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Arbeitsgruppe Hydrologie / Klimatologie

INTEGRATED WATER QUALITY MODELLING IN MESO- TO LARGE-SCALE CATCHMENTS OF THE ELBE RIVER BASIN UNDER CLIMATE AND LAND USE CHANGE

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"Wer nichts wagt, der darf nichts hoffen."
Friedrich Schiller

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"It always seems impossible, until it is done."
Nelson Mandela

Summary

In a changing world facing several direct or indirect anthropogenic challenges the freshwater resources are endangered in quantity and quality, and need protection as well as actions for improvement in order to ensure an adequate status for human and ecosystem wellbeing in the future. Various substances can influence the water quality of river ecosystems, including those naturally occurring in the watersheds. An excessive supply of nutrients, for example, can cause disproportional phytoplankton development and oxygen deficits in large rivers, leading to failure of the aims requested by the Water Framework Directive (WFD). Such problems can be observed in many European river catchments including the Elbe basin, where effective measures for improving water quality status are highly appreciated.

During the last decades computer-based modelling tools became more and more common in water resources management and protection. Models can help to understand the dominant nutrient processes in a watershed and to identify the main sources of nutrient pollution in the river network. Furthermore, they can be effective tools for impact assessments investigating the effects of changing climate or socio-economic conditions on the status of surface water bodies, and for testing the usefulness of possible protection measures. An important prerequisite for successful model applications is a sufficiently detailed process description in a model including all relevant ecosystem compartments, as well as a careful model setup and calibration/validation. Due to the high number of interrelated processes, ecohydrological model approaches containing water quality components are much more complex than the pure hydrological ones, their setup and calibration/validation require more efforts, and thus they are less applied in the scientific community for impact studies. Such models, including the process-based semi-distributed Soil and Water Integrated Model (SWIM), still need some further development and improvement for a more realistic water quality modelling, especially in large catchments.

Therefore, this cumulative dissertation focuses on two main objectives: 1) the approach-related objectives aiming in the SWIM model improvement and further development regarding nutrient (nitrogen and phosphorus) process description, and 2) the application-related objectives in meso- to large-scale Elbe river basins to support adaptive river basin management in view of possible future changes. The dissertation is based on five scientific papers published in international journals and dealing with these research questions.

Several adaptations were implemented in the model code to improve the representation of nutrient processes in the catchments under investigation. Firstly, the model application in the meso-scale Rhin catchment was improved by including a simple approach for a better simulation of specific water and nutrient processes in wetland soils. In the Saale case study, the ammonium pool was added to the model for a more comprehensive description of the nitrogen cycle. While calibrating the SWIM model for the Rhin and Saale catchments it was found, that the simple routing of nutrients through the river network is not sufficient to represent their seasonally observed concentrations, especially of those nutrients coming mainly from point sources. Therefore, a detailed in-stream module was added to the SWIM model structure, simulating algal growth, nutrient transformation processes and oxygen conditions in the river reaches, mainly driven by water temperature and light. This new approach created a highly complex ecohydrological model with a large number of additional parameters, which could be calibrated. However, testing less complex methods to represent retention processes in the

landscape and/or river network did not result in comparably good model performances for all nutrients under investigation.

The calibration and validation of the SWIM model enhanced by the new approaches in the selected subcatchment and the entire Elbe river basin delivered satisfactory to good model results in terms of criteria of fit. Thus, the calibrated and validated model provided a sound base for the assessment of possible future changes and impacts.

Simple climate sensitivity experiments were applied in the smaller catchments, and finally a detailed climate change impact assessment for the entire transboundary Elbe river basin was conducted, driven by a set of 19 regionally downscaled climate scenarios for the reference and two future periods. The ensemble of climate scenarios projects rising average temperature and precipitation for the Elbe watershed with increasing trends, leading to higher river discharge, and spatially variable changes in nutrient loads in future periods. The variability in water quality results can be explained by the heterogeneity of the large-scale case study area, as well as the high number of interrelated landscape and in-stream nutrient processes. Applying some land use and management change experiments, it could be concluded that some measures and their combinations have a potential to intensify or reverse climate change impacts, which could be helpful to derive feasible adaptation methods.

Modell-based impact studies always come along with a certain degree of uncertainty of results, which can be related to input data, model structure or scenarios, and further steps could be undertaken to reduce some of these uncertainties. A model with a large number of included processes and highly sensitive calibration parameters generally suffers from high calibration efforts and probable uncertainty related to parametrisation. It should thus be decided in advance, whether the new developed SWIM with the implemented in-stream module should be applied in a specific case study, or not. Depending on the research question, the original SWIM version could be sufficient, e.g. for pure nitrate nitrogen modelling or the assessment of diffuse nutrient pollution from agriculture.

Nevertheless, there are some research questions, where the new developed SWIM version would definitely be advantageous, especially in the large-scale and plankton dominated rivers. The new in-stream module is an important contribution to improve the representation of nutrient processes in the SWIM model, particularly for nutrients coming mainly from point sources directly to the rivers (e.g. phosphate phosphorus). The new enhanced modelling approach improved the applicability of the SWIM model for the WFD related research questions, where the ability to consider biological water quality components (such as phytoplankton) is important. The results of the impact assessments presented here can be used by decision makers and stakeholders for understanding future challenges and for applications aimed in adaptive management of the Elbe river basin.

Zusammenfassung

In einer sich ändernden Umwelt sind Fließgewässerökosysteme vielfältigen direkten und indirekten anthropogenen Belastungen ausgesetzt, die die Gewässer sowohl in ihrer Menge als auch in ihrer Güte beeinträchtigen können. Viele Oberflächenwasserkörper bedürfen daher besonderer Schutz- und Entwicklungsmaßnahmen zur Gewährleistung eines guten ökologischen Zustands in der Zukunft. Verschiedene – auch natürlich vorkommende – Stoffe können die Wasserqualität eines Fließgewässers beeinflussen. Ein übermäßiger Eintrag von Nährstoffen verursacht etwa Massenentwicklungen von Algen und Sauerstoffdefizite in den Gewässern, was durch Änderungen der Umweltbedingungen noch verstärkt werden und zum Verfehlen der Ziele der Wasserrahmenrichtlinie (WRRL) führen kann. In vielen europäischen Einzugsgebieten und auch dem der Elbe sind solche Probleme zu beobachten.

Während der letzten Jahrzehnte entstanden diverse computergestützte Modelle, die zum Schutz und Management von Wasserressourcen genutzt werden können. Sie helfen beim Verstehen der Nährstoffprozesse und Belastungspfade in Einzugsgebieten, bei der Abschätzung möglicher Folgen von Klima- und Landnutzungsänderungen für die Wasserkörper, sowie bei der Entwicklung eventueller Kompensationsmaßnahmen. Aufgrund der Vielzahl an sich gegenseitig beeinflussenden Prozessen ist die Modellierung der Wasserqualität generell komplexer und aufwändiger als eine reine hydrologische Modellierung, so dass sie bisher in der Wissenschaft seltener angewendet wird. Ökohydrologische Modelle zur Simulation der Gewässergüte, einschließlich des prozess-basierten und halb-aufgelösten Modells SWIM (Soil and Water Integrated Model), bedürfen auch häufig noch einer sorgfältigen Weiterentwicklung und Verbesserung der Prozessbeschreibungen, insbesondere in großen Einzugsgebieten.

Aus diesen Überlegungen entstand die vorliegende Dissertation, die sich zwei Hauptanliegen widmet: 1) einer Weiterentwicklung des Nährstoffmoduls des ökohydrologischen Modells SWIM für Stickstoff- und Phosphorprozesse, und 2) der Anwendung des Modells SWIM im Elbegebiet zur Unterstützung eines anpassungsfähigen Wassermanagements im Hinblick auf mögliche zukünftige Änderungen der Umweltbedingungen. Die kumulative Dissertation basiert auf fünf wissenschaftlichen Artikeln, die in internationalen Zeitschriften veröffentlicht wurden.

Im Zuge der Arbeit wurden verschiedene Modellanpassungen in SWIM vorgenommen. Für die Anwendung im Einzugsgebiet des Rhin wurde zunächst ein einfacher Ansatz zur Verbesserung der Simulation der Wasser- und Nährstoffverhältnisse in Feuchtgebieten getestet. Bei der Modellierung des Saaleeinzugsgebietes wurde Ammonium in den Stickstoffkreislauf im Boden integriert. Bei beiden Modellanwendungen zeigte sich, dass ein einfaches Routing der Nährstoffe im Fließgewässersystem nicht ausreicht, um die beobachteten Konzentrationen in ihrer saisonalen Dynamik am Gebietsauslass zufriedenstellend abzubilden, insbesondere für direkt eingetragene Nährstoffe aus punktuellen Quellen. Daher wurde ein Modul in SWIM integriert, das Umwandlungsprozesse, Sauerstoffverhältnisse und Algenwachstum im Fließgewässer selbst simuliert, was aber auch dazu führte, dass durch eine Vielzahl an neuen Parametern die Komplexität des ökohydrologischen Modells merklich erhöht wurde. Der Test weniger komplexer Ansätze zur Retention von Nährstoffen im Saalegewässernetz erzielte jedoch nicht für alle Stoffe zufriedenstellende Ergebnisse.

Die Kalibrierung und Validierung der erweiterten SWIM-Modellansätze führte zu guten Ergebnissen in den Teileinzugsgebieten und dem gesamten Gebiet der Elbe, so dass das Modell

zur Abschätzung möglicher Folgen von Klimavariabilitäten und veränderten anthropogenen Einflüssen genutzt werden konnte. In den kleineren Einzugsgebieten wurden zunächst einfache Experimente zur Klimasensitivität durchgeführt, worauf die detaillierte Analyse des Einflusses von 19 Klimaszenarien auf Wassermenge und -güte der Fließgewässer im Elbegebiet folgte. Die 19 Szenarien projizieren im Mittel steigende Temperaturen und Niederschläge für das Elbeeinzugsgebiet mit zunehmenden Trends in späteren Zukunftsperioden. Dies führte zu im Mittel höheren Durchflüssen in den Fließgewässern und räumlich variablen Änderungen der Nährstofffrachten, was mit der Heterogenität des großskaligen Untersuchungsgebietes, aber auch mit der großen Zahl an Prozessen und Rückkopplungen im Modellansatz erklärt werden kann. Analysen über Auswirkungen veränderter Landnutzung oder Managementmaßnahmen zeigten, dass einige Maßnahmen die Fähigkeit haben, Klimaauswirkungen zu intensivieren oder umzukehren, was wertvolle Hinweise für das Management liefern kann.

Die Ergebnisse modellgestützter Wirkungsstudien sind immer mit einem bestimmten Maß an Unsicherheit behaftet, die sich auf verschiedene Faktoren zurückführen lässt, und einige weiterführende Maßnahmen ließen sich denken, um die Spanne der Unsicherheiten zu reduzieren. Ein prozessbasiertes Modell mit einer großen Menge an sensitiven Kalibrierungsparametern geht generell mit einem großen Kalibrierungsaufwand und starker Parameterunsicherheit einher. Es sollte daher schon im Vorfeld entschieden werden, ob die Anwendung des erweiterten SWIM-Modells mit integrierten Fließgewässerprozessen in einer spezifischen Fallstudie wirklich notwendig ist. Abhängig von der Forschungsfrage könnte auch die originale SWIM-Version ausreichend sein, so etwa für die ausschließliche Nitratmodellierung oder bei der Abschätzung der diffusen Nährstoffverschmutzung aus der Landwirtschaft.

Darüber hinaus gibt es jedoch auch einige Forschungsfragen, bei denen die detaillierte Modellierung von Nährstoffprozessen im Gewässer vorteilhaft ist, insbesondere in großskaligen und planktondominierten Fließgewässern. Das neue Fließgewässermodul ist ein wichtiger Beitrag zur Verbesserung der Nährstoffmodellierung in SWIM, vor allem für Nährstoffe, die hauptsächlich aus Punktquellen in die Gewässer gelangen (wie z.B. Phosphat). Der neue Modellansatz verbessert zudem die Anwendbarkeit von SWIM für Fragestellungen im Zusammenhang mit der WRRL, bei der biologische Qualitätskomponenten (wie etwa Phytoplankton) eine zentrale Rolle spielen. Die hier dargestellten Ergebnisse der Wirkungsstudien können bei Entscheidungsträgern und anderen Akteuren das Verständnis für zukünftige Herausforderungen im Gewässermanagement erhöhen und dazu beitragen, ein angepasstes Management für das Elbeeinzugsgebiet zu entwickeln.

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CHAPTER 1

INTRODUCTION AND BACKGROUND

The availability of sufficient fresh water with an adequate quality for the human society and ecosystems is one of the most important challenges for the future. According to the Water Framework Directive (WFD; EC, 2000) it is a common aim in the European society to keep the surface water quality parameters below certain thresholds to ensure a “good ecological status” of water bodies in order to provide a suitable living environment for flora and fauna, including many endangered species, and to preserve the natural water resources for future generations.

Water and nutrient transport processes in river basins are strongly connected. The quantity and quality of water resources can be significantly influenced by natural or human-induced environmental changes in climate conditions, land use composition or inputs from urban and industrial sources. These are essential factors controlling the ecohydrological characteristics of catchments and the resulting water quality of the rivers.

The potential impacts can vary considerably at different spatial and temporal scales, and have to be studied in order to improve the preparedness of people and to assure the adaptive capacity of the individual catchments to possible future changes. Modelling tools and scenario simulations can be helpful instruments in impact assessments, subject to the condition that the models are well developed, set up and calibrated, and include all relevant water and nutrient transport and transformation processes occurring in the catchment under investigation and influencing water quality of the surface water bodies.

This cumulative dissertation is a combination of five scientific publications dealing with water quality modelling (nitrogen and phosphorus) and the nutrient’s reaction to possible climate and socio-economic changes in the Elbe river basin and its selected subbasins. The main task for this thesis was to develop further and apply the water quality modelling module of the semi-distributed ecohydrological watershed model SWIM (Soil and Water Integrated Model) (Krysanova et al., 2000) in meso- to large-scale river catchments under future climate and land use scenarios involving uncertainty. The model results should be a step towards an adaptive water resources management in the Elbe (sub-)catchment(s) under study.

1.1 Water quality and global change impacts

1.1.1 Nutrient processes in river basins of a temperate climate

Nutrients are elements and their combinations which are consumed by plants for primary production and creation of organic material. The basic elements in nature are carbon, oxygen and hydrogen, and the main nutritive substances for plants are nitrogen, phosphorus, sulphur, potassium, calcium and magnesium. Within the natural environment, the nutrients are subject to several adsorption and transformation processes, causing the occurrence of a high number of different stable and active nutrient forms in the soils and water resources of a landscape (Scheffer & Schachtschabel, 2002).

Normally, more than 98% of the nutrition material in soils is minerally or organically bound, and only 2% of nutrients occur removably sorbed or dissolved in the liquid soil phase (Schroeder, 1992). In dissolved form nutrients usually exist as anions or cations in the soil solution originating from weathering of inorganic material or mineralisation of organic matter, and can be uptaken by plant roots. The nutrient amount in soils can be increased by fertilisation, atmospheric deposition, groundwater inflow or fixation from the atmosphere, and decreased by plant uptake, leaching/erosion to the river network, or denitrification. The removal of nutrients and organic material from soils generally results in increased mobilisation processes (Hornbeck & Kropelin, 1982). Mobilisation and immobilisation processes are important parts of the soil's nutrient balance. They can be influenced by several factors, such as soil moisture, soil temperature or the redox potential.

However, if dissolved nutrient concentrations exceed a certain level in a water body (mainly caused by human activities), serious adverse effects for ecosystems and economy can occur. Then the intrinsically essential nutrients can cause eutrophication processes accompanied by oxygen deficits and a decrease of biodiversity in surface water ecosystems, or impact the quality of groundwater and the drinking water supply (compare section 1.1.2). The most important nutrients causing problems in this context are nitrogen (N) and phosphorus (P). Therefore, the general transformation and transport processes in river basins of these two nutrients will be described in more detail here.

Figure 1.1 shows conceptual diagrams of the N and P pools in soils, and main transformation and transport processes influencing them. The cycles have some similarities, but also differences, mainly depending on the stability and individual affinity of the nutrients to soil particles. Without anthropogenic influence the nitrogen cycle, including gaseous nitrogen components, proceeds much quicker in nature than the phosphorus cycle without gas involvement and with a high share of stably bounded phosphorus in stony material (Bayrhuber & Kull, 1989).

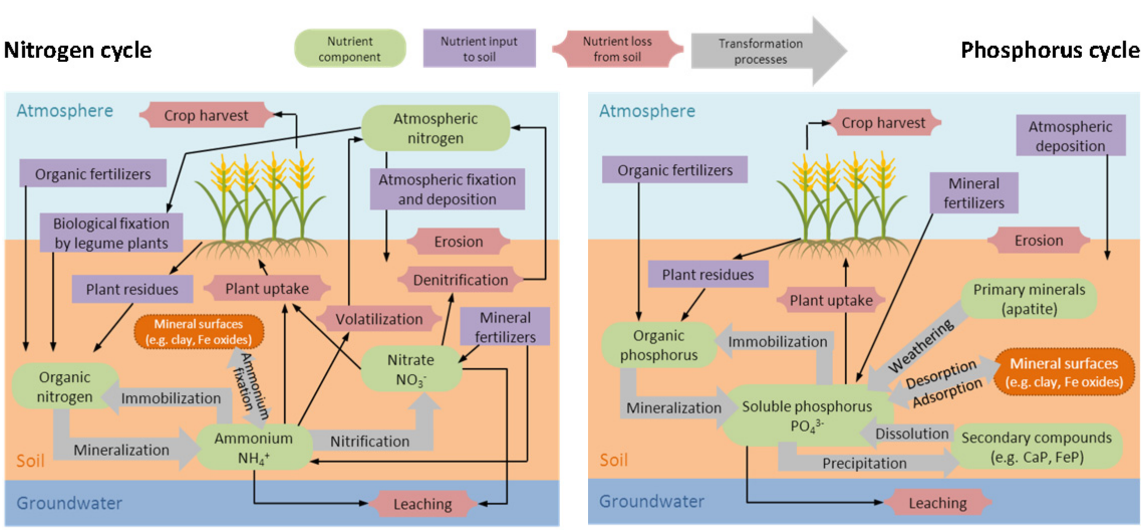

Figure 1.1 Conceptual diagrams of the nitrogen (left) and phosphorus (right) cycles in soils including the most important nutrient components, transformation processes and input / loss paths (altered from www.ipni.net).

The nitrogen cycle in soils

More than 90% of the soil nitrogen pool consists of organic compounds, e.g. humic substances, plant residues and organic biomass (Scheffer & Schachtschabel, 2002). Only a small part of the nitrogen pool has an inorganic character and is available for plants, especially the readily soluble and therefore easily leachable nitrate (NO_3^-) and, in lower concentrations, the more soil particle-affine ammonium (NH_4^+). Nitrogen is added to soils by mineral and organic fertilisers, plant residues, atmospheric deposition, and biological N_2-fixation from the atmosphere by legume plants. Nitrogen leaves soil by plant uptake and harvest, denitrification, volatilisation, erosion and leaching (Figure 1.1, left).

