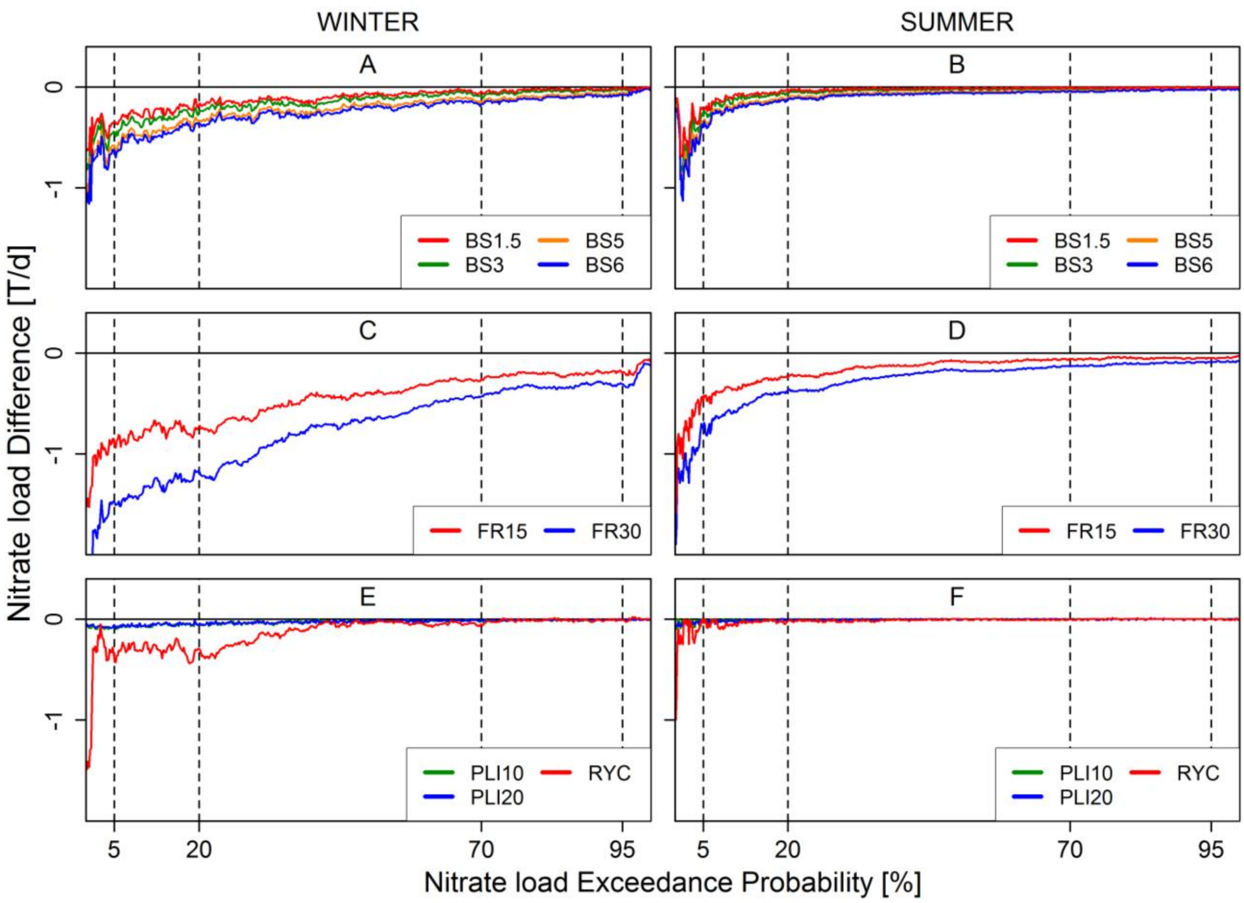

Figure 4.5: Difference of NDC between baseline and the BMPs simulations.

Likewise, Fig. 4.5-A,B also show that the BS6 presented the highest difference between the baseline and the scenario simulations. In this way, the reductions simulated for BSs indicated the response of the catchment to perennial vegetation in BSs. Lam et al. (2011) found a reduction of 15% in nitrate loads with BS with 10 m width in a sub-basin of the Treene catchment, which resembles to our results. Considering the geographic relief of the Treene catchment, with smooth slopes and lower surface runoff, the BSs will not necessarily demonstrate a key role in nitrate loads abatement. The BSs are effective in retain nutrients in shallow subsurface flow and surface runoff (Grismer et al., 2006; Ranalli and Macalady, 2010).

The FR simulation showed the more effective reduction of nitrate loads at the catchment outlet (Fig. 4.4). A fertilization rate reduction by 15% (FR15) led to less nitrate loads in the order of 15.1%. The reduction by 30% (FR30) represented less 25% nitrate loads reaching the river. There is a direct relation of fertilization rates and nitrate loads. Lam et al. (2011) obtained a reduction of 10% for nitrate loads by reducing the fertilization rate by 20% on croplands. The study of Laurent and Ruelland (2011) resulted in 19% reduction at the outlet by reducing nitrogen fertilization by 7% on wheat and by 39% on maize. Aouissi et al. (2014) found 22% of nitrate loads decrease by reducing fertilization rates by 20%. Furthermore, Holsten et al. (2012b) suggested the limit of 100 KgN/ha/year based on a fertilization of 157 KgN/ha/year, which represents a decrease of 36.3%. They indicated that this measure would lead to an average reduction of 37% on nitrate leaching.

The loads reductions were perceived in almost all phases (Fig. 4.5-C,D) for FR, for both the winter and summer periods. Winter presented the highest reductions, reaching 2 t/d in the very high phase (Fig. 4.5-C). The difference in loads compared to the baseline continued high until the beginning of the mid loads phase, but even so kept reductions until the very low phase (95% load exceedance probability). The reduction in all phases for FR indicates that also less nitrate will reach the river via groundwater and tile flow. For summer (Fig. 4.5-D), the reductions are marked for very high and high loads. This behavior is related to higher runoff presence due to precipitation, since greater plant uptake occurring in this period reduces the nitrate availability for leaching. In the phase with exceedance probability of 95% the changes were less marked for both periods. Once the loads are connected to discharge, the transport of nitrate until the river is smaller in this phase.

So, the results of this BMP implementation demonstrated the high impact of fertilization reduction on nitrate loads at the catchment outlet. Principally in lowlands as the Treene catchment, in which the drainage tiles interacts fast with the water from fields (Kiesel et al., 2010), this BMP was highly effective. Cerro et al. (2014) also pointed this relationship of subsurface runoff and nitrate transport for another lowland catchment in northern Spain. Despite the lowland nature, the results of FR also demonstrated that with less fertilization fewer nitrate will be leached with surface runoff in high precipitation events. This is an expected behavior that was confirmed since nitrate availability was reduced.

A FR may normally lead to yields reduction too. Generally, the greatest changes occurred for silage corn and pastures (Tab. 4.5). There was a decrease of yields for some crops and other apparently did not suffer high influences with FR15, like rye and winter barley. By FR30 some reductions doubled (silage corn and pasture), while others presented even stronger reductions, like rape, winter barley and winter wheat. The results reflected the strong dependency of nitrate as a limiting nutrient for growing processes for almost cultures. Only rye presented low variation in yields. As the less fertilized crop it was expected higher reaction to the fertilization changes. However, as part of a rotation it can possibly profit from the surplus of fertilizer of the previous crop.

Table 4.5: Changes in crop yields after BMP implementation.

Crop	Yield difference (%)	
	FR 15	FR30
Silage corn	-13	-26
Rape	-8	-17
Rye	0	0.5
Winter barley	-3	-8
Pasture	-10	-20
Winter wheat	-6	-14

The two variations of PLI implemented in the SWAT model showed that the increase of pasture areas will just have a minimum impact in nitrate loads reduction at the catchment outlet. By shifting 10% (PLI10) and 20% (PLI20) of silage corn and winter wheat to pasture areas in the catchment, only 1% less nitrate loads was registered at the catchment outlet. In principle a higher reduction could be expected with PLI, since soils are not so exposed during winter time by pastures and the fertilization is lower. However, a change of 20%, representing 700 ha in the catchment, did not affect significantly nitrate loads. Thus, the change of land use in 1.5% of the catchment area will not bring an evident change in nitrate loads in the river at the catchment outlet.

Nevertheless, in more detail, the sub-basins with HRUs in which PLI was implemented, the simulations showed higher changes for PLI20. In this case, 3% less nitrate loads reached Treia station. In this more specific spatial scale the effects are stronger, reflecting the change in nitrate transport processes. The interactions between soil, water and plant changed. Masters et al. (2016) reported the positive effects of grasses on nutrient leaching as showed here.

The nitrate loads reduction of PLI in the simulated conditions presented the highest reductions in extreme events regarding exceedance probability in winter (Fig. 4.5-E). This result evidenced the reduction of surface runoff and possible a higher plant uptake during winter periods. These periods were mentioned before as greater contributors of nitrate loads. For the summer period (Fig. 4.5-F), there was no marked difference in comparison to the baseline situation. At the observed scale and the changed area, no revealing nitrate reduction was observed.

The implementation of RYC reduced silage corn monoculture and showed a similar behavior as the PLI management practice. By replacing half silage corn areas in the catchment, which represents 2000 ha, the new crop rotation led to a decrease of 4.3% in the nitrate loads. The BMP demonstrated little significance in terms of nitrate loads reduction at the catchment scale and for the area size used. Considering the fertilization reduction and the presence of vegetation covering the soil during winter periods with this crop rotation, higher impact of the change on nitrate loads could be expected. Nevertheless, as this area represents only 4.2% of the catchment, the obtained reduction is a representative indication of the potential of this change.

Moreover, most decreases of RYC were registered in fall and winter. As a 2-year crop rotation, rye would be growing from fall 2011 to spring 2012 and also in 2013-2014 in the simulation period. Precisely in these intervals the decrease of nitrate leaching was between 10% and 22%. Figure 4.6 shows exemplarily the differences in these periods (black boxes). The less fertilization needed in the first rotation year and the soil covering during winter resulted in a decrease of nitrate leaching in the winter period for this year. So, rye presented a positive role in the crop rotation. (Lam et al., 2011) also demonstrated the benefits of rye cultivation in crop rotations.

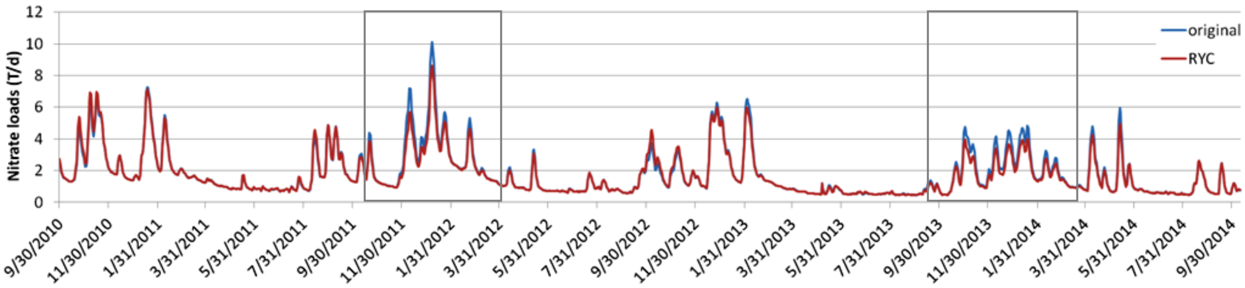

Figure 4.6: Rye effect on nitrate loads reduction.

Furthermore, the red NDC curve in Figure 4.5-E,F also demonstrated this behavior of reduction. In winter there is a significant loads reduction in the very high and high phases (Fig. 4.5-E). The presence of grasses and rye increase nitrate uptake by plants and less surface runoff. For summer, alike it was for the other practices, RYC showed differences to the monoculture of silage corn in the very high phase (Fig. 4.5-F). This behavior is also observed in Fig. 4.6, in which the difference between blue and red colors is mostly not discernible.

4.3.4 Combined BMPs

The BMPs were afterwards combined in model simulations to assess the nitrate loads reduction evoked by more than one BMP. All possible combinations up to an implementation of all BMPs in the same model simulation were tested and presented in Fig. 4.7.

The combined BMPs showed a reduction varying from a minimum of 4.7% to maximum of 38.2%. The lowest reduction would be obtained in the combination of PLI20 and RYC. The maximum reduction was estimated for the combination of one type from all BMPs, leading to the highest reduction in nitrate loads. A complementary positive effect was observed for many combinations, which means that the more BMPs were combined the more nitrate was reduced.

A clear trend from the combinations was noted: the presence of FR30 led to better results regarding nitrate loads reduction. Thus, the rate of less 30% fertilization was present in all the higher reductions. Afterwards there is a decay step in the reduction sequence when FR15 is implemented (Fig. 4.7, second row in small plots). The lowest loads reductions with a combination were registered in case without fertilization reduction (Fig. 4.7, third row in small plots).

The presence of BS also led to nitrate loads reductions. However, the BS width was important since BS5 and BS6 presented higher reductions. Indeed, the presence of BS6 and FR30 in the combinations showed highest nitrate reductions. The presence of RYC also contributed with nitrate reductions when observing the combinations without RYC (Fig. 4.7, top left big box) and with the BMP (Fig. 4.7, bottom left big box). Already with PLI the contributions are almost not visible comparing the combinations without the practice (Fig. 4.7, top left big box) and the combinations with PLI10 and PLI20 (Fig. 4.7, top second and third big boxes, respectively). Thus, increasing the pasture areas in a low proportion did not bring expressive positive effects on nitrate loads reduction. The positive effect of a joined implementation of different BMPs was also the behavior observed in the study of Lam et al. (2011) and Chiang et al. (2012).

Furthermore, the results showed that different BMPs combinations can lead to similar reduction. The implementation of BS3 with FR15 led to similar results as BS1.5 with FR15 and PLI10. The different width of BS or the proportion of land use change of PLI influenced the loads reduction. Furthermore, a BMP like PLI acts directly on the arable land and BSs will retain nitrate coming from the field. Moreover, with FR, once fertilization rates are reduced less nitrate will be available for be carried with precipitation. The combination of different BMPs will attain and influence different nitrate processes in the catchment, enabling more nitrate retention in the soil, more plant uptake and less nitrate leaching. Panagopoulos et al. (2011) registered the same behavior in their study. The use of different combinations is a good possibility for the consideration of catchments heterogeneity. The spatial differences can be taken into account with distinct proper practices. Indeed, despite similar reductions of some combinations, we reinforce that not all BMPs can be replaced for another. BSs, e.g., cannot be eliminated and changed by RYC, they are totally different. One can judge, however, if the BS width could be reduced in one specific combined case.