There are several processes transforming the nitrogen substances in soils. Organic substances and residues are converted to NH_4^+ by microorganisms (mineralisation or ammonification). This process enhances with increasing temperature reaching an optimum at about 50°C (Myers, 1975). The mineralisation is also facilitated by a C:N-ratio lower than 25; whereas soil moisture and the pH-value are less important (Scheffer & Schachtschabel, 2002). A part of the generated ammonium can be bounded to soil particles, mainly in soils with a high clay and low sand content (ammonium fixation). This bounding is subject to seasonal variations in the equilibrium of the soil solution. Other parts of the ammonium pool can be ingested by soil organisms or uptaken by plants to form very stable new organic material (immobilisation). Free ammonium forms are often converted to nitrate (NO_3^-) by microbial nitrification processes. This process is also affected by the soil temperature, and reaches an optimum at 35°C (Myers, 1975). As the nitrification process is faster than the ammonification, the ammonium concentration in soils is usually low (Scheffer & Schachtschabel, 2002). However, NH_4^+ enrichment can occur under low temperatures and in an anaerobic environment (e.g. at high groundwater levels).

The inorganic nitrogen forms can leave soil by plant uptake or by their transformation to atmospheric nitrogen (denitrification of NO_3^- to N_2 and volatilisation of NH_4^+ to NH_3). The denitrification is the most important reduction process for nitrate in soils, conducted by microorganisms, which use the oxygen of nitrate as electron acceptor, gradually changing the redox potential of nitrogen ($NO_3^- \rightarrow NO_2^- \rightarrow NO \rightarrow N_2O \rightarrow N_2$). Denitrification occurs only in anaerobic conditions, mainly at soil water contents higher than 60% (Bremner & Shaw, 1958; Shelton et al., 2000). The total nitrogen loss due to denitrification generally increases with higher soil moisture and finer soil texture, and is also a function of pH-value and available carbon and nitrate (Weier et al., 1993; Giles et al., 2012). The volatilisation of ammonium to gaseous ammonia occurs in alkaline soils or after organic nitrogen fertilisation. Amongst others the process is influenced by the pH-value, water content and temperature of the soils as well as by the exchange potential with the atmosphere (Fenn & Hossner, 1985).

The phosphorus cycle in soils

The main share of the soil phosphorus appears in a sorbed form (e.g. at mineral surfaces, in organic compounds, or in organic material), and only less than 0.1% occurs in the liquid phase. The inorganic soluble phosphate (PO_4^{3-}) in the soil solution usually has concentrations between 0.001 and 0.1 mg L^{-1}. In the upper soil layers this concentration can be increased up to 5 mg L^{-1} after fertilisation. Soils with a high binding capacity usually have lower soluble phosphate concentrations than soils with lower binding capacity (Scheffer & Schachtschabel, 2002).

Figure 1.1 (right) shows the general sources, loss pathways and transformation processes influencing the phosphorus pool in soils. Rocks and stones are the largest global storages of phosphorus, which comes to the pedosphere by weathering of primary minerals. Phosphorus also enters soils by atmospheric deposition, fertilisation or decomposition of plant residues, and is reduced by erosion, plant uptake followed by harvest, and – only a small share – by leaching.

The share of organic phosphorus in the total soil phosphorus varies between 25 and 65%, and is decreasing in the soil profile corresponding to the humus content from the top to the lower soil layers (Scheffer & Schachtschabel, 2002). It can be transformed to soluble phosphate phosphorus by enzymes originating from microorganisms or fungi (mineralisation). The mineralisation processes are enhanced with a lower C:P-ratio (Mafongoya et al., 2000), and the seasonal mineralisation rates depend on the activity of soil organisms as well as on soil texture (Magid et al., 1996). A part of the soluble P pool can be uptaken by plants or ingested by soil organisms to form stable organic material again (immobilisation).

Other parts of the soluble phosphate phosphorus pool are usually strongly sorbed to the mineral surfaces of soil particles (e.g. clay or iron oxides) to form a mineral complex (adsorption) underlying a specific equilibrium as a function of the soil phosphorus saturation, the soil type, as well as the number of available anions, which compete against phosphate phosphorus for free sorption places. Solution processes from mineral surfaces (desorption) occur rarely due to specific pH-values (Scheffer & Schachtschabel, 2002).

Soluble phosphorus can be bond to calcium and iron to form secondary compounds, which leave the soil solution by precipitation (Tunesi et al., 1999; Wandruszka, 2006) but can be returned to the soluble soil phosphorus pool by dissolution processes under anaerobic conditions (Jayarathne et al., 2016).

Lateral nutrient flows through the river catchment

Nutrient movement within a catchment to the river network is highly connected to the water cycle and lateral water flows in a landscape (Figure 1.2). Nutrients can be transported either by leaching of soluble nutrient forms (connected to the subsurface and groundwater flows) as well as by erosion of soil particles with adsorbed nutrients (connected to the surface flow). Organic nutrient forms are transported mainly by erosion processes.

Due to its high solubility, nitrate nitrogen is primarily transported by water leaching from soils to the surface water bodies. In contrast, the positively charged and therefore higher sorptive ammonium nitrogen is transported mainly by erosion (Scheffer & Schachtschabel, 2002). In case ammonium nitrogen is applied in excess to sandier soils with low clay content and limited sorption ability, or originates in groundwater influenced soils of lowlands, it can be also transported by water (Voß, 2007; Mancino & Troll, 1990). For phosphorus, erosion is the main pathway due to its high sorption potential (Scheffer & Schachtschabel, 2002). However, under deep sandy or high organic matter soils, or due to increasing phosphorus concentrations in many agricultural soils caused by fertiliser application, leaching processes and subsurface losses of phosphorus to groundwater and drains are now observed more often (Sims et al., 1998; Ilg, 2007). Therefore, leaching of phosphorus becomes increasingly important, especially in lowland catchments with small slopes and erosion rates. However, compared to nitrogen, the input of phosphorus from the catchments to the rivers is relatively low (Pieterse et al., 2003).

In general, there is a distinct seasonal dynamics in the lateral nitrogen transport to the rivers, as the nitrogen transformation processes in soils and soil water are temperature and precipitation dependent (compare above). Besides, the nitrogen leaching and erosion processes in soils are influenced by the soil conditions, water dynamics, rainfall, vegetation pattern and land use measures as well. For example, the nitrogen leaching rate is higher in sandy than in clay soils (Scheffer & Schachtschabel, 2002; Zotarelli et al., 2006), and higher fertiliser application rates also increase the rate of N leaching (Mancino & Troll, 1990). Of course, the date of fertiliser application is also important (van Es et al., 2005). Erosion processes are mainly influenced by soil properties, slope, vegetation cover and the intensity of precipitation. In agricultural areas nitrate nitrogen leaching as well as losses of ammonium nitrogen with erosion are generally highest in periods with missing or lower vegetation cover (September – April) due to reduced plant uptake as well as less rootage and resulting lower soil stability (Vos & van der Putten, 2004; De Baets et al., 2011).

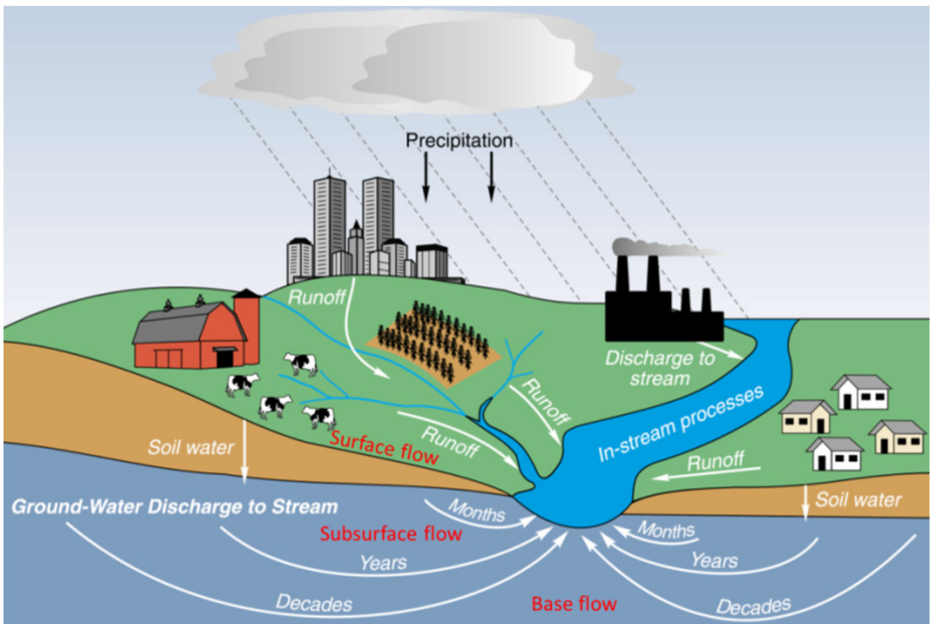

Figure 1.2 Nutrient movement in river catchments linked to water flows (slightly altered from Phillips et al., 1999).

During their lateral movement with the water flows to the river network, nutrients are subject to sorption and decomposition processes in the soils as described above causing a certain loss of nutrients in the soil water (nutrient retention) and a reduction of nutrients leaching to the river network. These processes are mainly a function of soil properties (e.g. soil texture, effective field capacity or depth of groundwater table) but are also influenced by management practices (e.g. drainage or riparian zones) (Wendland & Kunkel, 1999; Hattermann et al., 2006). Denitrification is the most important decomposition process of nitrate nitrogen, ammonium nitrogen is mainly reduced by adsorption to soil particles, but also by plant uptake, nitrification and volatilisation. Phosphorus adsorbs to sediments, organic matter and clay particles or can be taken up by microbial biomass. The general lag time of water in the catchment significantly affects the retention potential of both nitrogen and phosphorus in a catchment by facilitating physical, chemical and/or biological processes. The delay in nutrient transport to the rivers can have a time frame of years or even decades in the subsurface and base flows, so that changes in the nitrogen and phosphorus balance in the catchment are not immediately reflected by changes in nutrient emissions reaching the surface water bodies (de Wit & Behrendt, 1999).

In-stream nutrient processes

After reaching the river network, nutrients are additionally subject to transformation, retention, transport and fixation processes in the water column and the underlying sediments. These processes mainly reduce the nutrient concentrations and loads in the river waters and the resulting nutrient inputs to the oceans (Seitzinger et al., 2002). The in-stream nutrient processes are strongly influenced by algae or consumers' occurrence and growth, but also by physical boundary conditions such as light, water temperature, hydromorphology and – connected to it – flow velocity (Doyle et al., 2003; Munshaw et al., 2013; Lin et al., 2016; Bukaveckas et al., 2017).

Several nitrogen forms occur in the water bodies of catchments underlying a number of transformation processes (e.g. mineralisation, nitrification) as illustrated in Figure 1.3. A general nitrogen reduction can be achieved by denitrification processes (Hill, 1979). Volatilisation and uptake by algae/plants also cause a reduction of nitrogen in the water bodies. In contrast, for phosphorus the transformation processes in the rivers are less important. A reduction of phosphorus in the water column can be achieved mainly by sorption, sedimentation or uptake by algae/plants. Due to its high binding capacity, dissolved ammonium nitrogen can be also sorbed to particulate matter, and subsequently subject to sedimentation processes. Sedimentation and sorption are negatively correlated to the flow velocity (Behrendt & Opitz, 2000; Kronvang et al., 1999). Therefore, the importance of these processes is higher in lowland rivers with generally lower flow velocities than in rivers located in mountainous regions. For nitrate nitrogen, the sorption processes are less important. However, the denitrification intensity as well as phosphate desorption from sediments raises with increasing anaerobic conditions in slow flowing downstream river reaches (Triska & Higler, 2009).

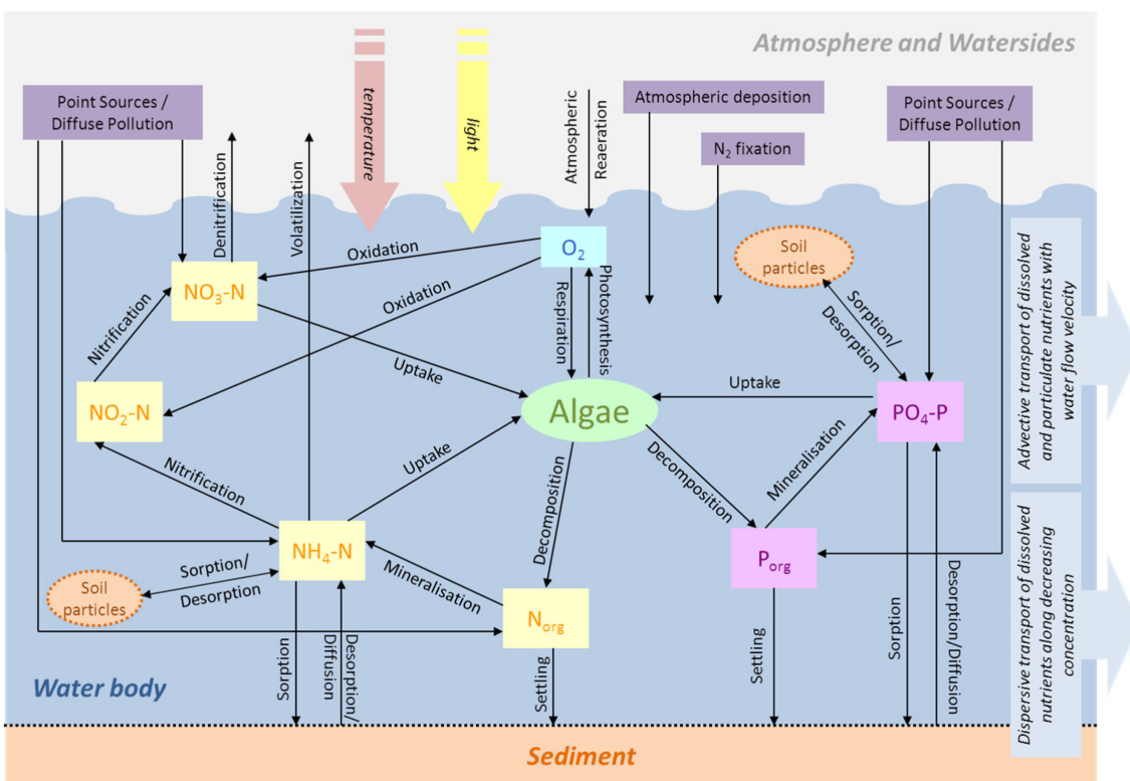

Figure 1.3 Main in-stream nutrient transport and transformation processes in rivers and streams influenced by nutrient inputs (violet boxes) and physical boundary conditions (italic).

Additional to a simple dispersive transport of nutrients along a decreasing concentration (diffusion) the advective transport of dissolved or particulate nutrients due to flow direction and velocity is the most important process influencing the concentration of nutrients at a certain river location in flowing waters. Therefore, the nutrient processes in rivers and streams cannot be really explained with a simple nutrient cycle. Several kinds of nutrient spiralling or river continuum concepts exists to describe the nutrient behaviour in rivers and streams taking into account the movement of water and substances within a river network, as well as the specific ecosystem conditions along the aquatic continuum from land to ocean (Bouwman et al., 2013).

The conversion and nutrient retention rates per meter of stream length generally increase with the stream order due to lower flow velocities, increased hydrologic residence time and resulting longer reaction time in downstream river reaches. However, quantifying the proportion of total nitrogen input that is removed as well as ranking the importance of small and large river reaches for nitrogen removal is difficult and depends on the level of spatial aggregation for which removal is reported, the underlying hydraulic and geomorphic factors and the magnitude of biological activity. Although larger river channels generally have the lowest reach-specific nitrogen removal, the proportional removal of upstream inputs by larger streams is several-fold greater than for smaller streams when considering the entire length of a stream of given order because of the cumulative effect of continued nitrogen removal along the entire flow path in downstream river reaches (Seitzinger et al., 2002; Wollheim et al., 2006).

In general, increasing the hydrologic connectivity, water surface area and residence time of water in a river ecosystem (e.g. by river restoration) significantly promotes the rate of nutrient retention at broader watershed scales (Newcomer et al., 2016) and helps to reduce negative effects on river water quality in order to improve the ecosystem services of river environments.

1.1.2 Nutrients as indicators of river water quality

In addition to a surface water quality assessment using hydromorphological river structures, indicator species or a saproby system, the water quality and ecologic potential of a surface water body can be detected by observing concentrations of nutrients and pollutants in the waters. For a good ecological status of a river it is important to minimise these concentrations, as high amounts of nutrients, heavy metals or organic pollutants may have negative impacts on the river ecosystem. Too high nutrient inputs can affect standing or flowing water ecosystems (eutrophication, see Figure 1.4) and, subsequently, the coastal sea areas.

According to Correll (1998), eutrophication is the overenrichment of receiving waters with mineral nutrients. The results are excessive production of autotrophs, especially algae and cyanobacteria. This high productivity causes extensive bacterial populations and high respiration rates, leading to hypoxia or anoxia in poorly mixed bottom waters and at night in surface waters during calm, warm conditions. Low dissolved oxygen causes a loss of aquatic animals, and release of many materials normally bound to bottom sediments including various forms of phosphorus. This release of phosphorus may reinforce the eutrophication. However, nitrification can also affect the oxygen availability in a river or lake by use of dissolved oxygen, causing time periods with too low oxygen concentrations for fishes and other species. Additionally, ammonia has a toxic effect on fish populations (Randall & Tsui, 2002). High concentrations of nitrogen also influence the usability of drinking water resources (Ward, 2009).

Depending on the N:P ratio in a water body, phosphorus is usually the limiting factor for primary production and even small additional amounts of it can cause eutrophication. In contrast, in the ocean, nitrogen often becomes the key mineral nutrient controlling primary production (Hecky & Kilham, 1988; Correll, 1998). Although several authors refer to phosphorus being the limiting factor for primary production, Dodds & Smith (2016) stated that both nitrogen and phosphorus control should be considered in the eutrophication management of streams.

Besides wet and dry atmospheric deposition (precipitation and fallout), many human activities cause water pollution with nutrient components. Pollutants can enter the river waters from point (e.g. sewage treatment plants) or diffuse sources (e.g. input with erosion or draining waters from agricultural fields). In an inhabited region a good ecological status of a water body can only be achieved by application of treatment measures for sewage waters and of adequate agricultural practices. Regarding the diffuse input of nutrients to water bodies, the main sources are substance-dependent according to its ability to be sorbed to soil particles. The phosphorus and ammonium inputs are mainly connected to erosion processes, whereas nitrate nitrogen is mainly leached from agricultural fields with water flows. Measures to reduce nutrient inputs and to apply a good agricultural practice should be connected to this special behaviour, as here are the most promising reduction potentials.