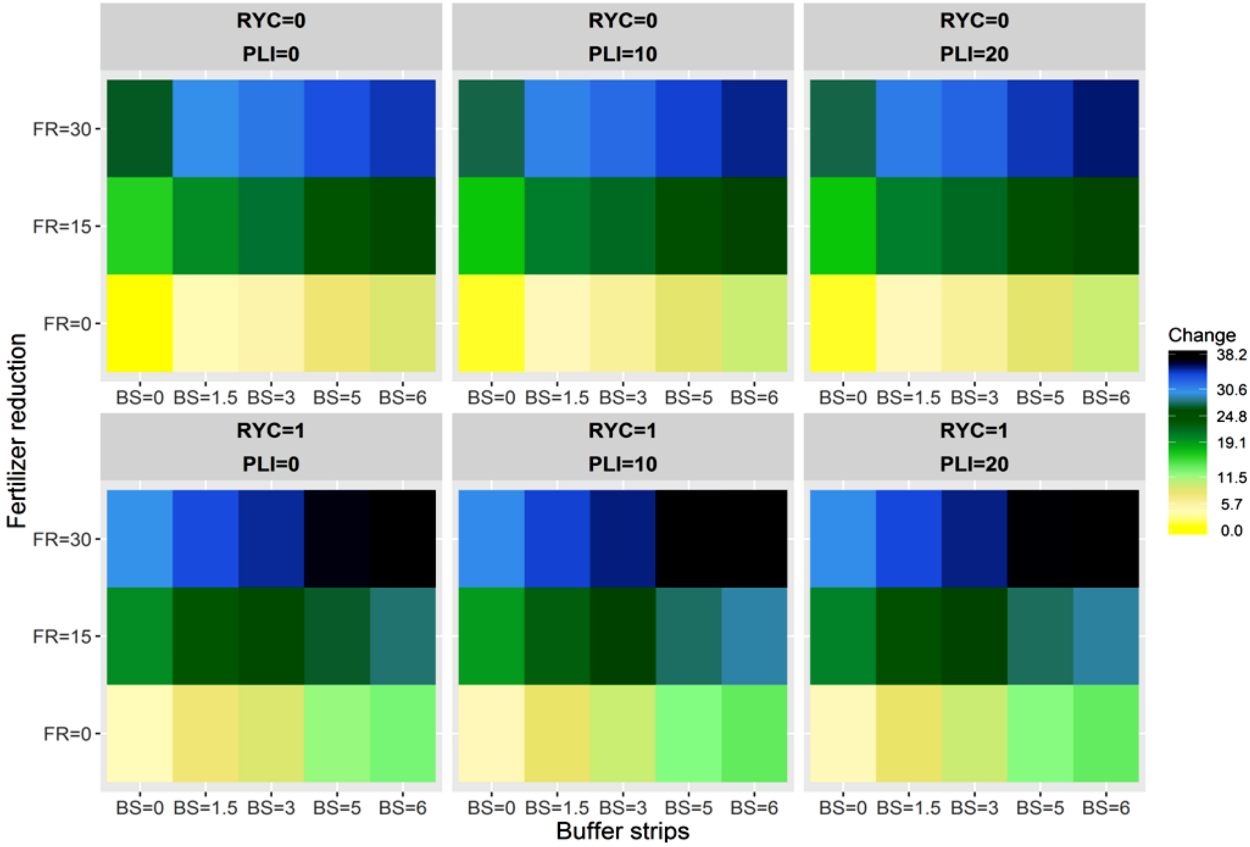

Figure 4.7: Nitrate loads reduction in the combined BMPs simulations for the catchment outlet Treia. BSs and FR are axis x and y, respectively. It is differentiated in RYC in rows and in PLI columns. The BMPs are abbreviated as described in Tab. 4.2. The darkest colors represent higher reductions in nitrate loads.

The temporal differences in the operating time of BMPs are also a benefit in a combined approach. The major affected processes were regarded to plant uptake and nitrate transport by runoff components as mentioned before in Haas et al. (2015). The special characteristics of lowland catchment influenced the BMPs simulations, principally lower surface runoff and drainage tiles presence. These features are related to a reduced efficiency of BSs and to faster response to FR, respectively. Gebel et al. (2013) also pointed to particular behavior of nitrate dynamics in lowland soil in Germany.

The greater reductions of nitrate loads in this study for the most BMPs and their combinations were observed in the winter periods, which generally presented higher precipitation and less plant growing processes. So, the combination of different BMPs presented greater nitrate loads reductions, principally in the most critical periods.

4.3.5 End-of-pipe approach (EP)

By the implementation of this BMP, nitrate loads reaching the river would present an abatement of 36%, 15% and 6% in summer, fall and winter, respectively. By considering the presence of EP together with other BMPs, additional reduction would be noted. The maximum reductions could achieve 60% in spring, 47% in fall and 41% in the winter period. Thus, EP can be an effective tool to reduce the nitrate loads reaching water courses.

The efficiency of EP is sensible to spatial and seasonal climatic conditions (Addy et al., 2016; David et al., 2016, 2015; Woli et al., 2010). The structure configuration at the end of tile like the size, materials, water availability (flow intensity and volume), carbon presence, and also temperature (for biochemical processes) are some important spatial and seasonal climatic variable aspects to consider. However, the field experiments of Pfannerstill et al. (2016) in a sub-basin of the Treene catchment showed the effectiveness for this area.

Furthermore, according to Schmidt and Clark (2012) the effects of EP after installation are perceived fast. The values obtained from EP implementation represented a high reduction of pollutants reaching the outlet. They would be very helpful additive tool in winter time, when the highest loads are noted in the catchment.

4.3.6 BMP costs

The costs for the BMPs implementation were addressed in Tab. 4.6. The table shows the cost in €/ha and €/structure and also for the catchment scale.

BSs only need a relatively small amount of direct investment funds for their implementation. The costs came from area preparation, soil sampling, grasses planting, start little fertilization, area closing off and also labor and equipment. Afterwards, BSs only need few cheap maintenance activities such as regularly visual inspection and weeds cleaning. Still, despite the cost for BS implementation is regarding to one (1) ha many farms in the catchment would probably dedicate less than this area.

In contrast, PLI implementation presented higher costs. The practice requires more activities due area preparation, soil sampling, seeding of grasses, fertilization and much labor for harvesting, transport, ensilage and storage of yields. However, the costs for soil preparation and seeding costs will be much lower for several years in the succession.

FR practices basically present a cost saving, since fertilization rates are reduced. A little reduction in machinery costs, fuel and labor is also expected. Nevertheless, the actual activities would remain the same with this practice. In this way, less fertilizer would represent less €21 and €42 in costs per ha for FR15 and FR30, respectively. We considered that the fertilization activity remained the same, in the same dates, only the rates were reduced.

The crop rotation in RYC was based on 3 crops (silage corn, rye and grasses), so the costs are a sum of their contribution margin divided by two (rotation years). As RYC represents a change in the used crop, the costs present the same values for all subsequent years. Considering the previous crop rotation, silage corn monoculture, which has a contribution margin of €484, RYC presented slightly higher costs.