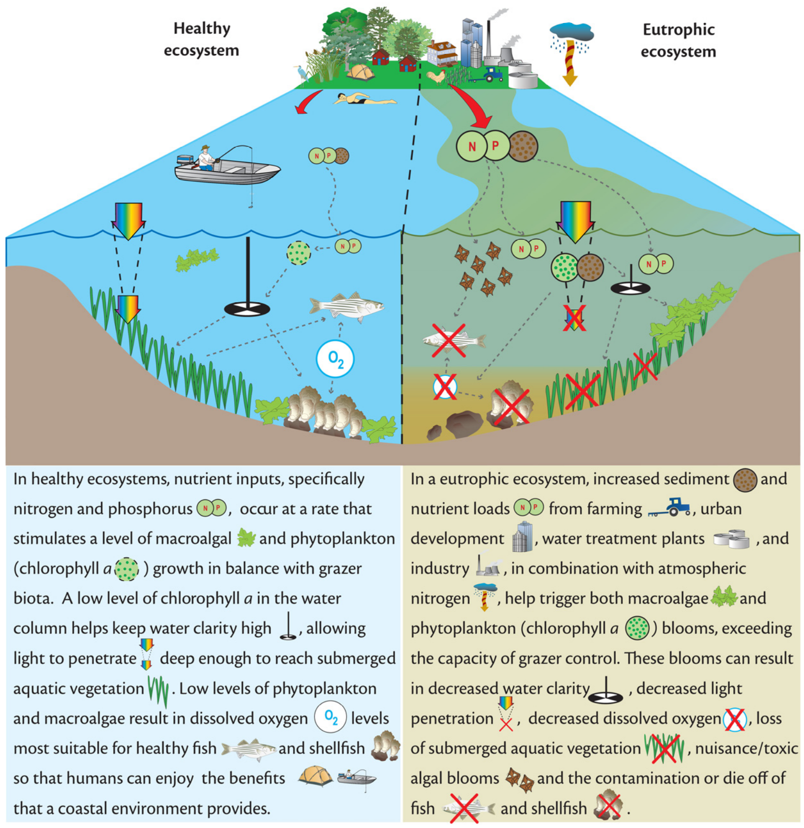

Figure 1.4 Comparison of a healthy water ecosystem to an unhealthy system exhibiting eutrophic symptoms (from Bricker et al., 2007).

Figure 1.5 gives an overview on the origin of nitrogen and phosphorus coming to German surface water bodies based on model assumptions for the period 2012-2014. The majority of nitrogen inputs come from the agricultural fields connected to groundwater and drainage flows (67% of all inputs) representing the nutrient's high leaching potential as a result of its low binding capacity to soil particles. Only a small share of the total nitrogen inputs is connected to erosion processes (1%). Total phosphorus, in contrast, comes mainly from urban and industrial areas and direct discharges (52% of all inputs). Due to phosphorus binding to soil particles, its relative inputs by erosion are notably higher than for nitrogen (16%).

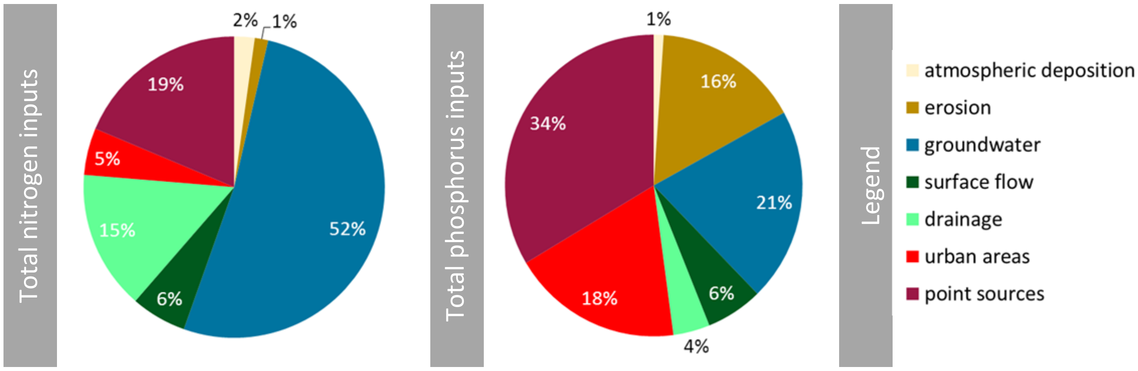

Figure 1.5 Origin of total nitrogen and phosphorus inputs to surface water bodies in Germany estimated for the period 2012-2014 based on MoRE/MONERIS model applications (data source: UBA 05/2017 - https://www.umweltbundesamt.de/daten/gewaesserbelastung/fliessgewaesser/eintraege-von-naehr-schadstoffen-in-die#textpart-1).

For an effective protection of water ecosystems the regular monitoring of water quality is a prerequisite. Considering protection of water organisms (including accumulation of harmful substances in the food chain and human health), the EU and national water quality standards for some priority substances (heavy metals, organic compounds) are available.

Although they can have negative effects on water ecosystems, nutrients do not belong to the polluting substances of the first priority according to the WFD. Before the implementation of the WFD in Germany, the German Working Group on water issues of the Federal States and the Federal Government (LAWA) and the German Environmental Agency (UBA) developed a water quality classification scheme including nutrient substances (LAWA, 1998). As there are no other mandatory standards for nutrients provided by the EU up to now, this classification system (see Table 1.1) is still used in Germany for surface water quality evaluation based on a network of more than 250 observation gauges in Germany.

In the LAWA water quality classification system, class I means the geogenic background value for naturally occurring substances such as nutrients and salt (without anthropogenic impacts). Class II represents target values determined by considering all subjects requiring protection (e.g. aquatic communities, drinking water supply, groundwater protection, corrosion prevention). The following three classes result from the multiplication of the target values of the previous class with factor 2 until the eightfold of the target value for nutrients. The highest pollution class IV is defined when nutrient concentrations exceed the eightfold of the target value, and oxygen concentration is below or equal 2 mg L^{-1}.

Table 1.1 Chemical water quality classes for nutrients investigated in this study as well as for dissolved oxygen according to LAWA (1998).

		Chemical water quality class (reference value: 90-percentile)						
Parameter	Unit	I No pollution	I-II Very low pollution (≤ ½ target)	II Moderate pollution (≤ target)	II-III Distinct pollution (≤ target × 2)	III Hightened pollution (≤ target × 4)	III-IV High pollution (≤ target × 8)	IV Very high pollution (> target × 8)
TN	mg L^{-1}	≤ 1	≤ 1.5	≤ 3	≤ 6	≤ 12	≤ 24	> 24
NO_3-N	mg L^{-1}	≤ 1	≤ 1.5	≤ 2.5	≤ 5	≤ 10	≤ 20	> 20
NH_4-N	mg L^{-1}	≤ 0.04	≤ 0.1	≤ 0.3	≤ 0.6	≤ 1.2	≤ 2.4	> 2.4
TP	mg L^{-1}	≤ 0.05	≤ 0.08	≤ 0.15	≤ 0.3	≤ 0.6	≤ 1.2	> 1.2
PO_4-P	mg L^{-1}	≤ 0.02	≤ 0.04	≤ 0.1	≤ 0.2	≤ 0.4	≤ 0.8	> 0.8
Oxygen*	mg L^{-1}	> 8	> 8	> 6	> 5	> 4	> 2	≤ 2

* 10-percentile

1.1.3 Past trends and future scenarios of climate and socio-economy

Air temperature

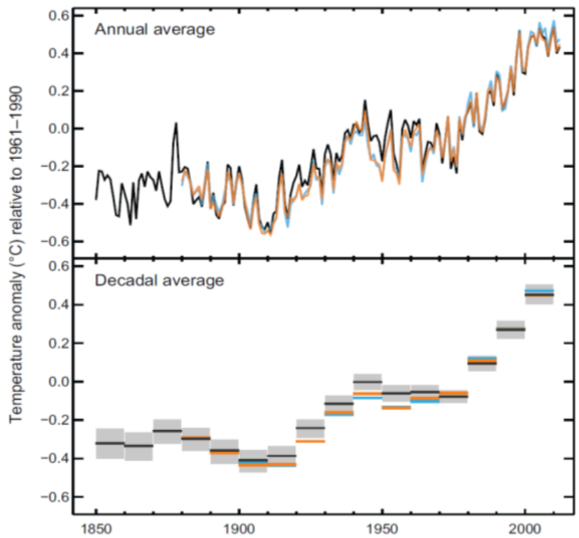

Figure 1.6 Observed global mean combined land and ocean surface temperature anomalies from 1850 to 2012 from three data sets. Top panel: annual mean values. Bottom panel: decadal mean values including the estimate of uncertainty for one dataset (black). Anomalies are relative to the mean of 1961-1990 (taken from IPCC, 2013).

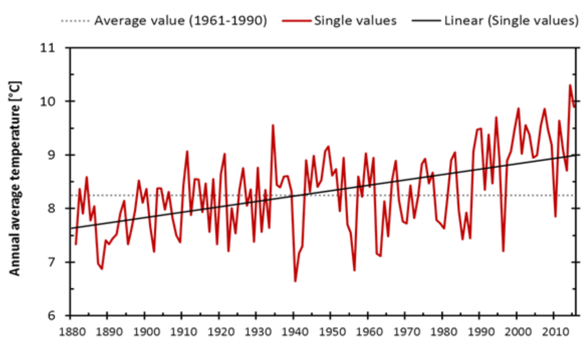

Figure 1.7 Annual average values and their linear trend of daily average temperatures in Germany 1881-2015 compared to the average value of the period 1961-1990 (Data source: DWD taken from https://www. umweltbundesamt.de /daten/klimawandel/trends-der-lufttemperatur).

Table 1.2 Linear trends of seasonal air temperature in Germany between 1881 and 2015 (Source: DWD taken from https://www.umweltbundesamt.de/daten/klimawandel/trends-der-lufttemperatur).

Season (months)	Linear trend	significance
Spring (Mar, Apr, May)	1.4 °C	yes
Summer (Jun, Jul, Aug)	1.2 °C	yes
Autumn (Sept, Oct, Nov)	1.2 °C	yes
Winter (Dec, Jan, Feb)	1.0 °C	no
Total year	**1.3 °C**	**yes**

According to the IPCC (2013) each of the last three decades has been successively warmer at the Earth's surface than any preceding decade since 1850 (Figure 1.6). The globally averaged combined land and ocean surface temperature data as calculated by a linear trend over the period 1880 to 2012 show a warming by 0.85°C. Almost the entire globe has experienced surface warming with some spatial and substantial decadal and inter-annual variability (IPCC, 2013). Up to now the year 2016 was globally the warmest year ever observed with a temperature anomaly of 0.94°C relative to the 20th century average (https://www.ncdc.noaa.gov/sotc/global/201613).

Similar trends in historically observed air temperature can be seen for Germany (Figure 1.7). For the year 2015 the temperature anomaly relative to 1961-1990 was +1.7°C. The linear trend of the average annual air temperature between 1881 and 2015 amounts to 1.3°C showing a slight seasonal variability (Table 1.2). The temperature increase in Germany is strongest in spring time, and has a lower intensity and no statistical significance in the winter months.

It is generally accepted that natural and anthropogenic substances and processes that alter the Earth's energy budget are drivers of climate change (IPCC, 2013). As long as total radiative forcing is positive (mainly caused by the increase in the atmospheric concentration of CO_2 since 1750), the climate system takes up energy resulting in global warming and climate change. The total anthropogenic radiative forcing has increased more rapidly since 1970 than during prior decades (IPCC, 2013), and this development is expected to endure in the future due to continued emissions of greenhouse gases. The future degree of global temperature change will substantially depend on the success in reducing greenhouse gas emissions.

Model-based scenario simulations including climate processes, anthropogenic pressures and feedbacks are used to project and quantify possible responses of the climate system in the future. Depending on the emission scenario applied (Representative Concentration Pathways, RCPs) the projections of possible future temperature dynamics by the end of the 21st century are different (Figure 1.8). However, warming is likely to continue and to exceed 1.5°C relative to 1850-1900 for all RCP scenarios except RCP2.6. The increase of global mean surface temperature in the period 2081–2100 relative to 1986–2005 is projected to be in the ranges 0.3°C to 1.7°C (RCP2.6), 1.1°C to 2.6°C (RCP4.5), 1.4°C to 3.1°C (RCP6.0), and 2.6°C to 4.8°C (RCP8.5). Warming will continue to exhibit interannual-to-decadal variability and will not be regionally uniform. The Arctic region will warm more rapidly than the global mean, and mean warming over land will be larger than over the ocean (IPCC, 2013).

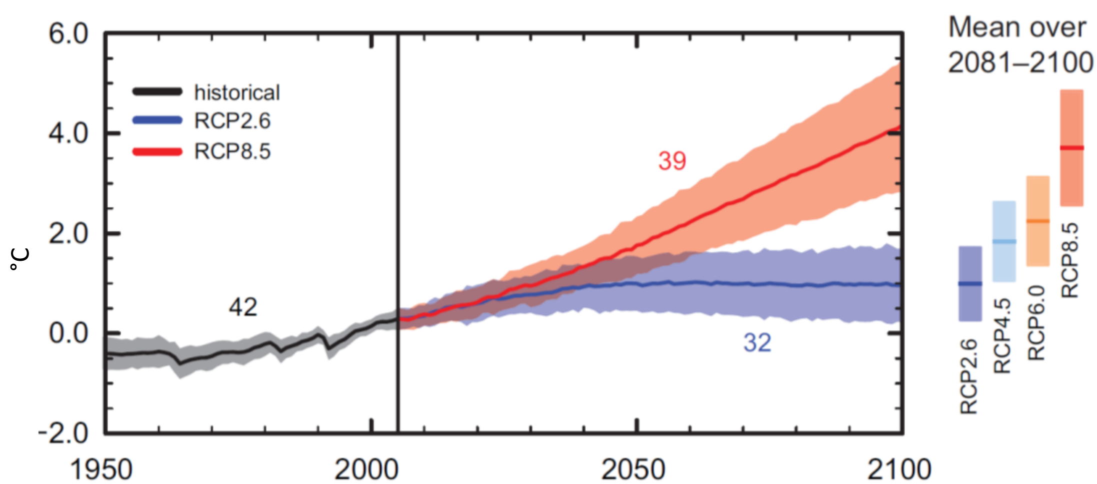

Figure 1.8 Multi-model simulated time series from 1950 to 2100 for change in global annual mean surface temperature relative to 1986-2005. Time series of projections and uncertainty (shading) are shown for scenarios RCP2.6 (blue) and RCP8.5 (red). Black (grey shading) is the modelled historical evolution using historical reconstructed forcings. The mean and associated uncertainties averaged over 2081-2100 are given for all RCP scenarios as colored vertical bars (taken from IPCC, 2013).

Precipitation

In contrast to the observed and projected trends in air temperature described above, the global trends in precipitation are less distinct. At the global scale, the confidence in precipitation change in the historical period averaged over land areas is low for the years prior to 1950, and medium afterwards because of insufficient data, particularly in the earlier periods of the records. Available globally incomplete records show mixed and non-significant long-term trends in reported global mean precipitation (IPCC, 2013; Hartmann et al., 2013).

Looking at selected latitudes (Figure 1.9), some spatial variability of observed trends can be distinguished but often with a low (prior to 1951) or medium (afterwards) confidence. Averaged over the mid-latitude land areas of the Northern Hemisphere (30°N to 60°N), precipitation has increased since 1901 (medium confidence before and high confidence after 1951) (IPCC, 2013).

For other latitudes the area-averaged long-term positive or negative trends have a low confidence (IPCC, 2013). Although there are some increasing or decreasing trends in precipitation for shorter time periods in the whole observation period of 110 years, the overall trends are not significant in the tropical land areas (30°S to 30°N) as well as in the mid latitudes of the Southern Hemisphere (60°S to 30°S). Due to different projections of the five global precipitation sets investigated, the evidence is often limited, and the estimated changes and trends in precipitation show a wide range of magnitudes and are quite uncertain (Hartmann et al., 2013).

A similar increasing trend in precipitation as estimated for the mid-latitudes shown in Figure 1.9 can be observed for Germany between 1881 and 2015 (Figure 1.10). The linear increase in annual precipitation amounts to +76 mm and is statistically significant; however, there is a large variability between the seasons (Table 1.3). The main increase can be observed in winter months, followed by the not significant increasing precipitation trends in spring and autumn, and there is even a slight decrease in summer months.

Projections of future global precipitation are difficult due to a general high spatial and temporal variability of precipitation patterns, as well as due to poor skills of current climate models in this respect. The changes in the global water cycle in response to the warming over the 21st century will not be uniform. It is supposed that the contrast between wet and dry regions and between wet and dry seasons will generally increase, but probably with regional exceptions influenced by natural internal variability and anthropogenic impacts (IPCC, 2013).

It is generally assumed that with increasing global mean surface temperature the extreme precipitation events over the mid-

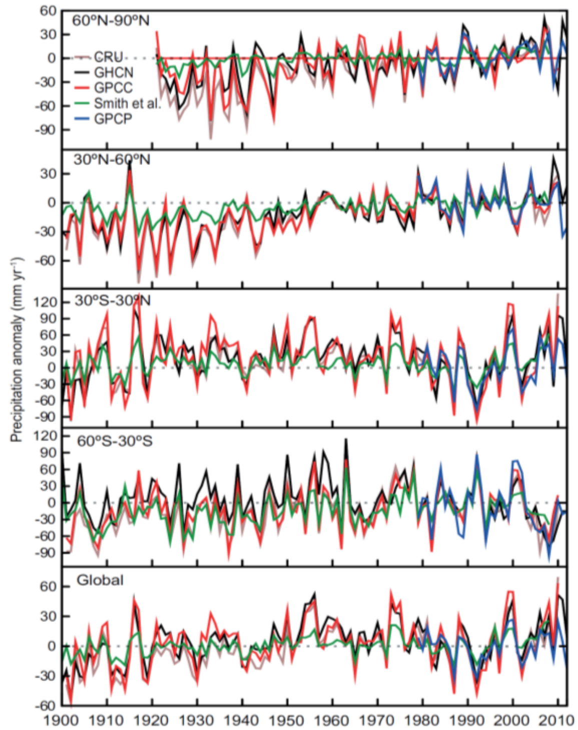

Figure 1.9 Annual precipitation anomalies averaged over land areas for four latitudinal bands and the globe from five global precipitation sets relative to a 1981-2000 climatology (taken from Hartmann et al., 2013).

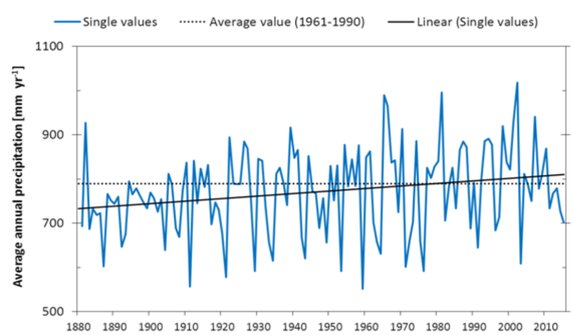

Figure 1.10 Average annual precipitation with linear trend in Germany between 1881 and 2015 compared to the average value of the period 1961-1990 (Data source: DWD taken from https://www.umweltbundesamt.de/daten/klimawandel/trends-der-niederschlagshoehe).

Table 1.3 Linear trends of seasonal sum of precipitation in Germany between 1881 and 2015 (Source: DWD taken from https://www.umweltbundesamt.de/daten/klimawandel/trends-der-niederschlagshoehe).

Season (months)	Linear trend	significance
Spring (Mar, Apr, May)	+19.1 mm	no
Summer (Jun, Jul, Aug)	-3.3 mm	no
Autumn (Sept, Oct, Nov)	+14.3 mm	no
Winter (Dec, Jan, Feb)	+47.3 mm	yes
Total year	**+76.3 mm**	**yes**

latitude land masses and over wet tropical regions will very likely become more intense and more frequent by the end of this century. Monsoons are likely to become longer lasting, wider spread and more intensive compared to the recent observations (IPCC, 2013).

Land use

In addition to the globally changing climate conditions described above, which could affect or alter natural nutrient processes in soils and water bodies, there can be also some direct anthropogenic impacts on natural resources caused by society and economy.

Anthropogenic impacts increase with a rising number of inhabitants in a region. The mismatch between the society's need for resources and space and the capacity of the land to support and adsorb these needs often leads to conflicts. According to the European Environment Agency (EEA), the European continent has the highest share of land used for settlements, production systems (including agriculture and forestry) and infrastructure (all together up to 80%) compared to other continents of the world, causing high land use pressure on natural resources like vegetation, soil and water (http://www.eea.europa.eu/themes/landuse/intro).

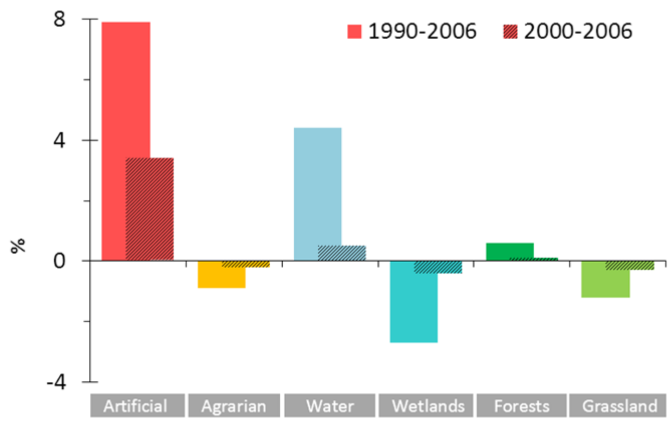

Figure 1.11 Land cover change in Europe between 1990 and 2006 (blank) and between 2000 and 2006 (striped) for major habitat classes: percental change of the end year relative to the initial year (Data source: http://www.eea.europa.eu/data-and-maps).

Due to a high pressure of a rising population, growing industry and increasing transport demands on landscape and natural vegetation, many changes in land use could be recognised in Europe in the past (EEA, 2010). According to the cited report, the area used for agriculture and pastures shows a small decreasing trend but with intensified management, the size of forested areas slowly increases but with declining share of old-growth forests, and urban areas are growing most notably in Europe as a whole in the period 2000-2006. Figure 1.11 depicts the percental changes of selected habitat classes in Europe for the two time periods 1990-2006 and 2000-2006. It is obvious that the main changes could be observed directly after the political turn in the last decade of the 20th century, but the direction of changes remained and did not change in the following years.

However, the national trends in land use may be different. For example, current tendencies include a decreasing trend in crop acreages in Spain (conversion to olive groves and vineyards), Czech Republic (to pasture) and Northern Germany (to fallow). Changes in forested areas occur mainly in Northern Europe (Finland: net loss of forest and Sweden: some uptake of forested areas by economic sites), Portugal (new forested land) and Hungary (transitional woodland creation). Notably growing urban areas can be found especially in France and Western Germany (EEA, 2007a; RIKS, 2010). Figure 1.12 shows percental land cover changes of selected habitat classes in Germany for the period 1992-2015 and six shorter subperiods. The direction of observed changes is similar to the European data shown in Figure 1.11, but with different amplitude. The human infrastructure experienced the most notable changes: settlements and transportation areas increased by more than 20% during the total analysed period. However, when analysing the shorter time periods, it is obvious that the increase intensity is continuously decreasing over time. In case this decrease will last, it could be possible that the ground sealing rate of 66.1 hectare per day in the period 2012-2015 will decrease to reach the aspired value of 30 ha d^{-1} in 2030 (Federal Statistical Office, 2016a).

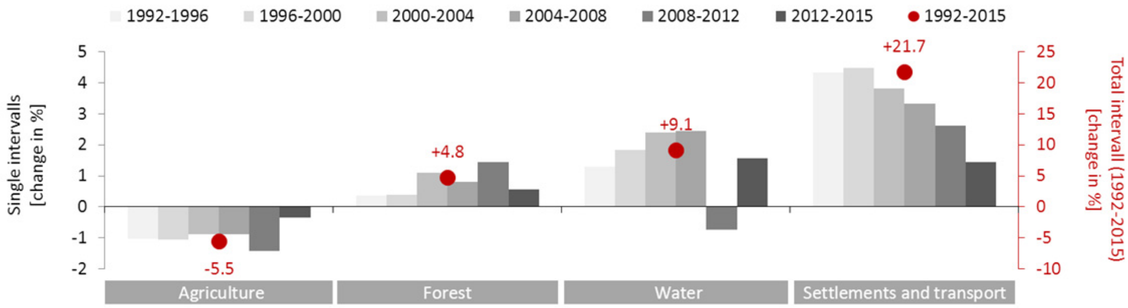

Figure 1.12 Land cover change in Germany between 1992 and 2015 for selected habitat classes: percental change of the end year relative to the initial year (Data source: Federal Statistical Office, 2016a).

Figure 1.13 (left) exemplarily illustrates the land use change heterogeneity in Europe by showing the percental decline of arable land area due to land take by economic site and infrastructure development. The largest changes can be seen in the Netherlands as well as on the Iberian Peninsula near the Mediterranean Sea, whereas only small changes occur in Northern and Central Europe. It is expected that the current European trends in land use patterns as described above will continue in the coming 10–20 years. Therefore, some decrease in arable land area was projected in recent EEA studies (EEA, 2007a; RIKS, 2010). However, the area of permanent crops may not change substantially in Europe. According to these reports, it is also expected that the area of forested landscapes will increase in Europe by ca. 5% between 2000 and 2020, whereas the share of urban areas will increase by approximately 1% in total. Figure 1.13 (right) exemplarily shows the projected increase in urban surface areas between 2010 and 2030 in Europe. The data also include a distinct spatial heterogeneity with main increases on the Iberian Peninsula, in Poland and in Ireland, moderate increasing trends in Scandinavia, France and Western Germany, and even negative changes (meaning a decrease in urbanisation) in the Baltic States, on the Balkan Peninsula and in Eastern Germany.

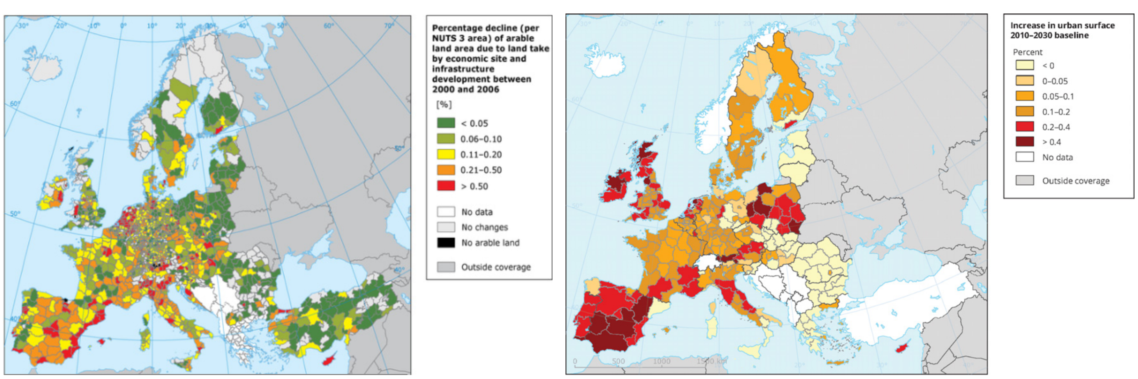

Figure 1.13 Percental decline of arable land area in Europe by change to artificial surfaces between 2000 and 2006 (left) and projected percental increase in urban surface area in Europe for the time period 2010-2030 (right) (maps from http://www.eea.europa.eu/data-and-maps).

Fertilisation

Since Liebig's law of the minimum developed in the mid of the 19th century, postulating that the yields of a plant are proportional to the amount of the scarcest of its essential nutrients (Liebig, 1840), crop cultivation and conventional farming on agricultural areas usually involve fertiliser application to increase soil fertility and crop yields. The amount of applied fertilisers slowly increased until 1950, but with the technological progress and the development of production facilities for mineral fertilisers, a considerable rise in fertiliser application could be recognised from the 1960ies worldwide. However, depending on the development status of a region, large differences in fertiliser application could be observed in the last decades (Tenkorang & Lowenberg-DeBoer, 2009; Alexandratos & Bruinsma, 2012). Significantly higher application rates are obvious in the Northern Hemisphere, with maxima centred on areas with intensively used cropland and high densities of livestock. Furthermore, some hot spots can be defined globally, covering approximately 10% of the treated land but receiving over 50% of the applied fertilisers (Potter et al., 2010).

Figure 1.14 (left) illustrates the temporal development of fertiliser use in Germany over almost 80 years. Starting from the same moderate level of application, the intensity of fertiliser use increased rapidly until a maximum in the 1970th (phosphate) or, respectively, 1980th (nitrogen) followed by a remarkable decrease afterwards (due to growing pollution problems and water protection efforts), and remaining at a constant reduced level during the last decade. The overall decrease is higher for phosphate than for nitrogen, even reaching an application level lower than in 1939. In recent time, nitrogen fertiliser use is five to ten times higher than phosphate fertiliser application in Germany.

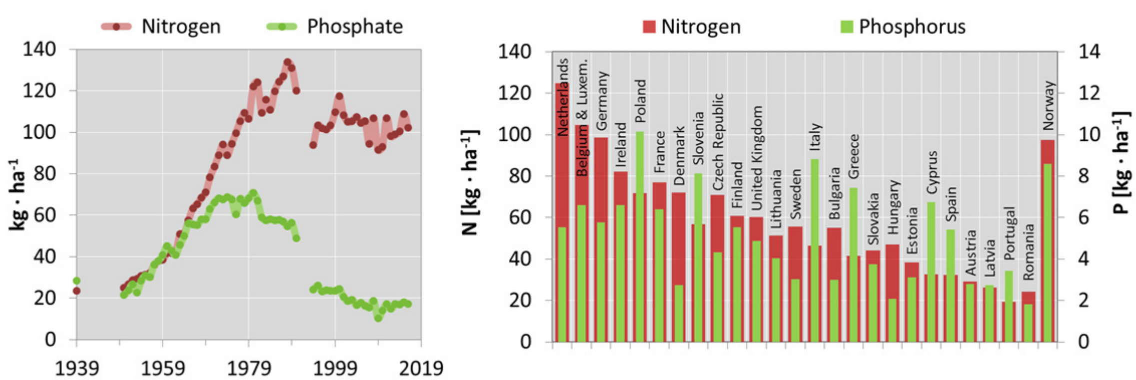

Figure 1.14 Development of mineral nitrogen (N) and phosphate (P_2O_5) fertiliser inputs on agricultural fields in Germany including fallow between 1939 and 2016 (left) (Data sources: Bührer, 2001; Federal Statistical Office, 2016b); and estimated consumption of manufactured fertilisers in 2009 at country level in Europe (right) (Data source: Eurostat 2016 - http://ec.europa.eu/eurostat/statistics-explained/index.php/Archive:Fertiliser_consumption_and_nutrient_balance_statistics).

However, large spatial differences in fertiliser application rates can be seen at the national level comparing 27 countries of the European Union (Figure 1.14, right). The highest nitrogen rates are obvious for the Benelux countries followed by Germany and Norway, whereas the highest phosphorus fertiliser rates are in Poland, Italy, Norway and Slovenia. Nitrogen fertiliser application rates in the Netherlands are about six times higher than in Portugal, and phosphate fertilisation rates in Poland are five times higher than in Romania.

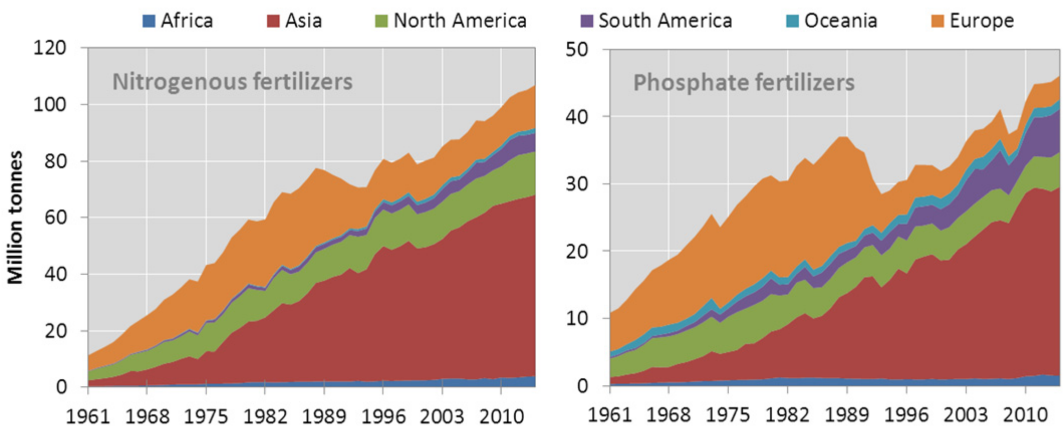

Figure 1.15 Past trends in fertiliser consumption per continent between 1961 and 2014 (Data sources: FAOSTAT 04/2017 - http://www.fao.org/faostat/en/#data/RF and http://www.fao.org/faostat/en/#data/RA).

Looking at the continental scale (Figure 1.15), the main increase in global fertiliser consumption during the last half of century is in the Asian countries. A distinct decrease can be observed only for the European countries after the political changes in 1989.

The worldwide fertiliser use is projected to further increase with the world's population and with the progress of emerging markets and in developing countries. Though, mineral fertiliser application in general is highly diverse across countries and regions due to the heterogeneity of natural resources, soil properties, irrigation practices, additional manure application and/or economic incentives. Aggregated over all crops and countries, fertiliser consumption could increase from 166 million tonnes in 2005/2007 to 263 million tonnes in 2050 (Alexandratos & Bruinsma, 2012). However, the growth of fertiliser application rates per area (kg ha^{-1}) and/or of fertiliser efficiency per crop yield (kg t^{-1}) is expected to slowdown, especially in the developed countries and East Asia. Growth in industrial countries, mainly in Western Europe, is expected to lag significantly behind the growth in other regions or even decline due to already high level of fertilisation, new techniques such as biotechnology and precision agriculture, higher shares of organic farming practices, and the increasing awareness of and concerns about environmental problems caused by excessive fertiliser use (Alexandratos & Bruinsma, 2012; OECD, 2012).

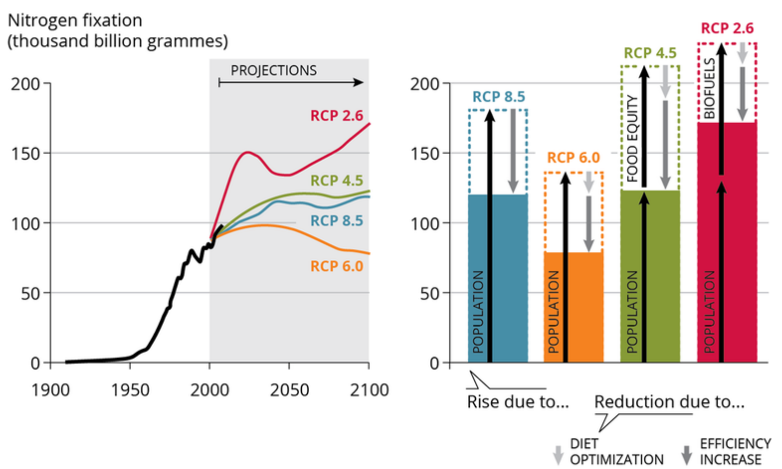

Figure 1.16
Historical trend in global demand for industrial nitrogen fertiliser 1910-2008 and projections to 2100 based on RCP scenarios (left); and drivers of the projected changes in demand in 2100 (right).

(taken from http://www.eea.europa.eu/data-and-maps/figures/historical-trend-in-global-agricultural)

Projections on global future fertiliser applications and needs are difficult, as they depend on assumptions regarding population growth, consumption patterns, biofuels use, and fertilisation efficiency. Winiwarter et al. (2013) calculated different projections on future nitrogen fertiliser demand based on the four IPCC RCP emissions scenarios (Figure 1.16). The projections suggest that there may be trade-offs between greenhouse gas mitigation and pollution abatement. In the lowest global warming scenario (RCP 2.6) intensified biofuel production could lead to high nitrogen fertiliser consumption, which cannot be compensated by new techniques regarding diet optimisation (refers to a shift in consumption towards food produced with more effective nitrogen uptake) or efficiency increase (refers to the ratio of nutrients taken up by crops to the total amount of nutrients applied to soil) in agriculture (EEA, 2015a).

Point sources

In addition to the diffuse nutrient inputs to surface waters leached or swept off from agricultural fields and urban areas, nutrients can also be directly emitted to the river systems by point sources, such as wastewater treatment plants or industrial facilities. Nutrient inputs by point sources are more important for phosphorus than for nitrogen (compare Figure 1.5). Due to a rising awareness about environmental pollution, the nutrient inputs from direct dischargers were continuously decreasing in the past decades. This effect can be clearly seen in Germany at the end of the 20th century (Figure 1.17).

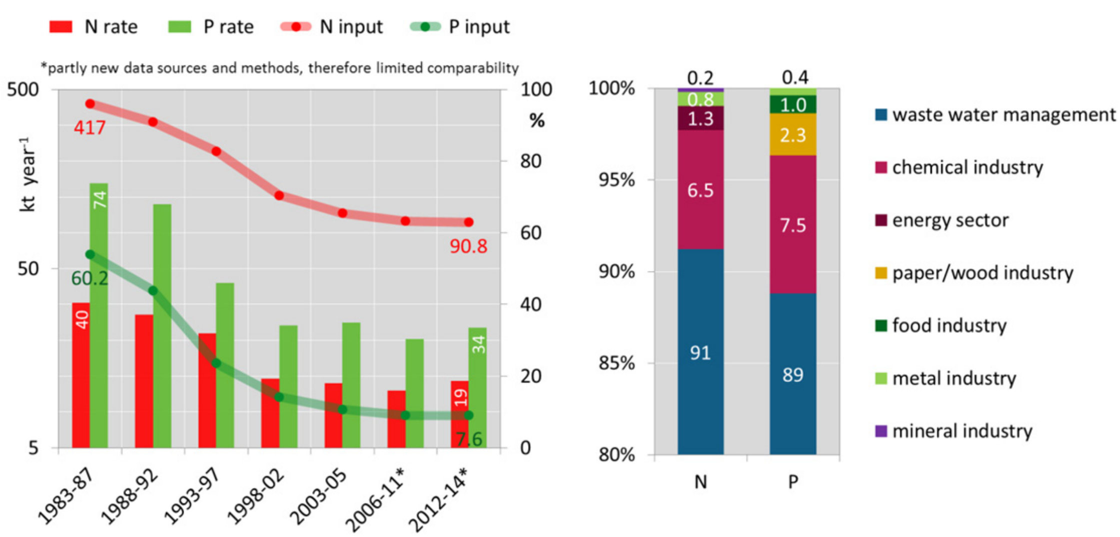

Figure 1.17 Nutrient inputs from point sources to surface water bodies in Germany and the rates of total nutrient inputs based on MoRE/MONERIS model applications (left; data source: UBA 05/2017 - https://www.umweltbundesamt.de/daten/gewaesserbelastung/fliessgewaesser/eintraege-von-naehr-schadstoffen-in-die#textpart-1); and origin of PRTR-obligated nutrient releases to water in Germany in the reporting year 2015 (right; data source: UBA, 2017).