For EP, the costs calculations considered the construction of one structure. The calculations considered by Schipper et al. (2010) showed similar costs to our study. Most likely more structures would be necessary in a farm, which would increase the costs. After the installation only maintenance costs for monitoring of the structure and material conditions are necessary for many years.

Regarding to the BMPs combinations, the costs can be, in principle, assumed as simple summation. In this way, logically, the more BMPs would be implemented the greater would be the costs (only FR is subtracted). Because of this another table is not necessary.

Table 4.6: Costs for BMPs implementation considering ha at the catchment scale:

BMP	Implementation Costs	Area in catchment (ha)	Implementation costs catchment (in 1000 €)
BS	160 (€/ha)	150 (BS1.5)	28.5 (BS1.5)
		301 (BS3)	57.2 (BS3)
		501 (BS5)	95.2 (BS5)
		601 (BS6)	114.2 (BS6)
FR15	-21 (€/ha)	41794	-877.7
FR30	-42 (€/ha)	41794	-1755.3
PLI	1234 (€/ha)	350 (PLI10)	432 (PLI10)
		700 (PLI20)	864 (PLI20)
RYC	578 (€/ha)	2000	1156
EP	1100 (€/structure)	-	-

* The negative mark (-) indicates a saving of money.

The investigation of BMPs costs can be helpful for comparisons with current activities and for enable future considerations on possible approaches. The costs brought here are immediate, concerning implementation. However, the BMP operation can be long lasting, which would attenuate their costs over time. BSs and EP have this possibility and advantage. Robertson (2010) and Schmidt and Clark (2012), e.g., affirm that bioreactors have the benefit of many years durability, reaching a decadal life time. According to Borin and Bigon (2002) it is possible to observe the effectiveness of older trees in BSs in nitrate retention. These characteristics attenuate costs in a medium term. Furthermore, FR practice has the possibility of significant alleviation of nitrate inputs to water in a mid and long term. So, the benefits can be higher since the environment system response to nitrate pollution reduction measures can be slow (Bouraoui and Grizzetti, 2014; Meals et al., 2010).

Looking from the catchment scale, the costs obtained for the BMPs implementation (Tab. 4.6) may seem high. However, considering a catchment approach in IWRM, for instance, these costs could be minimized once buying materials in more quantity from suppliers or working in contiguous farms initiatives, e.g., could reduce costs.

Furthermore, in addition to the costs, also the yields losses due to the implementation of BMPs need to be considered. These values are important factors for decision making since it implies less revenue for the farmer. The mean observed yields for the study period and the current market prices of the considered crops (LKSH, 2016) are shown in Table 4.7. The adjacent columns in the same table show the income differences related to yields reduction by area reduction due BS or less yield due FR or also to land use changes for PLI and RYC. The farmers would perceive important income losses. Illustrating the case of yields loss for BS implementation and considering silage corn as crop in these areas (with productivity of 38.9 t/ha), the farmer would perceive a difference of less €1522 per ha in a year together with the implementation.

PLI implementation needs to be observed with attention, since the yields can be sold, feed livestock or be used as fuel for biogas stations, bringing profits in a midterm time scale, making this income difference calculation complex. For this study case, the yields of PLI were considered sold and the income losses in comparison to the previous crops would be €1752.

Only the implementation of RYC would bring positive incomes for this situation. Despite silage corn monoculture is very productive, RYC present the advantage of rye growing during winter, which characteristic the monoculture does not have. Furthermore, the implementation cost for grass and rye are a little lower than silage corn, which possibilities better results.

Table 4.7: Income difference in a year considering BMPs implementation costs and less incomes from area losses (€/ha).

Crop	Observed yields (T/ha)	market price (€/T)	Income difference (€/ha)				
			BS	FR15	FR30	PLI	RYC
Silage corn	38.9	35	-1522	-156	-312	-1752	267
Rape	4.1	372	-1685	-177	-355	-	
Rye	7.1	124	-1040	-21	-187		
Pasture	8.1	100	-1201	-114	-229		
Winter barley	8.2	127	-970	-84	-169		
Winter wheat	8.8	147	-1454	-147	-294		

Following, the investigation of BMPs efficiency in relation to all related costs (covering the implementation and revenue differences) and nitrate loads reduction demonstrated that this approach can also be important for decision making. Figure 4.8 shows these relations by associating the BMPs efficiency to colors. The clearer the color, the better was the relationship (€/ha/nitrate t reduction).

In this way, firstly BS showed better efficiency when considered lonely. BS1.5 showed the best result, since the implementation costs are low, it requires little area and reduced nitrate loads by 3.9% per year. Together with other BMPs, the efficiency of BSs showed worse results. This is related to the fact that arable land was lost, leading to revenue losses and influencing the efficiency.

The introduction of FR was generally an efficient practice, since basically represents saving money in its implementation. The colors are green shaded due the higher yields losses with this practice. FR showed moderate efficiency even with the combinations.

The implementation of PLI demonstrated worse efficiency (darkest boxes). Considering the implementation features (10% and 20%), the nitrate loads reduction and the income losses in comparison to the previous crops at the areas (silage corn and winter wheat), the efficiency was worse. This situation showed the strength of the economic variable, once PLI implementation needs higher investment and profits are minor in comparison to silage corn in a first moment. However, the initial costs for PLI will reduce in the following years, improving the efficiency. PLI efficiency was slightly better only when RYC was combined in the simulations. As mentioned before, RYC presented benefits on yields, which affects the efficiency. Furthermore, excluding the worse efficiency case, showed by PLI, the mean value would be by 0.3 € per ha and nitrate t reduction. This means a good efficiency for the other BMPs and their combinations.

The EP was not included in Figure 4.8 since it is a theoretically approach in the study. Nevertheless, considering the reduction for summer, fall and winter, the efficiency of one structure was higher in summer due its high nitrate loads reduction rates. Keeping in mind that the structure for EP normally has a long lifespan, the efficiencies probably would be better in the following years after installation.