Figure 1.17 (left) depicts the development of point source pollution in Germany for nitrogen (N) and phosphorus (P) in the period 1983 until 2014 estimated by model application. The annual effluents from point sources could be reduced by 78% for N and by 87% for P in this period. The share of nutrients coming from point sources compared to the overall nutrient inputs to surface water bodies in Germany could be reduced as well. However, point sources are still the main source of phosphorus input to the surface water bodies in Germany (compare Figure 1.5).

According to the "Pollutant Release and Transfer Register" (PRTR) required by the EU for pollutants emitted to the environment exceeding predefined thresholds (>50.000 kg $year^{-1}$ for TN and >5.000 kg $year^{-1}$ for TP) the majority of N and P inputs in Germany originates from waste and waste water management followed by the chemical industry, and only small shares come from other sources (Figure 1.17, right).

Future projections for emissions from point sources to aquatic ecosystems are based on scenario assumptions. While emissions are not expected to distinctly increase in Germany and other developed European countries in future due to the already high standards in waste water treatment facilities and environmental legislation, the global N effluents are projected to grow rapidly by 180% and the P effluents by 150% between 2000 and 2050 without new policies (OECD, 2012). The expected increase is due to population growth, rapid urbanisation, and an increasing number of households with connection to sewage systems, but lagging nutrient removal in wastewater treatment systems, which are not fast enough to counterbalance the large projected increase in nutrient inflows. The largest increases of N and P effluents from wastewater to surface water bodies are expected in China, India and Africa (Figure 1.18). Following these assumptions under current global policy settings, the nutrient loads coming from rivers to the oceans will vary considerably across the world's main seas with highest amounts for the Indian and Pacific Ocean, but only slight increases of nutrient discharges to the Mediterranean and Black Seas (EEA, 2015a).

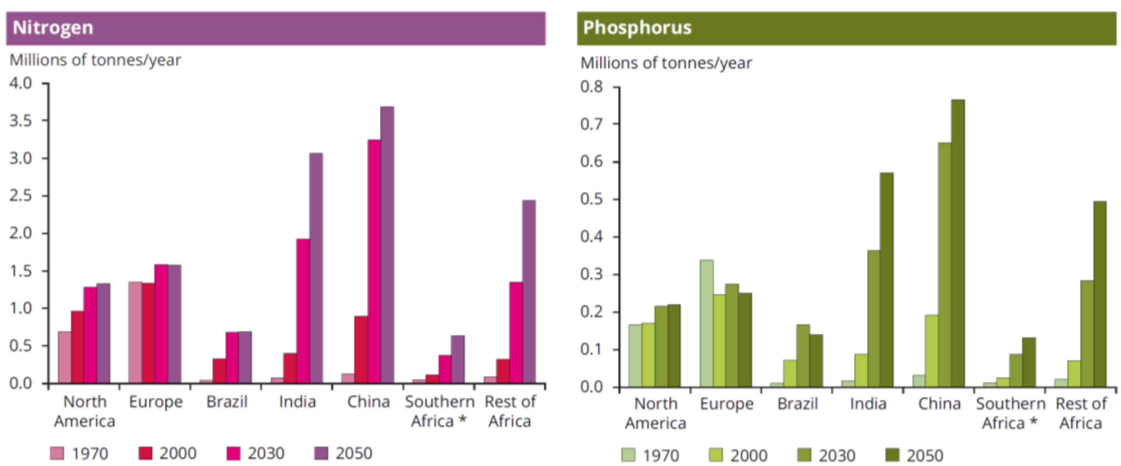

Figure 1.18 OECD-projected effluents of nitrogen and phosphorus from wastewater to surface water bodies, 1970-2050 (from EEA, 2015a).

1.1.4 Impacts of global changes on nutrient processes and water quality

Climate and land use are two essential factors controlling the ecohydrological characteristics of river catchments such as river discharge and water quality (Bronstert et al., 2002; Hörmann et al., 2005). As described above in Section 1.1.3, changes of the climate system and increased anthropogenic pressures on natural resources have already been detected in the past in Europe and worldwide, and this development is likely to continue in the future (IPCC, 2007; IPCC, 2013; EEA, 2010; Cassardo & Jones, 2011; RIKS, 2010; Alcamo et al., 2007b).

Variations in climate conditions and management measures will probably have impacts on the environment and the natural conditions of ecosystems with more or less distinct feedbacks and effects on the water cycle, vegetation, biodiversity, human health and economy. The effects of altered climate conditions on diverse ecosystemic and social functions can already be detected, such as a longer plant-growing season, changes in species distribution and biodiversity, retreating of glaciers, humans suffering from heat waves, and electricity generation problems (see Linderholm, 2006; Gabriel & Endlicher, 2011; Vittoz et al., 2013; Wang et al., 2013b; Koch et al., 2015). Possible impacts of climate and socio-economic changes on nitrogen and phosphorous processes in a watershed and on the overall river water quality will be discussed in this section. As water quality is always coupled to water quantity in a catchment, the impacts on the general water cycle will be shortly described, too.

Climate change impacts

The already observed climate changes in Europe are characterised by increasing temperatures and shifting rainfall patterns, with drier conditions mainly in the South and on the Iberian Peninsula, and wetter conditions in the North European regions around the North and Baltic Seas (EEA, 2012). According to Alcamo et al. (2007a), potential warming in Europe could reach values from +1 to +6 °C by the end of this century causing various effects on the water cycle.

Figure 1.19 illustrates possible impacts of changed climate conditions on the water cycle. The warmer atmosphere leads to increased evaporation and transpiration rates followed by higher air humidity, cloudiness and precipitation events, but also to a decrease in snowfall and glacier coverage in mountains, changing snowmelt regimes, altered river runoff and sea level rise. Generally, climate change is expected to go along with more intense and frequent precipitation causing increased flood events and higher sediment loads, but also a decrease in light rains, and even more severe drought periods between rains are very likely. The late summer discharges are expected to decrease with increased water temperature.

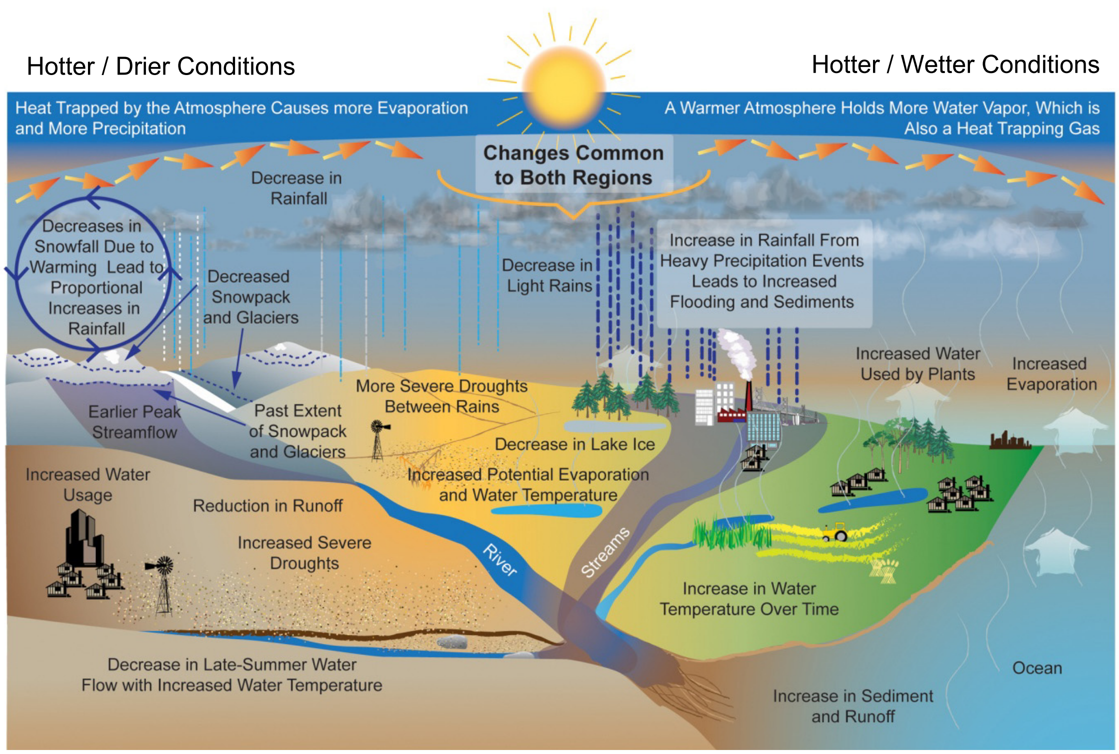

Figure 1.19 Possible climate change impacts on the water cycle (taken from USGCRP, 2009).

The described changes in climate conditions and water cycle can have various effects on nutrient occurrence and behaviour in a river catchment (Whitehead et al., 2009; Arheimer et al., 2012; Øygarden et al., 2014; Stuart et al., 2011). The determining factors are the river flow volumes, but also the water and soil temperatures in the rivers and catchment, as well as extreme events and adaptation measures.

Altered river discharge affects the mobility and dilution of nutrients and sediments in river waters. Lower flows following precipitation decrease imply higher concentrations of nutrients downstream of point sources foiling the efforts to improve water quality and to achieve the European WFD objectives (Whitehead et al., 2009). Especially phosphate phosphorus is characterised by this inverse relationship with water flows, as it originates to a large extent from point sources (see Figure 1.5). Nitrate nitrogen, coming mainly from diffuse sources, is more affected by increasing precipitation amounts causing higher leaching rates to the river system.

The terrestrial nutrient turnover and transport processes in the catchment (denitrification, nitrification, volatilisation and leaching) are also impacted by climate change, additionally influencing the river water quality at the outlet of a basin (Barclay & Walter, 2015; Whitehead et al., 2006; Macleod et al., 2012). The nitrate concentration in river waters, for example, increases over time with rising temperatures, as soil mineralisation in the catchment is facilitated, and the emerged nitrate components could be easily washed out (particularly significant under the high flow conditions following drought).

More river flow also means more stream power and sediment loads, which can have impacts on the freshwater habitats by an altered morphology of rivers and the sedimentation of lakes. As hydromorphology is a key factor controlling the ecosystem behaviour and its ecological status, climate change may have an important role for surface water bodies in this respect. However, there are different opinions and observations about the potential consequences of climate change impacts on the hydromorphology of rivers. While Orr and Walsh (2006) postulate that climate change may act against restoration of rivers, making it difficult to return to the desired previous ecosystem status, Hering et al. (2009) showed that habitat restoration for water quality indicator species may be enhanced by the effects of a more variable flow regime.

Due to projected climate change, an increase in both flood frequency and drought frequency is expected for many regions (Hirabayashi et al., 2008). The extreme river flows due to heavy precipitation events can cause flash-flooding and uncontrolled discharge from urban areas with increased amount of contaminants and nutrients. On the other hand, very low flow volumes with reduced water velocities and higher water residence times go along with lower oxygen levels and often toxic algal blooms, or re-dissolution of phosphorus from sediments to the water column. Especially in the middle and lower river courses and standing waters the risk of deoxygenation increases in hotter summers with low discharges and higher water temperatures (Whitehead et al., 2009).

In general, water temperature is an important factor controlling the chemical reaction kinetics and the ecological status of a freshwater ecosystem (Whitehead et al., 2009). Higher water temperature causes a reduced saturation concentration for dissolved oxygen and an increased risk of fish death. A temperature rise by 1-3°C could be already observed over the last 100 years in large European rivers (Rhine, Danube) in parallel to the globally observed air temperature increases (EEA, 2007b). At higher temperatures chemical reactions and bacteriological processes run faster, and, for example, ammonium concentration decreases while nitrate concentration increases due to intensified nitrification processes.

However, a changing temperature regime affects not only the chemical nutrient transformation processes in river waters, but also controls the growth rate and behaviour of aquatic organisms. Species are often temperature sensitive, and have a limited range of thermal tolerance. Changing boundary conditions regarding heat and flow can cause the invasion of better adapted alien species, as the exotic species are often out-competing the native species in a changing environment. This could have implications in meeting the WFD objectives regarding water quality and for achieving the requested good ecological status, which is always defined by comparing with the reference conditions in species composition (Whitehead et al., 2009).

According to Whitehead et al. (2009), the nutrient loads in rivers are generally expected to increase under climate change. Arheimer et al. (2012) simulated phosphorus increase but nitrogen reduction in the Baltic region under changing climate, whereas Øygarden et al. (2014) detected a clear seasonality in nitrogen losses from agricultural fields coupled to the growing season. In general, a wide range of nitrogen loss projections can be found in literature (Stuart et al., 2011). However, it should be taken into account, that eutrophication occurs as a result of the complex interplay between nutrient availability, light conditions, temperature, residence time and flow conditions, so that no ultimate conclusions can be easily drawn regarding the future conditions of surface water bodies under climate change.

It should also be kept in mind that various indirect impacts of climate change can affect water ecosystems and quality, too, as, for example, the impacts of management and policy measures applied in a catchment in order to adapt to climate change (e.g. bio-fuels or emission control). Possible management measures – are they adaptation measures or simple economic activities – represent the second important factor controlling surface water quality in a river catchment, and they will be discussed in more detail in the following section.

Effects of management measures

Since centuries, hydromorphology and water quality of river systems in Europe were affected by anthropogenic impacts causing reduced ecosystem services of river catchments (Figure 1.20). The ecosystem's potential of natural river flood-plains and catchments for water and nutrient storage, water and food supply, human recreation and living space for flora and fauna species has been heavily impacted by urbanisation and pollution with contaminants or nutrients, changes in land use patterns and crop type composition, tillage methods and hydraulic engineering (Tockner et al., 2009; Søndergaard & Jeppesen, 2007; Schinegger et al., 2012; Grizzetti et al., 2017). All these management measures can also have direct and indirect impacts on nutrient behaviour and occurrence and the resulting river water quality in a catchment.

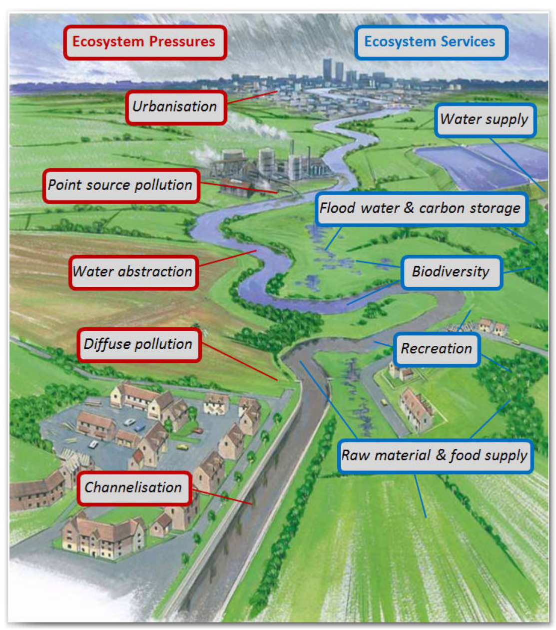

Figure 1.20 Ecosystem services of a healthy river system and catchment (blue) and impacting pressures (red) influencing the ecological status and water quality of the river (taken from http://www.therrc.co.uk/why-restore).

The population density and human activities are important underlying factors for point and diffuse nutrient pollution entering rivers (Seitzinger et al., 2010). As already mentioned in Section 1.1.2, nutrient pollution originates from factories and sewage treatment plants (point sources) as well as from agricultural fields (diffuse sources), and can lead to eutrophication processes and a general decrease in river water quality (Vollenweider, 1968; Anderson et al., 2002; Pieterse et al., 2003; Schindler, 2006). Due to these negative impacts on natural ecosystems and biodiversity, increasing nitrogen and phosphorus pollution has become a major concern at the global scale.

A significant increase in food production could be achieved by the application of synthetic mineral fertilisers, but if global loads of nitrogen and phosphorus on water systems continue to increase, the natural nutrient cycles could be significantly perturbed even to the point of unsustainability (EEA, 2015a). The total occurrence of nitrogen in the environment has more than doubled since the 1970s as a result of global population growth, agricultural intensification and omnipresent inefficiencies in nutrient uses (Galloway et al., 2008). The effluent quantities in agriculture generally depend on the intensity of fertiliser use and the efficiency in fertiliser application in combination with soil properties (e.g. texture) and timing of the fertilisation. Point source emissions mostly depend on the number of inhabitants, the industrial development and the level of water treatment. Hence, changes in agricultural, industrial and wastewater treatment practices will cause changes in nutrient inputs to the river systems.

During the last decades, many efforts were undertaken to reduce nutrient inputs to the rivers by construction and improvement of sewage treatment plants and optimisation of fertiliser application on cropland in Europe (compare with parts 'Fertiliser' and 'Point sources' in Section 1.1.3). They resulted in a remarkable reduction of total phosphorus emissions (which originate mainly from point sources), but only a small decrease of total nitrogen inputs (coming mainly from diffuse sources, compare Figure 1.5) due to the lag time of diffuse nutrients in soils (Bouraoui & Grizzetti, 2011; de Wit et al., 2002; Grizzetti et al., 2012). It is widely recognised that the control of diffuse source emissions is much more difficult than a technical improvement of sewage water treatment methods from primary (physical), over secondary (biological) to tertiary (chemical) treatment in order to release wastewater that is close to the quality of the receiving waterbody. So, it is expected that the inputs of nutrients from households and industry will be further reduced in Europe in the future, and diffuse inputs from fertilisers and manure will become the main sources of nutrient pollution on the continent (de Wit et al., 2002).

The type of crops cultivated on the agricultural acreages is an additional factor controlling the danger of diffuse nutrient inputs to river waters. Crop types have different water and nutrient needs and vegetation cycles, causing diverse stages of vegetation cover, nutrient consumption and water demands (FAO, 1986; Fageria, 2009). The cultivation of more water and nutrient demanding late-sprouting crop types (e.g. maize) is characterised by long phases of bare soil, and can cause nutrient and sediment pollution problems in the draining rivers as well as surplus nutrient leaching to groundwater without adequate agricultural practices (Finke et al., 1999; TLL, 2011b; Manevski et al., 2015). Cover crops during winter time can help to stabilise nutrient balance, and to hamper unnecessary sediment, nitrogen and phosphorus losses to the river systems (Cooper et al., 2017; Dabney et al., 2007; Kaspar et al., 2012; Plaza-Bonilla et al., 2015).

An excessive water abstraction for irrigation purposes on agricultural fields or for water supply of the inhabitants can have additional negative impacts on water quality and ecosystem functioning of a river system (Carolli et al., 2017). High nutrient leaching rates can be found under irrigated crop areas or during cultivation of some special nutrient demanding crop types. Crop type specific agricultural practices and fertilisation, taking into account the individual growth stages of different crops, are important measures to reduce excessive nutrient and sediment inputs to surface water bodies, although the lag time of nutrient storage in soils often does not allow to achieve fast improvements of water quality (Meals et al., 2009). However, fertiliser amounts, tillage methods and irrigation times should generally be adapted to soil properties and special needs of the cultivated crops (as much as necessary, as little as possible) and should be oriented to the concept of "good agricultural practices" (GAP; FAO, 2003).

Additionally, land use type composition and pattern can have significant impacts on water quality and nutrient inputs to a river system, too. Riparian zones and wetlands along the river courses or forests within a river catchment can help to store water and nutrients in the basin, to stabilise the soil banks, and to protect surface water bodies from extreme nutrient and sediment inputs (Aguiar et al., 2015; Dosskey et al., 2010; Verhoeven, 2014). The stored water with slow lateral flow velocities and delay in reaching the river network (e.g. in wetlands and shallow lakes) is an important factor to prevent/control extremely high and low flow periods in rivers and streams, to protect the human infrastructure, to provide a stable water supply for the inhabitants and to deliver sufficient water volume for dilution of point source emissions coming to the river networks (Robinson et al., 2003; EEA, 2015b).

Clear-cutting and deforestation measures can have far-reaching consequences for the water and nutrient cycles in a watershed. It often causes the disruption and change of the hydrologic regime, coming along with increased surface runoff and decreased groundwater recharge or even with the loss of perennial streams. These changes affect the surface water quality by decreasing flows in dry periods and concentrating nutrients and contaminants in surface waters. They are often additionally impacted by increased erosion rates, leading to high levels of turbidity and sedimentation in rivers and lakes, often connected with phosphorus contamination (FAO, 1996; Sweeney et al., 2004).

According to the WFD, a good ecological status of a surface water body is connected to its hydromorphology. Water engineering measures, such as transverse structures in river courses (dams and weirs) and channelisation of former meandering river reaches, decrease the ecological potential and biodiversity in ecosystems, hamper the passability for fish species and increase the downstream vulnerability to extreme events (Elosegi et al., 2010; Elosegi & Sabater, 2013; Liermann et al., 2012; Poff et al., 2007). The dammed river reaches are characterised by a decreased water flow velocity, whereas straightened rivers flow faster and have a diminished water surface, both acting in the direction of reduction of the oxygen reaeration potential. The resulting decreased concentrations of dissolved oxygen in water bodies impact water quality and biota by interrupting nutrient transformation and decomposition processes and losing basic survival needs of organisms (Horsák et al., 2009; Sharma, 2015). Furthermore, oxygen deficit facilitates the release of sorbed contaminants (phosphorus, heavy metals) from bottom sediments additionally affecting the water quality (Wu et al., 2014; Tammeorg et al., 2017). Several renaturation measures (e.g. afforestation of riparian zones, connection of formerly abandoned channel parts, or construction of fish passes to overcome dams or weirs) could be applied in anthropogenically impacted river ecosystems to improve the river ecosystem services and to increase the habitat diversity of the flowing water bodies (Bullock et al., 2011; Kupilas et al., 2017).

Combined changes impacts and scaling effects

In inhabited regions of a continuously changing and quite vulnerable world human impacts on river ecosystems occur not only as a single pressure, but often in combinations (Schinegger et al., 2012). This can have additive and multiplicative effects on the river functioning (Vinebrooke et al., 2004), and complicate the efforts to find measures to protect and improve the ecological status of a river ecosystem. It should be additionally kept in mind that an already affected ecosystem is not able to adapt to stresses and pressures in the same way as an unaffected one. Roux et al. (1999) remarked that the impact of further pressures can be even greater than normally expected when the assimilative capacity of an ecosystem is already reduced.

The interpretation of multiple impact effects will actually be more complicated by addition of expected climate change impacts. Climate as well as human societies are important co-designers of the environmental situation of the vulnerable river ecosystems in Europe. It cannot be expected that future development will take place without any additional changes in climate conditions, human behaviour, land use patterns and economic activities. Alterations in any of these characteristics can influence water resources and nutrient cycles in the drainage basins, and, consequently, in the river systems themselves.

However, climate as well as socio-economic change impacts will probably occur with individual intensities and magnitudes, which are also dependent on the scale of impact investigation. There is some evidence that the detected effects of land use change are scale-dependent, and that the effects are getting smaller at a larger case study catchment (Hörmann et al., 2005). A high spatial variability is often obvious when looking at the climate change impacts in regional impact studies. Some regional trends can even be opposite to the overall trend for large areas (Arheimer et al., 2012), and some local effects can be masked by the large-scale aggregation of results (Piniewski et al., 2014).

The climate and socio-economic change impacts on river water quality superimpose each other, and create a very complex system of interactions and feedbacks (Dunn et al., 2012; Huttunen et al., 2015; Mehdi et al., 2015). Climate change may intensify or even reverse certain current trends in river discharge and nutrient loads caused by the socio-economic developments. The nitrate loads in the rivers, for example, are climate-dependent, and were probably influenced by former climate variations, so that it is difficult to identify and interpret the pure effects of management changes in the past (Bouraoui & Grizzetti, 2011). In many impact cases direct and indirect effects on river water quality can be observed. Adaptation measures and policy responses to the projected climate change, e.g. subvention for bio-fuels or control of greenhouse gas emissions, can be direct management change impacts but indirect climate change impacts affecting freshwater quality (Whitehead et al., 2009).

Therefore, assessing possible future changes of river water quality and derivation of suitable adaptation measures for maintaining or improvement of the river's ecological status can only be properly done by a combined interpretation of climate and management change impacts. A combined land use and climate change impact assessment supported by the application of a well calibrated ecohydrological model can be an important step facilitating the integrated river basin management. This allows to take into account the system characteristics and variable boundary conditions, which should be requested by default in modern management strategies (Scharfe et al., 2009) to support the implementation of adaptation measures in river basins, and to come closer to the requirements of the WFD in Europe in future.

1.2 Ecohydrological water quality modelling

Ecohydrology is an interdisciplinary, multidimensional scientific concept investigating the relationships between hydrological processes and biotic dynamics at the catchment scale. The concept is applied in order to solve environmental problems for a sustainable development of water resources, which is dependent on the ability to restore and maintain evolutionary established processes of water, plant and nutrient circulation. The aim is an enhancement of the carrying capacity of the global ecosystem related to water resources, biodiversity, ecosystem services for societies and the resilience to an increasing variety of impacts (Zalewski et al., 1997; Kundzewicz, 2002; Zalewski, 2002; Jørgensen, 2016; UNESCO, 2017).

The field of ecohydrology is very complex, containing a high diversity of research directions, methods and approaches and bringing together scientists from many disciplines (e.g. biologists, hydrologists, ecologists, landscape architects and water managers). It reflects the high complexity of the studied terrestrial and connected aquatic ecosystems characterised by a high number of interactions and feedbacks, often influenced by regional and global climate change as well as management measures (Porporato & Rodriguez-Iturbe, 2002; Müller et al., 2014).

The areas of research in ecohydrology include, for example, transpiration processes and plant water use, adaptation of organisms to their water environment, influence of vegetation on stream flow, and feedbacks between ecological processes and hydrological cycle. However, not only the biotic (and direct or indirect human) impacts on water flows and availability are studied, but also effects on nutrient cycles and the resulting water chemistry, which could be used for the characterisation of water quality and the status of an aquatic ecosystem.

For this purpose, mathematical models deliver helpful tools, as they allow the quantification of water and nutrient flows at different scales by combining many processes and feedbacks in the ecosystems. Water quality modelling involves the prediction of surface and groundwater pollution (e.g. by nutrients, salts or heavy metals) using mathematical simulation techniques. A typical water quality model consists of a collection of formulas representing physical mechanisms that determine position, form and amount of pollutants in a landscape or a water body. The models are available for different scales, substances and processes with various levels of complexity (meaning the number of natural processes taken into account). Due to the high amount of interacting processes and impacts, usually large and complex computer models are required to achieve adequate results close to real observations. The following sections give an overview on history, methods and types of applied water quality models, as well as on their usability for impact assessments at the catchment scale.

1.2.1 State of the art in water quality modelling

Modelling of water quality issues has a long history. Streeter & Phelps (1925) are counted as the pioneers in applying mathematical descriptions to aquatic processes (Wang et al., 2013a). Their model described the development of dissolved oxygen concentration (DOX) in a river or stream along a certain distance by degradation of the biochemical oxygen demand (BOD) and is, in enhanced and expanded form, still used in several present-day complex water quality models.

Until the 1960s, water quality modelling approaches concentrated mainly on improving the description of oxygen behaviour in surface water bodies (Wang et al., 2013a). However, with the increasing computational possibilities in the following decades, also the complexity of water quality models and the number of simulated processes and substances increased. Starting in the 1970s with conservative substances (e.g. salt) (Refsgaard et al., 1999), the models became more and more complex by incorporating also transport and transformation processes of different reactive substances and aquatic organisms: from nutrients (nitrogen and phosphorus) and sediments to pesticides, heavy metals and bacteria. Nowadays, most often the conventional substances, such as nitrogen, phosphorus and sediments are modelled in water quality modelling applications (Krysanova et al., 2009).

During more than 40 years of intensive model development, the surface water quality models have made a big progress: from considering a single factor to multifactors of water quality, from steady-state to dynamic models, from the point source model to the coupled model involving point and diffuse sources, and from a zero-dimensional model stepwise up to three-dimensional models, counting of more than 100 surface water quality models up to now (Wang et al., 2013a). This high number of different water quality models can be hardly structured combining single models in groups with common characteristics. As a result, many different classifications of the water quality models exist. Compiled from Tsakiris & Alexakis (2012) and Woldegiorgis et al. (2015), the differentiation could be exemplarily done by using the following characteristics:

- the pollutant item (nutrients, sediments, salts, etc.),
- the temporal resolution (from steady state to dynamic systems),
- the dimensions in space (0D, 1D, 2D, 3D),
- the area of application (catchment groundwater, river system, coastal waters, integrated),
- the nature (deterministic or stochastic),
- the spatial analysis (lumped or distributed),
- the discharge routing simulation (e.g. Muskingum or variable storage),
- the transport processes (fully mixed tanks versus advection-dispersion equations),
- the methods used to solve the differential equations used for description of the biological and physico-chemical processes in the river, or
- the data requirements (extensive databases or minimum requirements models).

Another approach to classify water quality models could be connected to the scale (small-, meso- or large-scale) of typical model application or connected to the spatial resolution (lumped, semi-distributed or fully-distributed models) as described in Krysanova et al. (2009). In meso- and large-scale river basins the spatially distributed or semi-distributed models are usually required for an adequate representation of ecohydrological and biogeochemical processes in view of land surface heterogeneity. Several models covering multiple of these possible model groups exist. They could be of intermediate or mixed types, like a model based on physical laws with some empirical and statistical equations, a deterministic model including some statistical relationships, or a semi-distributed model (Krysanova et al., 2009).

Consequently, it would be practically impossible to review and classify the water quality models in a comprehensive way. Furthermore, the direct comparison and valuation of them would be even not fair, since many organisations have developed water quality models for particular special purposes, and therefore they are simply not comparable (Tsakiris & Alexakis, 2012).

Nevertheless, Figure 1.21 tries to give an impression of a possible classification system of water quality models together with their short description, advantages and disadvantages, and providing some examples. According to Bronstert (2004), three main hydrological model types can be distinguished. A similar classification can be also applied in water quality modelling (Thorsen et al., 1996). Krysanova et al. (2009) used the terms 'conceptual', 'process-based' and 'physically-based' for describing these three main approaches in water quality modelling. They represent an increasing level of complexity meaning the number and spatial representation of physical, chemical and biological processes and feedbacks taken into account.

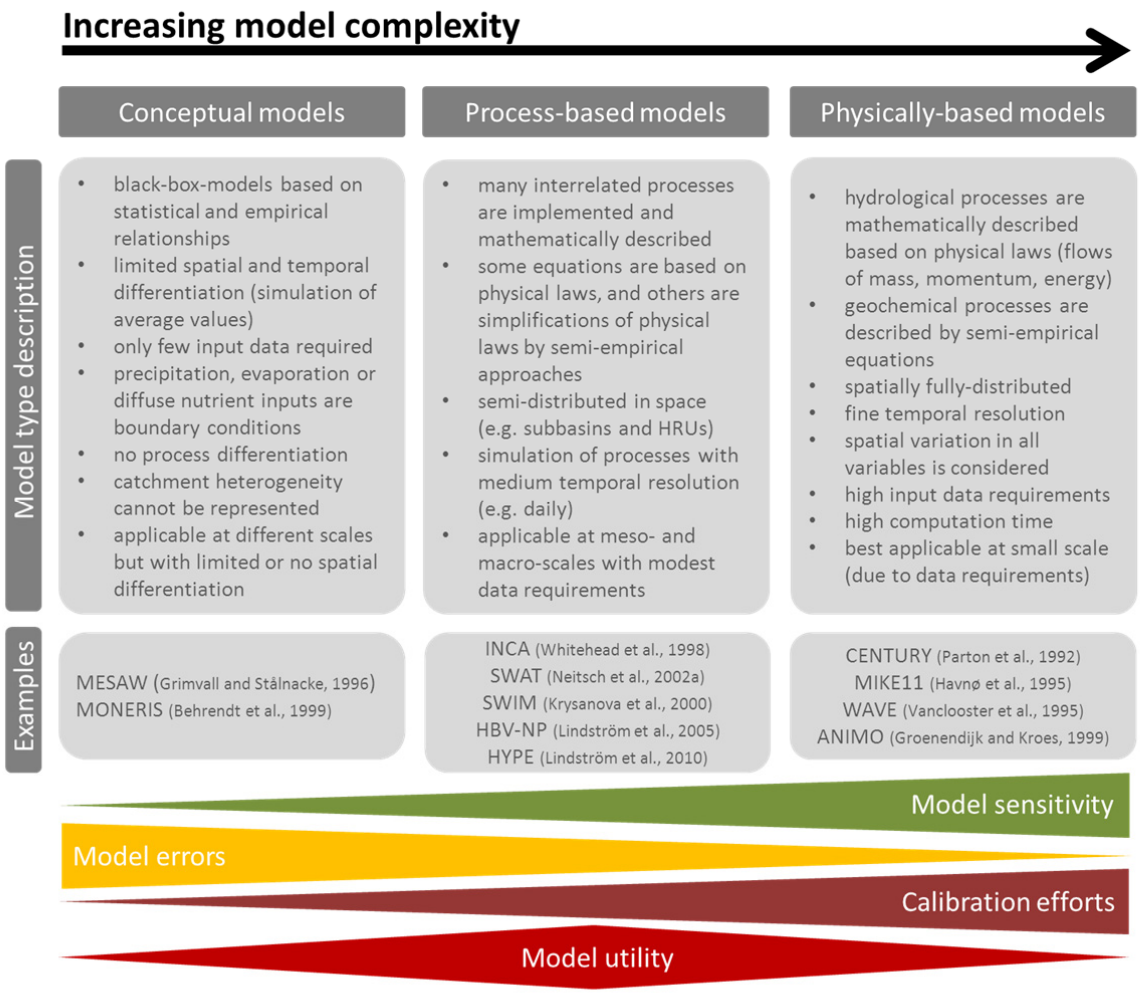

Figure 1.21 Types, description and examples of water quality models, supplemented by an evaluation of their characteristic benefits and demands.

The presentation of the three model classes in Figure 1.21 is supplemented by evaluation of their typical characteristics and benefits to be expected according to Lindenschmidt et al. (2006). With the rising model complexity the potential model error (meaning the difference between the simulated and the really observed water quality parameters) is expected to decrease due to the higher number of considered interactions and feedbacks influencing the resulting water quality in the modelled system. However, a higher number of simulated processes also leads to higher model sensitivity to certain calibration parameters, and often disproportional calibration efforts to achieve sufficiently good model results. Lindenschmidt et al. (2006) concluded that the maximum model utility can be achieved by minimising both error and sensitivity. Krysanova et al. (2009) also stated that the chosen model complexity should be generally defined as a compromising solution, as overparametrisation of very complex models is dangerous, and can lead to the problem of equifinality (meaning that there are several calibration parameter sets leading to similar results due to limitations of both the model structure and input data).

Although the development of water quality models reached a quite high level since the mid of the 1990s (Wang et al., 2013a), the models were mainly applied to catchments smaller than 1000 km^2, and the large scale applications are still rare (Krysanova et al., 1999). The ecohydrological modelling of catchments larger than 1000 km^2 is often suffering from limitations caused by the spatial heterogeneity and uncertainty of input data related to crops and fertilisation practices, which can be only partly solved (Poor & McDonnell, 2007; Rode et al., 2000).

Furthermore, it can be generally stated that water quality modelling is much more complex and difficult than solely hydrological modelling, and could not yet achieve the accuracy level and applicability of specialised hydrological models (Voß, 2007; Krysanova et al., 2009). These difficulties and restrictions can especially be identified in lowland catchments, where water and the connected nutrient flows are less influenced by straight and quick downhill runoff processes, but are subject to retention due to the low flow velocities causing water storages in soils and generally higher groundwater levels (Wriedt & Rode, 2006).

Nevertheless, an increasing demand for water quality modelling could be observed in the last decades due to recently evolved requirements of the national and European legislations and laws regarding environmental protection and sustainable management of natural resources (e.g. Water Framework Directive 2000/60/EC or Nitrates Directive 91/676/EEC), and adaptation needs to emerging global climate and socio-economic changes (Horn et al., 2004; Tsakiris & Alexakis, 2012; Wang et al., 2013a). To fulfil these requirements, the water quality models should be easily applicable, and their evaluation by decision makers and water managers should be possible. However, the large family of water quality models is still quite far away from being easily applicable and really user-friendly. Several authors complain about the lack of standardisation to improve the practicability of water quality models and the comparability of their results, and they mention this as the main task in water quality modelling for future (Moriasi et al., 2012; Wang et al., 2013a; Gao & Li, 2014).

In addition to this, some authors also detected a current tendency for devising integrated watershed models, in which the water quality component is a module. Such models are expected to account for the cross interactions of various processes affecting water quality by using the high capacity of computing facilities and the advanced tools for mapping and retrieving spatial and temporal data (Tsakiris & Alexakis, 2012). However, only a limited number of such studies could be found in literature up to now (Horn et al., 2004).

The choice of a model to be used for a case study depends on the objectives of model application and availability of measured data. The spatial and temporal resolution of a model should be appropriate for its use. The fine spatial resolution of a fully-distributed physically-based model may be required to study water flow components and related nutrient transport in a small catchment, whereas a lumped conceptual model may be sufficient for the case where only precipitation-runoff-relations and nutrient balance are roughly evaluated in a homogeneous small or medium-sized catchment. And a semi-distributed process-based model with a coarser resolution could be applied in a meso-scale or large river basin for integrated water resources assessment, including water quality, and climate impact studies (Krysanova et al., 2009).