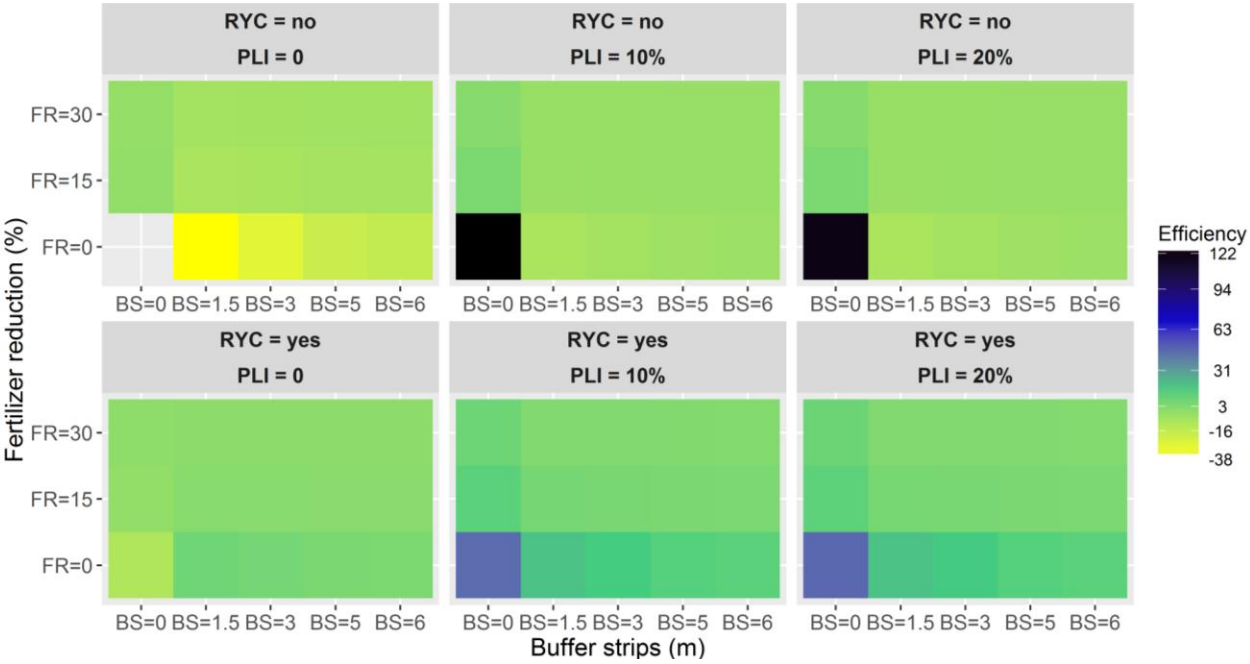

Figure 4.8: Efficiency of BMPs considering costs related to nitrate loads reduction (€/ha/nitrate t reduction). The darkest colors represent lower efficiency.

As observed, the efficiency of the BMPs showed the benefits of FR and BSs. They have no or low implementation costs and present long-term lifespan. These are great advantageous and influence the results. PLI and RYC, in turn, showed higher costs and lower loads reduction. Nevertheless, these BMPs need attention because both are important, presenting distinct roles in different times of nitrate dynamics regarding plant growing (nitrate uptake) and soil covering.

Furthermore, this assessment of BMPs efficiency would be important if carried out at the farm scale too. The farm scale is actually the administrative unit, where the financially driven decisions are made. Thus, what is important regarding indirectly to costs but is directly determinative of the actions in agricultural areas: the area loss and so possible less income.

4.3.7 Policies and Integrated Water Resources Management

The simulated BMPs, their cost and efficiency evaluation give us an idea of the difficulty of reaching consensus between WFD and EEG. Both the policies differ in a core point: the kinds of profit seek. They are important for society and can exert strong pressure on the environment.

Table 4.8 gives an overview of the pros and cons for each policy regarding the simulated BMPs and also the challenges to overcome the barriers. The discussions about how to deal with these issues can be done in the perspective of IWRM.

Under ecology perspective BSs are proven an advantageous approach. They play an important role for ecosystem services (McVittie et al., 2015). They act as networks, being fundamental for habitats connection. In the same way, BSs contribute for biodiversity conservation (B.-M. Vought et al., 1995). However, they are commonly not unanimous for many farmers, since their implementation in agricultural catchments means loss of arable land. For example, in our study area, considering only the implementation of a buffer strip with 6 m width at the river margin with 4.5 Km extension in a sub-basin, it would represent less 0.52% of arable lands (5.4 ha). It is a little area for the catchment, but if this area belongs to one unique farm it represents higher impacts in the incomes. In this way, BSs implementation may lead to less incoming and consequently contribute to the questioning and resistance to such a BMP. In other words, for an economy point of view a BS represents loss of revenue in the current market relations, since BS areas will not produce rentable yields or biomass. The WFD also demand the implementation of measures under the possibility of penalties in case of negligence. These efforts for WFD can frustrate EEG perspective without dialogs and investigations.

Thus, intermediate measures should be found, like the simulated combination of BS with other BMPs, attenuating this area loss. Government policies regarding possible payments for the BSs implementation and maintenance would be important too.

In principle is FR a simple management practice, with good results for reducing nitrate loads to rivers. In terms of WFD goals, it would be a very good BMP, by showing strong responses perceived in the water quality. However, a fertilization reduction by 15% led to less 13% silage corn and 10% pasture yields (Tab. 4.6). The reduction of 30% resulted in less 26% silage corn and 20% pasture yields. Thus, for EEG this BMP is negative, since represents less yields for energy generation.

The adoption of FR needs to be carried out in more detail as the generalization for this study. Varying the reduction rates considering every crop and soil conditions could be helpful. Modern techniques using GPS for specific fertilization placement can enhance this practice. These practices can be positive for both policies.

The FR can be implemented regarding mineral fertilizer or manure reduction. In case of mineral fertilizer reduction, the farmer would basically save money. However, considering manure reduction a surplus of this substance can be registered at the farms. This can trigger a net of problems from the farm level to the national scale, considering the case of great adoption of this practice in a country. To find alternative uses for manure is an issue concerning WFD.

Furthermore, despite benefits for environment quality, FR evokes yields loss when higher amounts are spared. Fewer yields represent less food for human and livestock and/or fewer raw materials for biogas generation. For WFD it would not be a problem, but, as for BS, this practice leads to less incoming for the farmers. Consequently resistances face FR may arise, even more with incentives to increase the productivity coming from EEG. Thus, alternative measures should be found for equalize the actors involved.

PLI implementation could be positive for both the ecology and economy directions simultaneously. This BMP require less fertilization, the soil is less disturbed and stays less time uncovered, which are benefits for ecology. Even so, PLI produces yields potentially useful for economic activities as for livestock and bioenergy production. However, the suppression of silage corn areas could go against EEG initiatives, since it is a valuable energy crop in Germany nowadays. Indeed, the goals and posterior management of increased pasture areas will influence the direction of gains. If the cultivation of these areas turns intense, with extensive use of manure, fertilization and pesticides, PLI will be only economically rentable.

PLI is also an initiative which goes in direction of the new EU policy, the Common Agricultural Policy (CAP, EU/European Commission, 2013) in which greening initiatives with land use diversification are required for specific farms. These activities seek to ensure a wide sustainable development of rural areas, considering all aspects from social, economical to environmental conditions. Nevertheless, the model simulations showed less efficiency in the relation to nitrate loads and implementation costs for this space scale. Thus, there is a need for further investigations and initiatives.

The use of RYC would be positive for WFD since promotes land use diversification, benefiting soil, biota and the water resources. It is an alternative in accordance with WFD and inside the new policy seeking for more rotation in agriculture. The efficiency evaluation also showed a positive result for this practice. However, looking only for energy generation potential the monoculture of silage corn would be more rentable according to the simulations. It would be also easier from the labor point of view, since it is less diversification. These are reasons for farmers not change the land use.

According to Masters et al. (2016), there is a great potential for nitrate loads reduction by shifting from great areas with silage corn to more grasses and rye, for example. These crops, if well chosen, can be used for biogas generation, need less fertilization and keep soils covered during winter. Nevertheless, according to our simulations these changes need a greater spatial scale for higher loads reductions. Thus, such practices would be positive for WFD and EEG and a dialogue between the policies is necessary in order to harmonize the interests.

The practice based on EP, as an additive structure with other BMPs, indicated high efficiency in nitrate loads reduction. This BMP does not interfere much in the crop fields itself; it is basically a structural modification in areas with no crops, specifically at the end of tile drainages. The EP would be an attractive BMP for both the WFD and EEG policies since does not requires arable land. Certainly the structure requires an area for construction that needs to be considered, but the proportion is less than for BS, for example.

A major question arising from this discussion is the payment of the BMPs costs. There are different valuations in discussion. The WFD and EEG have important but conflicting goals. Ample society spheres are involved and affected, direct or indirectly, with these discussions and decisions. The IWRM apprehend this situation and spectrum. Important research contributions with aids for decision makers at the catchment scale already showed the possibilities and challenges (Dong et al., 2013; Giupponi, 2007; Hu et al., 2014; Jin et al., 2015; Mazvimavi et al., 2008; Volk et al., 2008). Garnier et al. (2014) also pointed the importance of coordinated actions of *in loco* investigations and model simulations.

Bouraoui and Grizzetti (2014) mentioned that partial reasons for still having the nitrogen pollution problem are: a lack of full implementation of the legislation; delayed responses of the environment and the inappropriate choice of mitigation measures. The three elements are connected and the decision about appropriate approaches (as BMPs) at a farm, landscape or catchment scale is worthy to be discussed. It will interpose in the costs for the BMPs implementation, for example. Beyond this, as stated before, the costs are strongly related to arable land loss, which specifically makes the implementation in small farms difficult. The CAP stimulates the farms for greening initiatives with higher subsidies, so they can stay competitive face to big farms. This configuration can also be a positive scenario for BMPs implementation at the farm scale. Indeed, the farm activities should be connecting to other farms and then to the catchment scale afterwards.

Thus, the approach with BMPs, even if only simulated in a model, can enhance the contributions to this hard task inside the IWRM. Panagopoulos et al. (2012) well pointed that BMPs show possible scenarios and consequences of soil use changes at the catchment scale. Even if BMPs simulations have uncertainties, they can help in the discussions. Decision makers like public authorities, experts, managers and all general public in the catchment can benefit from this approach. Carr (2015) made a good discussion about the importance of the participation of stakeholders and public in IWRM.

Furthermore, the ultimate discussion regarding costs of BMP implementation cannot be made only on the farm level because, since it is a unit aiming also to an economic development, the implementation of any activity that incurs loss of area and productivity is not well seen. To know that BSs play an important role for ecosystems not necessarily persuade the farmer to implement them. The consciousness about costs and benefits can be diverse.

The costs discussion showed that it is difficult to encompass ecologic and economic factors. A political willingness is essential for changes in the assignment of importance weights. As mentioned before, compensation initiatives should be created and managed. An integrated approach, which can be due IWRM, is highly desired and indicated for this purpose. It is necessary consider about ecological, social and economic variables, which have different weights for each different social actor.

Table 4.8: Overview of BMPs pros and cons from the perspective of WFD and EEG and challenges to overcome:

	For the WFD		For the EEG		Challenge
BMP	**Pros**	**Cons**	**Pros**	**Cons**	
BS	Nitrate retention; Habitat connection; Biodiversity	-	-	Arable land lost	Cost restitution of arable land reduction; Valuation alternatives of ecosystem services Spatial distributed actions
FR	Soil biota; Less nitrate reaching; Less water courses pollution	-	-	Less yields	Studies regarding fertilization needs and productivity; Alternatives for cost restitution of yields reduction; Increase soil sampling and popularize use of GPS techniques for fertilizing.
PLI	Less erosion; More nitrate retention; Biodiversity	-	Bio energy generation	Area loss with more rentable crop	Balance between arable land lost and pasture areas increase Valuation alternatives of ecosystem services
RYC	Soil biota; Less erosion; More nitrate retention	-	Bio Energy generation	Area loss with more rentable crop	Different efficient crops and crop rotations for bio energy generation and environment protection
EP	Less nitrate reaching water courses	Possible negative side reactions	-	-	Efficient and stable structures for nutrient reduction

4.4 Conclusions

This study investigated the effectiveness of BMPs implementation in reducing nitrate loads in the Treene catchment. The investigation was carried out with the SWAT model and the results were investigated under the view of two different policies, the WFD and EEG.

Initially, the SWAT model showed to be able to simulate nitrate dynamics in a lowland catchment like the Treene catchment. The model was sensitive to spatial and temporal processes variations. The nitrate dynamics simulated highlighted the influence of drainage tiles presence and the seasonality, in which are included plant uptake and soil covering differences. In this sense, the spatial differences in the catchment need different approaches. The BMPs need to be adapted to each area. This was showed through the test of the different BMPs and their distinct results. Likewise, temporal differences were strong highlighted and need different approaches.

Furthermore, different assessment scales for apprehend more details in the effectiveness of the BMPs are highly indicated. The use of one catchment outlet like in this study allowed observing the effects of BMPs implementation for the whole area. Thus, the changes, even if not expressive, were significant at the gauging station. This means there is a response signal at the outlet, principally in crucial winter periods. On the other hand, the low changes in nitrate loads with some implemented BMPs showed that these practices need greater changes for generating a remarkable result. Larger initiatives are needed for achieve the goals of the WFD. This emphasizes the importance of an integrated catchment approach.

From the outcomes of this study it is important to highlight the remarks of Arabi et al. (2006b) and Laurent and Ruelland (2011) about scale dependence. The observed efficiency of BMPs implementation in reducing the nitrate loads at the catchment outlet is not the same as the efficiency at field scale or also at sub-basin scale.

As the study of Holsten et al. (2012a) already affirmed, one isolated action is not enough to reduce significantly the nitrate pollution. This study showed and reinforced the necessity of joined actions. Each BMP has its benefits and a core effectiveness timing and place. There is no one solution, but there are different possibilities for each situation and the best options are combined BMPs, space and time targeted adapted. They have higher nitrate loads reduction potential, as the implementation of buffer strips, the fertilization reduction and end of pipe structures.

As observable in the literature, installation of BMPs is rarely followed by long-term monitoring effectiveness of BMPs to analyze their success in meeting the original goals. Long term data of flow and water quality within catchments before and after BMPs placement is not generally available. It will be very important for further studies of water (and environment) management. Other initiatives, adapted to each area, should be investigated and tested in field studies. This is exemplarily the case of the remoistening of moor areas (Holsten et al., 2012a). They are numerous in the region of the study catchment as a lowland area. Investigate them in real and by model simulations is highly recommended.

In the way that is practically impossible to reduce nitrate leaching until zero, BMPs help to reduce this process. Indeed, a joint action of environmental agencies, farmers and administration agencies is needed for a progress with more BMPs alternatives together with effective agricultural practices. The different policies need to find convergence through joint acts. Thus, greater, broader, strongly and clearly initiatives are demanded to conciliate the economic development with an effective and lasting environmental protection.

4.5 Acknowledgements

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5 Summarizing discussion and conclusion

5.1 Summary discussion with key achievements

This dissertation presented a methodical approach for the improved understanding of nitrate processes in models by focusing on accurate process representation in ecohydrological modeling, resulting in more reliability in the simulations for environment analyses. Based on this, more realistic scenario simulations are obtained. This goal was achieved by (i) the detection of temporal dominant nitrate processes, (ii) by the development of a new calibration approach considering discharge and nitrate simultaneously and (iii) by analyzing the impact of different management practices on nitrate loads at the catchment scale using the well-calibrated SWAT model. The central findings coming out from the three research questions as stated in the introduction are highlighted below. Likewise, the limitations and the potentials for future research are addressed afterwards.