1.2.2 Model-based impact assessments for adaptive river basin management

For an environment facing changes in climate conditions and/or human activities (compare Section 1.1.3) the possibility of adaptation is essential to cope with potential future problems and challenges. Water management in the last decades was characterised by the prediction-and-control approach and emphasis on technical solutions. However, it has to become more adaptive and flexible under the fast changing socio-economic boundary conditions and climate change (Pahl-Wostl, 2007). Managing the probable future development of natural resources requires a good understanding of recent and possible upcoming problems, and an integrated view on relationships and feedbacks between the compartments of ecosystems and the society. Therefore, water management has to take into account all aspects of water systems (human, physical, biological and biogeochemical) and their interactions in an integrative way to allow a holistic approach for sustainable management of water resources in future.

There is a growing recognition of the necessity for Integrated Water Resources Management (IWRM) for the effective and efficient management of water resources (Rahaman et al., 2004). The Global Water Partnership (GWP) defines IWRM as “a process which promotes the co-ordinated development and management of water, land and related resources, in order to maximise the resultant economic and social welfare in an equitable manner without compromising the sustainability of vital ecosystems” based on the three principles: social equity, economic efficiency and environmental sustainability (GWP-TAC, 2000). However, some authors complain about the too static and formalised approach in IWRM by shutting out alternative thinking on pragmatic solutions of existing water problems, so that it seems to be not really able to cope with future changes, where more flexible adaptation is supposably needed (Pahl-Wostl, 2007; Gain et al., 2013; Giordano & Shah, 2014). A more adaptive water management is defined by the authors as an approach that addresses uncertainty and complexity by increasing and sustaining the capacity to learn while managing.

In order to be not too much surprised while managing water resources, the model supported impact studies using scenario simulations involving possible future changes of climate and socio-economy could be helpful instruments in water resources management. The applied models should be able to deal with the recent water management problems and the politically requested water protection measures regarding water quality and good ecological status. This means that water modellers have to develop and apply tools capable of linking the physico-chemical variables with hydromorphological and biological elements in watershed models. In this context, the integrated ecohydrological model approaches applied for the entire catchment scale should be the appropriate methods of choice.

According to Whitehead et al. (2009), the complex interactions between aquatic and terrestrial systems can be efficiently explored using integrated modelling at the catchment scale. The models have to represent climate, soil, land use, lakes, rivers and coastal waters, so that the responses of the whole catchment system can be simulated, and the models can be used to assess the impacts of alternative catchment management decisions to aid in finding adaptation possibilities. However, the majority of the modelled impact studies so far have addressed mainly the hydrological effects. Nevertheless, more and more scientific papers are published dealing with ecohydrological model applications in order to assess the (historical, recent and future) biological and geochemical integrity of rivers and streams together with their adjacent catchments (e.g. Peng et al., 2015; Woznicki et al., 2016)

Process-based regional-scale ecohydrological models can play an important role in river basin management. Their direct connection to land use and climate data provides a possibility to use the models for analysis of climate and land use change impacts on hydrological cycle, agricultural production and water quality. Such models can simulate impacts and effects of possible future changes, and help to find measures for improving the adaptive capacity of river basins. In the process-based models of intermediate complexity the vertical and lateral fluxes of water and nutrients in a catchment are generally modelled separately, whereas climate is usually not modelled but used as an external driver. The land use, crops and agricultural methods are mostly considered as stable. The models are usually semi-distributed, and apply two- or three-level disaggregation schemes, e.g. in subbasins and hydrotopes, which are based on the overlaying of subbasins, land use and soil maps. Numerous studies have demonstrated that such models are able to adequately represent natural processes at the catchment scale, and can be used for meaningful integrated impact assessments (Krysanova et al., 2009, 2015).

The regional impact assessment usually follows certain steps of procedure. Firstly, all necessary spatial (e.g. digital elevation, land use, subbasins, and soil maps) and temporal (time series on climate parameters, e.g. minimum, maximum and average temperatures, precipitation and solar radiation, on point source emissions, and on water abstractions) input data for the model setup are prepared. After that the model should be carefully calibrated to historically observed data regarding water discharge and water quality parameters measured at least at the outlet of the river basin. Data at the intermediate gauges can optionally be taken into account during the calibration as well. This would increase the spatial informative value of a heterogeneous catchment and the quality of the model results.

After the calibration of the watershed model, data on climate and/or land use scenarios should be prepared by adjusting/changing the relevant input files of the calibrated model (land use map and/or climate data) but not changing the calibrated parameter set. For a meaningful climate impact assessment the model runs should be performed covering reference and scenario time periods of at least 30 years. By comparing the long-term average annual or monthly model outputs of the scenario period with the corresponding values of the reference period and calculating the absolute or relative changes, the conclusions can be drawn regarding possible impacts on the water resources quantity and quality.

1.3 Motivation, research questions and objectives

Large river floodplains close to natural status have always been the embodiment of an ecosystem deserving protection for me. Intact rivers are lifelines of nature – with this idea in mind I grew up close to the Elbe, and consequently chose the surface water research to be my main subject while studying geoecology. Hence, the theme of my dissertation was also chosen close to this topic.

I fully agree with Zalewski (1997) that the integration of hydrology and ecology should be the most important goal in future water management, and could create the basis for sustainable development of freshwater resources. The freshwater management should not be mostly the elimination of threats such as floods, droughts and point source pollution by technical measures in and close to the river reaches, but rather an amplification of chances by a holistic view on the complex ecosystem processes and services of the entire river basin. Water research should be focused on integrating the functioning of freshwater ecosystems with the large-scale hydrological processes for the maintenance of the equilibrium between water quantity, water quality and biodiversity.

Therefore, ecohydrological methodologies are needed in sustainable water management. Process-based semi-distributed ecohydrological watershed models, taking biota in the landscape as well as in the connected river reaches into account, could be helpful tools for the holistic view on the catchment and its analysis, especially in regard to the recently growing demand for global change impact assessments. The process-based SWIM model (Soil and Water Integrated Model) could be a good base for such approach, but it needs some improvements in the water quality modelling routines to fulfil the increasing requirements for the in-stream processes consideration.

Water quality modelling lags behind the pure hydrological model approaches in the computer-assisted watershed research. Water quality modelling is complex and more difficult due to the high number of interrelations and feedbacks between the simulated pollutants and the environmental abiotic and biotic compartments. The difficulties especially increase in lowland river basins due to the high lag time of water and nutrient movement in such smoothly sloped watersheds facilitating nutrient transformation and retention processes. Model results for nutrients do not yet reach the model accuracy of river discharge simulation, and the number of water quality related research studies is still lower than the studies on water flows and availability. Therefore, this research field needs some further enhancement and improvements. The dissertation is intended to be a step forward in this direction.

When I started working at the Potsdam-Institute for Climate Impact Research (PIK), my work was focused on the Elbe case study of the EU FP6 project NeWater („New Approaches to Adaptive Water Management under Uncertainty“) aiming in the development of sustainable water management measures increasing the adaptive capacity of large-scale river basins, which are facing pressures of climate and socio-economic changes. So, the river basin for investigation was easily chosen.

The Elbe river basin is characterised by several water related problems. In the Framework of the NeWater and the German GLOWA-Elbe („Globaler Wandel des Wasserkreislaufes“, Teilprojekt Elbe) projects a questionnaire was compiled and disseminated between different groups of stakeholders and inhabitants working or living within the Elbe river basin in Germany and the Czech Republic (Hesse et al., 2007). The survey asked for people's opinions about the most important ecohydrological problems and research needs within the Elbe river catchment. The three problems, which were mentioned most often, are: 1) more intensive floods, 2) diffuse pollution influencing water quality, and 3) droughts in summer. The most important research needs identified by the German stakeholders were related to water availability and possible climate changes. The Czech stakeholders were mostly interested in the flood risk research. The next important research need mentioned was finding measures for improving water quality.

It is interesting to compare the opinions of stakeholder groups in regard to the causation of a decreased water quality. The German stakeholders see the diffuse pollution as the most important problem, whereas the Czech respondents more often name the point source pollutants. Their responses reflect differences in the stages of development of the water treatment facilities in both countries, as well as the increasing problems with diffuse nutrient pollution in lower river reaches and lowland tributaries located in Germany. Therefore, this aspect requested by stakeholders and water managers was chosen for deeper investigation in this study.

Hence, the main aim of the dissertation in hand was the improvement of the SWIM model for better representation of lowland and large-scale ecohydrological nutrient processes in the model, and its application for the Elbe river basin to support water resources management in this region. In particular, the following research questions were defined for the thesis:

- How is the standard SWIM version able to simulate nutrient (nitrogen and phosphorus) processes in meso-scale and lowland river basins?
- How can nutrient modelling with SWIM be improved for applications in lowlands and in meso- to large-scale basins?
- Which model approaches are most appropriate at different scales?
- Which effects have climate and land use changes on nutrient loads and concentrations in the Elbe river basin and its selected tributaries?

According to these questions it is obvious that there are two research fields and objectives to be covered in this work: 1) ***approach related objectives*** aiming in the model improvement and further development regarding nutrient process modelling, and 2) ***application related objectives*** dealing with the model set-up, calibration and impact assessments for selected river basins to support adaptive river basin management in the Elbe river basin.

Figure 1.22 illustrates the planned steps to fulfil the research objectives and to answer the research questions of this thesis. After a deep literature review, data collection and model setup for selected subcatchments of the Elbe river, the ability of the original SWIM version to model nutrient concentrations and loads in river basins will be investigated. After that modifications of the SWIM model code for better representation of nutrient processes in soils and river reaches will be done and tested in the meso-scale catchments. Finally, the modified SWIM model should be applied for the total Elbe river basin to assess impacts of possible climate and socio-economic changes in this large-scale catchment. This work and the results will be described in several scientific publications of this cumulative dissertation, supplemented by an overall evaluation of the different model approaches and the achieved results, and by recommendations for further development and improvements of the SWIM model and its applications.

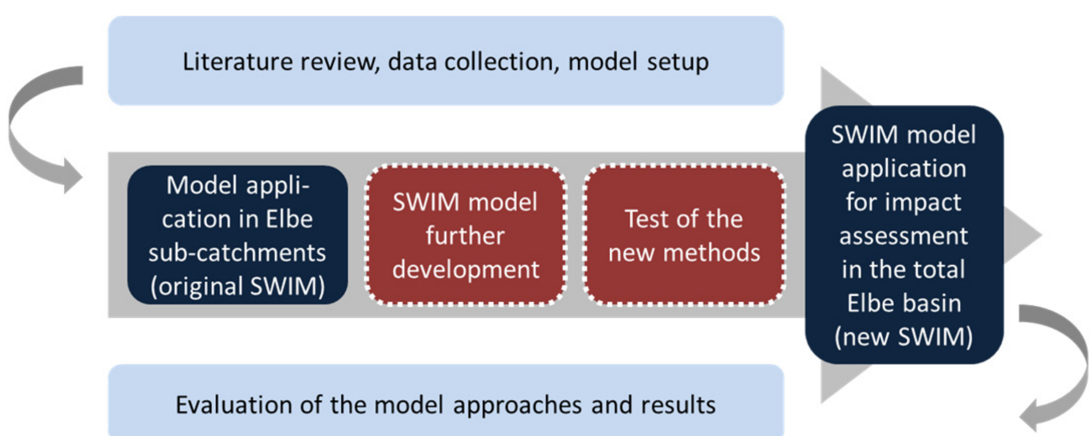

Figure 1.22 Scheme of the steps to answer the research questions and to achieve the objectives of the thesis. The tasks for model calibration and impact assessments are in dark blue, and the tasks dealing with the model further development and test of new model approaches are coloured in dark red.

1.4 Structure of this thesis

This thesis is a cumulative dissertation containing five original research articles published in different scientific journals. The included papers are in chronological order regarding the date of publication as well as regarding the catchment size of the studied areas rising from the meso- to the macro-scale within the Elbe river basin. It includes both, the more theoretically inspired research papers dealing with the comparison of different model approaches to answer a specific nutrient related research question, and the more practically oriented papers using the results of the best modelling approach for climate and land use change impact assessment on water quality conditions in the case study river basins (see Figure 1.23).

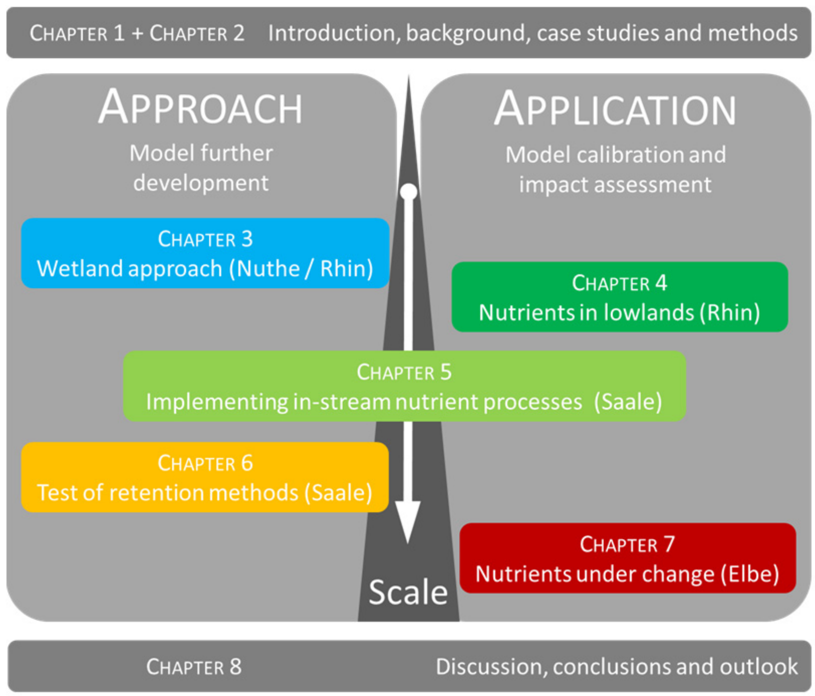

Figure 1.23
Structure of the cumulative dissertation with attribution of the included five scientific articles to the overall aims of being primary the model development papers describing new approaches in SWIM, or publications to present results of model application for impact assessments in meso- to large-scale river basins.

In particular, the introductory ***Chapter 1*** describes the general nutrient behaviour and importance in rivers and their drainage areas and the possible impacts of future global changes, the state-of-the-art in water quality modelling and global change impact assessment, as well as the motivation and objectives of this research study.

After that, ***Chapter 2*** presents the Elbe river catchment and selected subcatchments as study areas for the model approaches and applications, and a condensed description of SWIM and the model code adaptations implemented during this research work.

The following five chapters present the research papers already published in scientific journals:

- ***Chapter 3*** delivers a comparison of two different approaches implementing the specific water and nutrient conditions in wetlands in meso-scale ecohydrological modelling, and is aimed in the improvement of the model results for two catchments situated in the north German lowlands within the Elbe river basin.

- ***Chapter 4*** describes an implementation of SWIM to the meso-scale lowland Rhin catchment simulating nutrient cycling in the basin and evaluating the sensitivity to changes in climate or land use in order to find measures for improving water quality.
- While water quality modelling in the lowland catchment, it could be seen that it would be advantageous to account for possible nutrient retention and transformation processes within the river water. Thus, the subsequent ***Chapter 5*** describes the method and results achieved after implementing nutrient processes and algal growth in river reaches in SWIM to simulate water quality of the large-scale Saale river basin.
- Due to the fact that the new implemented in-stream processes in SWIM seemed to generate an overparameterised model demanding high calibration efforts with a high parameter and process uncertainty, ***Chapter 6*** analyses different nutrient retention approaches implemented in SWIM and tries to respond the research question, whether a more simple retention approach would be also able to reflect the measured water quality parameters at the outlet of the large-scale Saale river catchment sufficiently well.
- After applying the model to rivers of third and second (classical) orders, the SWIM with implemented in-stream processes was used in ***Chapter 7*** to simulate the first order river Elbe and its entire transboundary catchment for climate and land use change impact assessment, and to identify specific large-scale problems in water quality modelling.

Finally, ***Chapter 8*** discusses the results derived from the model applications presented in this thesis, draws conclusions, points out on uncertainties in conjunction with water quality modelling and impact assessments using SWIM, and outlines further research needs.

CHAPTER 2

STUDY AREAS, DATA AND METHODS

2.1 The Elbe river basin and its selected subcatchments

The Elbe river basin covers an area of 148,268 km². It is the fourth largest river catchment in Central and Western Europe, and the most important river draining the Eastern part of Germany. Before flowing into the North Sea near Cuxhaven, the Elbe river follows a course of 1094 km length, originating at 1386 m a.s.l. in the Giant Mountains situated between Poland and the Czech Republic. The Elbe drainage area is shared by four countries: 65.5% of the catchment area lies in Germany, 33.7% in the Czech Republic, 0.6% in Austria and 0.2% in Poland. The catchment is inhabited by 24.5 million people, and includes the large cities Berlin, Hamburg and Prague (IKSE, 2005).

The main tributaries of the Elbe river are the Vltava, the Saale and the Havel rivers, occupying more than 51% of the Elbe drainage area. In order to give an idea about the heterogeneity and comparability of the different subregions within the large-scale Elbe river basin, the characteristics of these three large tributaries will be additionally analysed and shown in this chapter, together with those of the entire Elbe river basin. The meso-scale Rhin catchment, which was one of the case studies described in Chapters 3 and 4 of this thesis, is also added to the analysis in this Chapter. The Saale river basin was used as case study area in Chapters 5 and 6, whereas the entire Elbe river basin was the final study area (presented in Chapter 7). Further descriptions of the individual case study areas, and their specific data preparation and model setups can be found in the corresponding chapters below.

2.1.1 Topography, climate conditions and discharge regimes

Large parts of the Elbe river basin (Figure 2.1) have characteristics of a lowland river with a wide alluvial valley downstream of Dresden (Grossmann, 2012). More than a half of the river basin is located at altitudes lower than 200 m a.s.l., mainly forming the Northern German Plain, almost 33% of the catchment has altitudes between 200 and 500 m a.s.l., representing the hilly land, and almost 17% of the drainage area belongs to the low mountain ranges, of which only 2% is located at altitudes of more than 800 m above sea level (IKSE, 2005).

The Elbe river basin is situated in the transitional zone between the maritime and continental climates, and belongs to the temperate climate zone. The continental influence can be seen in relatively low precipitation levels and large differences between the summer and winter temperatures. The main climate parameters reflect the orographic situation of the Elbe river basin. Precipitation levels increase and temperature decreases with the rising altitude in the low mountain ranges, so that significant differences between the individual regions can be observed.

The average annual air temperature is 8-9°C in the lowland, and 1-3°C at the peaks of the low mountain ranges. The most extreme temperature values in the river basin were measured in its southern Czech part with a more continental climate: +40.4°C in Dobřichovice near Prague on 20 August 2012, and -42.2°C in Litvinovice near Česke Budějovice (Upper Vltava river basin) on 11 February 1929. The lower part of the Elbe basin close to the mouth near Hamburg is characterised by more balanced seasonal temperatures, and relatively high precipitation levels, which are typical for a maritime climate (IKSE, 2005).