Nitrate process dynamics investigation is from the beginning a hard task due to processes interactions and data scarcity. These complexities challenge scientists in applied environmental investigations as well with the use of ecohydrological models. The conception and assessment of models for nitrate processes simulation requires firstly knowledge about the process dynamics. In this sense, this issue evoked this first question:

- *Is an ecohydrological model able to reproduce realistically temporal patterns of dominant model parameters for the complex nitrate cycle?*

To answer this research question, temporal variations in dominant nitrate parameters and processes in ecohydrological modeling were analyzed. It was answered using Temporal Dynamics of Parameter Sensitivity (TEDPAS). The method provided the sensitivity of the investigated model parameters in a daily resolution and was innovatively applied for the first time to a water quality variable (nitrate). The results shown in Chapter 2 indicated high variations in the sensitivity of nitrate parameters within the modeling period for the study area. These variations are strongly related to nitrate transport processes and the plant uptake processes.

The model simulations considered well how nitrate transport is related to surface and subsurface flow. Furthermore, the ability of intense precipitation events to leach nitrate was highlighted (see Section 2.4.3, Fig. 2.6). Plant uptake also evoked high sensitivities in the associated model parameters in times of crop growth indicating a plausible representation in the SWAT model (see Section 2.4.3, Fig. 2.6). Moreover, the sensitivity of nitrate parameters in the aquifers in these periods indicates the relevance of nitrate transport via subsurface flow.

Thus, TEDPAS method for nitrate investigation provided additional model diagnostic information regarding the nitrate process dynamics. It detected important parameters for the representation of complex process dynamics related to nitrate transport and transformation and also its removal from soil by plants. The capture of these temporal sensitivities by the model indicated a consistency of the process dynamics for each time step. Thus, analyzing temporal varying sensitivities helps to achieve consistent process representation in the model.

As TEDPAS method identified parameters that dominate the nitrate simulations in specific periods, these outcomes could also be used for further model calibration. In this way, the next step was to proceed to a model calibration approach considering more specific nitrate parameters. For simulating and investigating nitrate processes in ecohydrological modeling, both hydrologic and nutrient cycles need to be well calibrated. This assumption resulted in the second question:

- *How can river discharge and nitrate loads be jointly calibrated for ecohydrological modeling considering their interactions?*

For reliable representation of the nitrate dynamics in the catchment, a calibration procedure of the SWAT model had to be carried out which considers the relationship of nitrate to water movement. Following this, the second research question was answered by developing a procedure for joint calibration of discharge and nitrate loads (Chapter 3). It consisted of a multi-metric calibration considering traditional statistic performance metrics and signature measures for both variables simultaneously. The multi-metric approach was able to represent distinct phases and/or conditions for discharge and nitrate. In this way, this approach enhanced model evaluation by considering more details of the simulated discharge and nitrate processes. The transfer of 5FDC (Pfannerstill et al., 2014) to 5NDC leads to the use of different magnitudes of nitrate loads separately for the multi-variable calibration approach.

Furthermore, a good simulation of nitrate indicates a satisfactory reproduction of hydrological processes by the model. This is not only related to total discharge, but also the different phases of the hydrograph as emphasized by the use of the flow duration curve (FDC). For example, a good discharge simulation does not guarantee an appropriate reproduction of the runoff components. However, a good nitrate simulation is impossible with an inaccurate simulation of the runoff flow paths such as too high values of surface runoff. Thus, achieving good nitrate calibration means a better calibration of runoff components.

The calibration approach contributes to achieve higher confidence in the selection of good model runs. The performance measures considered in the procedure are also a way to reduce equifinality among model parameters (Beven, 2006) by a more precise identification of the model parameters using contrasting performance measures and a separate evaluation of distinct phases of the hydro- and nitrograph. In this way, the calibration approach led to plausible simulations of discharge and nitrate loads. The results of such investigations and the achievement of reliable model simulations is a basis for future applications of models in environmental and water quality studies. Based on this, the third question that came up was:

- *How effective is the implementation and simulation of different Best Management Practices (BMPs) for nitrate loads reduction at the catchment scale?*

To answer this question, the SWAT model was used for the simulation of different BMPs in the Treene catchment. With the results coming from the calibrated and validated SWAT model, it was possible to use the model results to further investigations of nitrate dynamics regarding land use and management changes.

In this sense, the last research question showed a SWAT model application after the previous nitrate process dynamics investigation and calibration approach. As an actual issue, the nitrate pollution in the river derived from agricultural activities and also land use changes were investigated with a well understood and better calibrated model. The simulation of BMPs showed in Chapter 4 indicated the ability of the SWAT model to account land use changes and management modifications at the catchment scale. Small, mid and large changes were simulated in the catchment and, even if slight, there were responses in nitrate loads at the outlet. So, the considered management practices indicated substantial potential for nitrate loads reduction. In particular, the joint use of different management practice led to higher reductions.

The outputs of the scenario simulations are useful for extended activities like economic evaluations. They were shown in the costs evaluation regarding pollutant reductions and management changes. This approach could be helpful for decision makers for future strategies of sustainable development. Likewise, the complexity and importance of a dialog between different governmental policies was highlighted in the light of the simulated BMPs and their results.

5.2 Research limitations

Despite the detailed investigation of nitrate dynamics in models and the achievement of reliable model simulations, there are still limitations in the applied methods which need to be known for further and deeper investigations.

Firstly, the sensitivity patterns as derived by the TEDPAS method (Chapter 2) strongly depend on the accuracy of the existing model structure. Thus, TEDPAS can be used as a step for model plausibility evaluation, as for example proposed by Pfannerstill et al. (2015). Furthermore, in a joint approach of parameter sensitivity and model performance, intern model structure deficiencies can be detected as shown in Guse et al. (2014). By using TEDPAS with modeled time series, it is only to a certain extent possible to affirm that a specific process representation in the model is totally well represented without using long-term and spatially distributed observation data.

The data availability for model parameter investigations is strongly related to this point. Data scarcity is still a limitation to achieve better model results (Rode et al., 2007). For example, detailed data related to nitrate cycle such as denitrification and mineralization rates could lead to better parameter estimation. The whole influences of water table level, temperature and soil properties on these processes are unknown. All nitrogen modifications are very sensitive to environmental conditions and this situation can lead to uncertainty in parameter estimation. The lack of information to parameter estimation can increase the uncertainty in the model simulations (Pechlivanidis et al., 2011). Likewise, the absence of longer nitrate time series is a limitation for the investigation of model performance. Model calibration and validation need data for simulation performance assessment (Epelde et al., 2016).

The parameter set chosen from the model calibration approach (Chapter 3) is strongly related to the considered performance measures. These metrics symbolize the representation quality of specific processes, but no performance measure can totally assess the representation of nitrate processes. This situation is not properly a complete limitation, however understanding about the degree of simulation efficiency is still under debate in the scientific community (Shafii et al., 2015) and would be an improvement for the calibration topic. In this way, probably different parameter sets and thus modeled time series would arise by utilizing distinct performance measures. The research focus influences the choice of specific performance measures to account for particular processes. However, appropriate performance measures were used, investigating details in dynamics and magnitudes in a balanced way for this calibration procedure. The selected performance measures support the developed method and model simulations well.

The BMPs simulations with the SWAT model for a larger catchment (Chapter 4) demonstrated good simulation of nitrate processes by the model. However, in general simplifications are required for model applications at this spatial scale. By using spatial distributed land use and soil information, the spatial heterogeneity within the catchment is considered in the input data. However, the calibration at this scale does not consider the spatial heterogeneity within the catchment when only using time series of the catchment outlet as representation for the whole catchment. Thus, nitrate process dynamics investigations are impaired at this scale.

5.3 Future research

Based on the previous discussions and statements as well as on limitations, recommendations for future research can be given. First, one can investigate the applicability of the steps in this thesis to other models and catchments. This approach is important to improve nitrate processes understanding and so enhance the modeling for environment applications.

Even though the TEDPAS analysis for nitrate is in principle applicable to other models and catchments, further investigations of the modeling processes in different models and also for different catchments are required. With this, important temporally dominant parameters and processes for different eco-hydrological conditions can be investigated and compared, indicating possible determinant characteristics, which will influence nitrate process dynamics in the study catchment. For instance, catchments covered with crop monoculture, uniquely by forest or also with predominantly urban areas would probably lead to different TEDPAS results. Likewise, catchments in mountainous areas, with different geologic formations or with predominantly sandy soils or much humus would result in varying behavior. These features alter the runoff components, nitrate residence time in soil and also plant uptake. Consequently, other biochemical reactions will affect nitrate processes. This last point is very important for temporal parameter sensitivity investigation in catchments with different climatic conditions.

The calibration procedure developed in this thesis is independent from catchment and model. However, it should be further tested in other ecohydrological models and conditions as mentioned above. These environmental variabilities will equally influence the calibration approach once different processes will be more or less sensitive to the model performance. The investigation regarding interrelations of hydrologic and nitrate parameters and processes under different environmental conditions is worthy of further studies.

Following this principle, the BMPs implementation approach should be carried out in other catchments, with different sizes, geographic realities and management practices. Moreover, other ecohydrological models should be tested for the same scenarios of this study and study area, but also for other BMPs. An investigation of the effectiveness of a specific BMP in reduce nitrate loads under different conditions can lead to better process dynamics understanding. By knowing the differences between two or more models and assessing their outputs of BMPs, simulations can be helpful for management decisions.

A further step would be transfer of the procedures to other variables. The verification of TEDPAS applicability with other nutrients such as phosphorus and also for sediment is an important further study. In this context, the relevance of certain hydrological processes such as surface runoff might be of higher relevance. The soil properties in the catchment will also affect temporal dynamics due to its composition and structure, for example. Nevertheless, for these variables it will also be important to take into account human activities related to water quality.

The joint multi-metric calibration approach developed could also be tested for phosphorus and sediments and other variables with strong relation to hydrology processes. It would be an important achievement to investigate model behavior and evaluate the parameters with stronger relationship in a joint calibration.

The transfer of BMPs implementations to other variables is quite well known. However, simulating BMPs after applying the first two steps of this thesis would be positive to obtain a more reliable model simulation. This can also be a good exercise to compare model performance with other modeling approaches.

Moreover, the verification of TEDPAS with other variables as well as the calibration approach with other variables can also contribute to the investigation of structure deficiencies in processes simulations. Regarding TEDPAS this occurs once the parameter sensitivities do not fit with the expected process dynamic behavior. In regard to the calibration approach there can be a deficiency once no parameter set would achieve plausible results. Surely, previous knowledge of process dynamics is needed to determine whether the sensitivities match reality, when the performance is good or not. In this sense, other methods need to be additionally implemented to evaluate the uncertainty source in model simulations.

There are many studies about model structure investigation and process understanding regarding hydrological aspects (Euser et al., 2013; Guse et al., 2014; Hrachowitz et al., 2014; Pfannerstill et al., 2015). Indeed, the hydrologic processes are complex by themselves; a further transfer of these approaches to water quality variables is even more complex due to the processes interactions. By investigating water quality variables the hydrologic components cannot be excluded; there is an additive complexity, and so this is an important future research topic. Up to now there are few studies involving processes understanding and model evaluation regarding nitrate, and considering the two first steps of this thesis, there is a high potential for the application for other water quality models.

In further studies, the spatial resolution should be considered in addition to the temporal resolution, bringing the temporal and spatial scales closely together. Likewise, the consideration of differences in the spatial scale can also be a further research step with TEDPAS investigation as well as the implementation of BMPs in larger catchments. This means an investigation utilizing different sub-basins simultaneously in one approach. The development of an extension from the steps of this thesis to spatial distributed investigations is therefore a future research possibility. The establishment of nutrient measures at strategic hot spot areas in the Treene catchment would be a new approach. Keeping in mind that this catchment is characterized by the landscape units Östliches Hügelland and Geest, a measurement station located at the transition point between both landscapes can enhance the understanding about the differences in the environment process dynamics between both landscapes.

Nevertheless, it is important to consider the scale-dependence of natural processes (Buck et al., 2004) by investigations using more spatial details. This will not cover all spatial data lacking for a calibration approach since the catchment heterogeneity can be huge. Data from one sub-basin is generally not equally applicable for others in a large catchment. However, the consideration of available spatial differentiations can improve processes modeling using spatial distributed models and also improve real approaches at the catchment scale. Furthermore, one approach which applies TEDPAS to nitrate and the developed calibration procedure in different spatial scales can also lead to process dynamics understanding improvement.

For future research possibilities it is still worth emphasizing the importance of water quality monitoring. The permanent measurement activity is crucial for investigations about the reality in the catchments, the impacts of soil use and is further important for the modeling approach and management implementation assessment.

5.4 Conclusion

This dissertation investigated nitrate processes in ecohydrological modeling at the catchment scale. The three steps of this thesis address nitrate in different research shapes. The consideration and investigation of the temporal patterns of dominant model nitrate parameters is highly important to model process dynamics understanding and evaluation. Temporal dominant parameters give insights about the model process dynamics representation in comparison to reality.

Furthermore, a calibration approach which considers the importance regarding the relationship of hydrology components with nitrate process dynamics leads to a model with more reliable outputs for further investigations. Once the model is consistently simulating hydrologic and nitrate process dynamics, the outcomes can be used for environmental application. A reliable model brings more confidence to the outputs simulated. This reliable model was achieved by the sequential application of the three steps within this thesis.

The knowledge of the thesis contributes to enhance the nitrate processes understanding, their improvement and also further implementing in empirical studies. Further investigations and tests regarding these topics will improve this knowledge and make the modeling approach even more useful for society.

6 References

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Erklärung

Hiermit erkläre ich, dass ich die vorliegende Dissertation, abgesehen von der Beratung durch meine Betreuer, selbständig verfasst habe und keine weiteren Quellen und Hilfsmittel als die hier angegebenen verwendet habe. Diese Arbeit hat weder ganz noch in Teilen bereits an anderer Stelle einer Prüfungskommission zur Erlangung des Doktorgrades vorgelegen. Ich erkläre, dass die vorliegende Arbeit gemäß den Grundsätzen zur Sicherung guter wissenschaftlicher Praxis der Deutschen Forschungsgemeinschaft erstellt wurde.

Kiel, 05.08.16

Marcelo Batista Haas