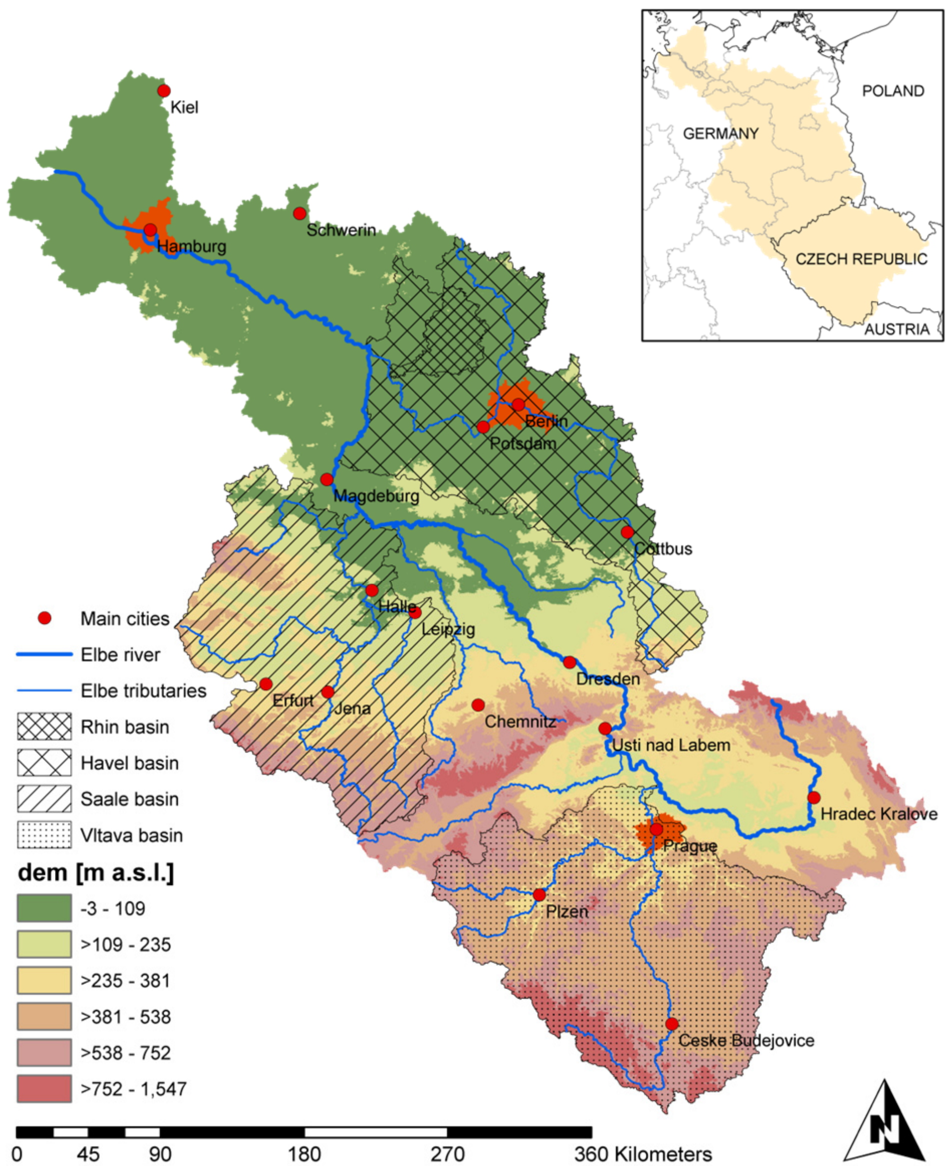

Figure 2.1 Location and topography of the Elbe river basin and its three largest tributaries Vltava, Saale and Havel (including the Rhin catchment) and location of the most important cities in the catchment.

The annual precipitation amounts range from 450 mm·a^{-1} in lowland up to 1,700 mm·a^{-1} in the highest mountainous regions, with an average value of 628 mm per year for the entire basin. The central parts of the Elbe river catchment in Germany as well as in the Czech Republic are located in the rain shadow of several mountainous ranges, and receive only little precipitation amounts during the cyclonic westerly and north-westerly weather situations. In about one third of the total Elbe river basin the annual precipitation is below 550 mm·a^{-1} (IKSE, 2005).

Resulting from these climate conditions, the Elbe river is characterised by a rain-snow-type runoff regime, typical for such transitional climate. The discharge regime of the Elbe river (861 m^3·s^{-1} on average) usually shows high water levels in winter and spring, and low water levels in summer and autumn (Figure 2.2). Due to snow melt in the low mountainous regions the runoff maximum is usually observed in the months of March and April. The lowest runoff can be registered in September. Additionally, extreme floods can be caused by regional heavy precipitation events in summer, such as the flood events in August 2002 and June 2013.

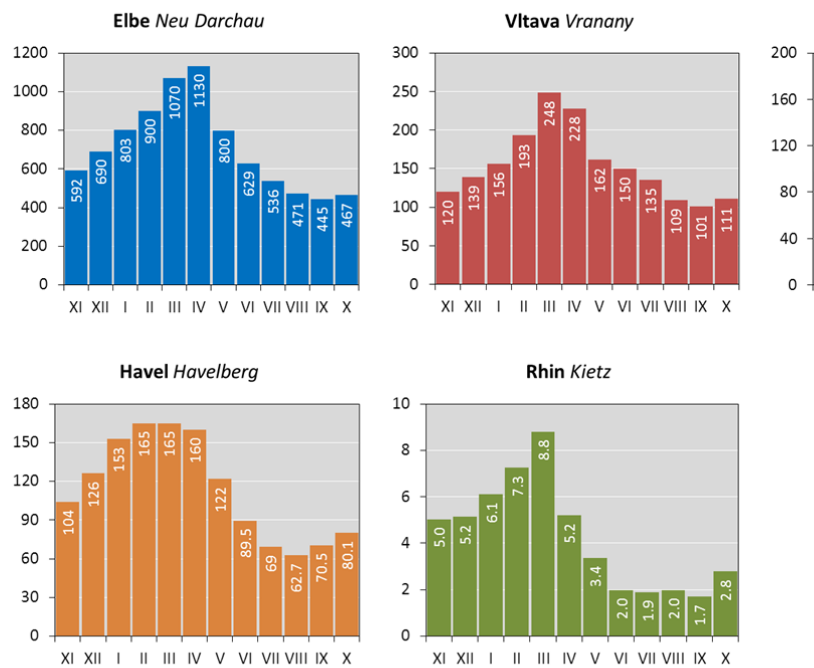

Figure 2.2
Long-term (1931/1946-2000) average monthly discharges (m^3 s^{-1}) at the downstream gauges of the Elbe river, its three largest tributaries, and the Rhin river (1980-2005).

The three main Elbe tributaries show quite similar runoff regimes on the long-term as the Elbe river (Figure 2.2). However, the maximum discharge can be observed earlier, in March, in the Vltava and Saale rivers, and the Havel has a more prolonged period of high discharge, from January to April. The longer high flow period in the Havel is caused by the lowland character of its catchment, with more rain and less snow cover in winter, and by a high share of dammed river reaches with low flow velocities.

The meso-scale Rhin river is characterised by average monthly discharges lower than 10 m^3·s^{-1}. The relation between the highest discharge in March and the lowest one in September is larger than for the large-scale rivers presented in Figure 2.2. Additionally, the summerly low flow period starts earlier and lasts longer than in the large-scale Elbe tributaries due water management impacts, water consumption and a higher evapotranspiration potential in this lowland catchment with vegetation connected to the groundwater.

In the Elbe river basin, 71% of the average annual precipitation is lost by evapotranspiration (FGG-Elbe, 2005). With the reference to the Neu Darchau gauge, which represents 89% of the whole Elbe drainage area, the average annual runoff rate amounts to 5.4 $L \cdot s^{-1} \cdot km^{-2}$. Thus the Elbe basin belongs to the river catchments with the lowest runoff rates in Europe (IKSE, 2005).

Table 2.1 gives an overview on the main natural characteristics of the Elbe river basin and the four selected subcatchments.

Table 2.1 Natural conditions of the total Elbe river catchment and, in comparison, differentiated for four of its subcatchments (discharge and climate parameters for the time period 2001-2010).

	Unit	Elbe	Vltava	Saale	Havel	Rhin*
Catchment area	km^2	148 268	28 090	24 079	23 858	1716
Average altitude	m a.s.l.	256	523	287	74	49
River length	km	1094	430	434	334	132
Mean discharge	$m^3 s^{-1}$	799	145	117	114	4
Average annual runoff rate	$L s^{-1} km^{-2}$	5.4	5.2	4.9	4.8	2.3
Average temperature	°C	9.0	7.8	9.2	9.6	9.4
Av. sum of precipitation	$mm y^{-1}$	708	713	680	616	513

* climate data: period 1996-2005 (DWD climate station Neuruppin)

2.1.2 Land use pattern, soil properties and management impacts

The dominating land use and vegetation cover in the Elbe river basin are agricultural acreages, followed by forests and grassland. The land use map of the entire catchment based on CORINE land cover (CLC2000) is presented in Figure 2.3, which also shows maps of point source emissions (sources: FGG-Elbe (2004a) and IKSE (1995)), soil properties (sources: BÜK1000 and Košková et al., 2007) and fertiliser application classes assumed for setting up the SWIM model.

The land use patterns in the Elbe river basin reflect the orographic, climatic and soil conditions. Forests can be found in the mountain ranges and on less fertile sandy soils. Predominantly agricultural use prevails on fertile brown and black soils in the middle and lower courses of the Saale basin and in the central Czech part, and grassland is widespread on wetland soils with a high groundwater table, as in the Havel catchment, and in the lower Elbe part close to the mouth.

The map of the soil properties in the Elbe river basin in Figure 2.3 is based on two main features important for water and nutrient behaviour in a river catchment: a) the sand content and b) the easy connection to groundwater (wetland soil). The sand content in soil is one essential parameter reflecting the water and nutrient retention potential in a landscape: the higher the fraction of sand in soil texture, the lower is its retention potential (Scheffer & Schachtschabel, 2002; Zotarelli et al., 2006). The wetland soils shown as grids in Figure 2.3 mark those lowland areas (e.g. fens, floodplains) characterised by an increased evapotranspiration (and nutrient uptake) potential due to a higher percentage of plant roots reaching the groundwater.

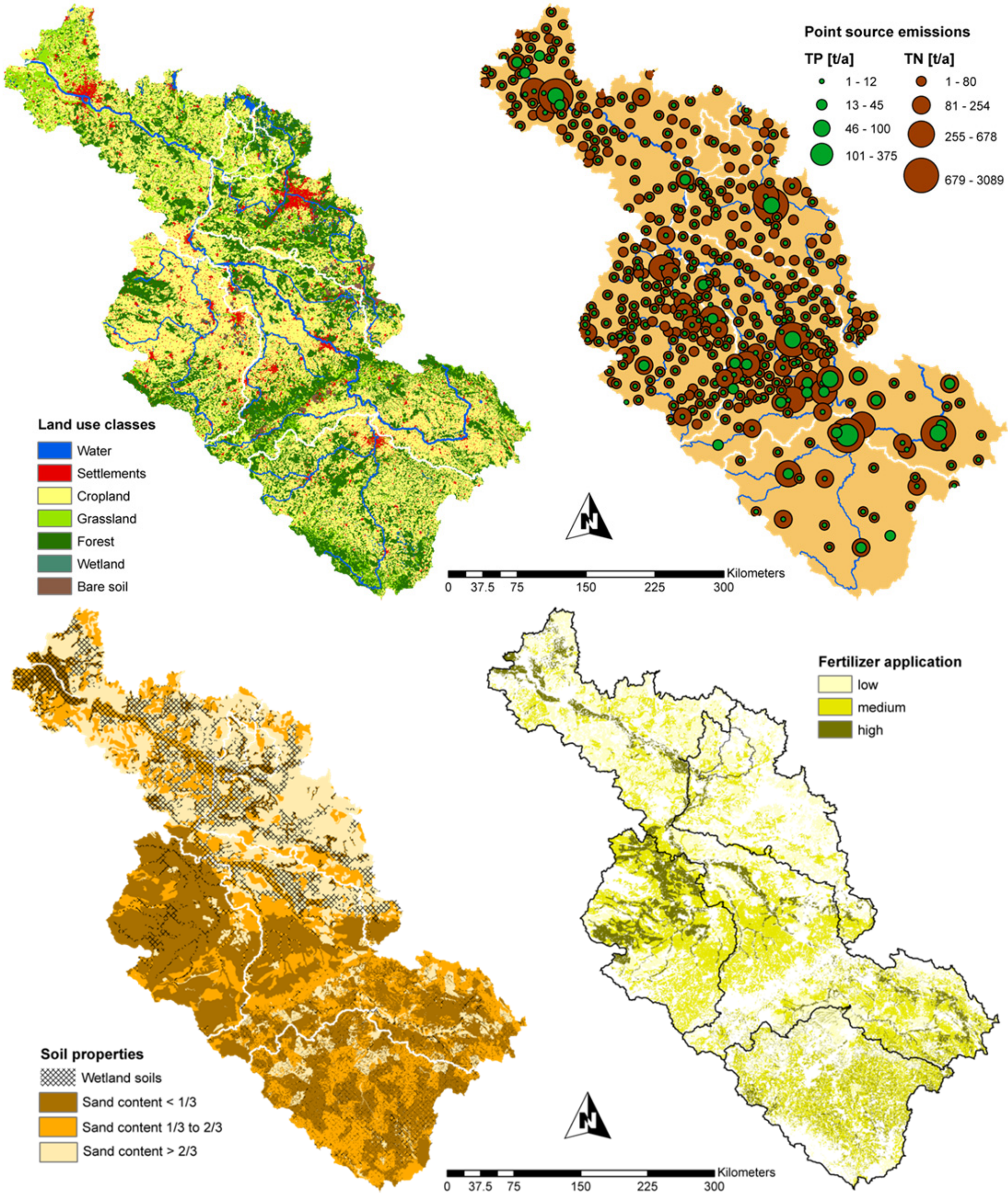

Figure 2.3 Spatial distribution of land use classes, point source emissions of total nitrogen (TN) and total phosphorus (TP), soil properties, and fertiliser application levels (as used in the study for the entire Elbe river basin).

Point and diffuse nutrient sources in the Elbe basin are mainly connected to human activities in the catchment. Large cities or industrialised regions usually come along with intensive point-borne pollution to the river network originating from water treatment plants and industrial sites. The diffuse pollution is linked to agricultural areas, and additionally depends on soil types and climatic conditions. Fertiliser application on agricultural fields is usually recommended to be increased with increasing crop yield expectations (TLL, 2011a), which can be defined by soil quality, water availability and climate conditions. Following this rule, the very fertile soils in the lower Saale basin can be expected to receive more fertilisers than the sandy less productive soils dominating in the Havel river basin. The fertiliser application map presented in Figure 2.3 illustrates the fertilisation rate classes as assumed for SWIM model application in the Elbe river basin based on model simulated potential yields under historically measured climate conditions in the time period 2001-2010 (compare Chapter 7).

Resulting from the maps and facts described above several additional characteristics of the Elbe river basin and its four subcatchments under consideration can be calculated, summarised and comparably listed. The comparison can be found in Table 2.2.

Table 2.2 Comparison of land use composition, selected soil conditions and point and diffuse nutrient sources of the Elbe river catchment and four of its subcatchments for the time period 2001-2010.

	Unit	Elbe	Vltava	Saale	Havel	Rhin*
Land use, major types						
Agriculture	%	51	50	63	39	41
Forest	%	30	37	23	38	34
Grassland	%	10	8	5	11	19
Settlements	%	7	4	8	8	3
Soils by sand content						
Sand <1/3	%	38	50	78	12	22
Sand 1/3-2/3	%	29	41	18	18	10
Sand >2/3	%	33	9	4	70	68
Wetland soils	%	23	16	10	34	40
Point sources						
Total nitrogen	$t\ y^{-1}$	26626	4704	3557	2768	25
Total phosphorus	$t\ y^{-1}$	2144	564	357	167	3
Total nitrogen	$kg\ y^{-1}\ km^{-2}$	180	167	148	116	15
Total phosphorus	$kg\ y^{-1}\ km^{-2}$	14	20	15	7	2
Fertilisation class						
Low	% *of agr.*	27	18	11	56	58
Medium	% *of agr.*	52	63	55	37	42
High	% *of agr.*	21	19	34	7	0

* point sources: period 2001-2005 (LUA Brandenburg)

The natural flow regime of the Elbe river and its tributaries is influenced by several anthropogenic measures, such as creation of reservoirs, regulation of rivers, drainage of wetlands and brown coal mining (Klöcking & Haberlandt, 2002). A large number of dams with a reservoir volume of more than 0.3 million m^3 can be found in the Elbe river basin, 175 of them are located in Germany and 137 in the Czech Republic. They comprise a total reservoir volume of approximately 4.12 billion m^3 (IKSE, 2005). The hydraulic engineering measures can influence water quality, discharge regime, structural diversity, particulate matter and groundwater, often seriously affecting the vulnerability of the ecosystem (Rode et al., 2002).

For example, in the upper course of the Saale basin, the river morphology and hydrological regime is modified by a series of five reservoirs for water harvest, flood protection and a salt-load control system in order to dilute high industrial and mining salt emissions downstream in the low flow seasons. The natural water flow in the lower reaches is influenced by several weir and lock systems to store water for enabling inland navigation also in the drier summer months.

The meso-scale Rhin river basin is characterised by an intensive water regulation system including more than 300 small dams and weirs. The large fens and wetland areas in this lowland catchment are meliorated for agricultural purposes and for use as pastures. Water storage, irrigation practices and water transfer to and from adjacent catchments influence the natural hydrological cycle, and have significant impacts on river discharge.

The extensive brown coal mining activities, as e.g. in Southern parts of the Havel river catchment (Lusatia), led to a wide-spread decrease in groundwater level and an artificial increase in river discharge by dewatering. After closure of the open-cast mining the pits are often refilled with river water causing a decrease of discharge. A temporary decreased groundwater level usually induces oxidation processes in the soils of the influenced regions, and often causes ferric sulphate pollution problems in the draining rivers after the rerise of the groundwater table.

Nevertheless, large parts of the main Elbe river in Germany are still free-flowing and are not influenced by barrages. Especially the areas around the middle course of the Elbe river in Germany contain several protected natural areas with a high diversity of flora, fauna and landscape types. But the originally broad floodplain areas around the middle and lower courses of the Elbe river are reduced and influenced by flood protection measures for settlements and agricultural or industrial activities. During the last two centuries approximately 84% of the floodplain along the Elbe river course in Germany has been protected by dikes, and cut off from the natural river ecosystem, whereas the narrower upstream valleys have experienced lower losses of floodplain than the wider lowland valleys downstream of Dresden (Grossmann, 2012).

The reduced flooding area around the river reaches causes problems not only in times of very high water levels (e.g., during the last decades when immense flood events and damages occurred), but also hinders the natural nutrient retention capacity of the river. The water engineering measures and construction of dams also influence the eutrophication status of a water body. They lower the river's flow velocity, impact sediment transport and planktonic growth rates and reduce oxygen concentrations in the river reaches. This often induces an intensification of nutrient pollution problems in the river waters.

2.1.3 Nutrient pollution and water quality

A water quality monitoring network was established along the Elbe river and its main tributaries in the last decades, and data can be found online and used for evaluation of the former and recent water quality status of the Elbe river and selected subcatchments (FGG-Elbe, http://www.fgg-elbe.de/elbe-datenportal.html). This was done for the most downstream stations of the Vltava (Zelčin), Saale (Groß Rosenburg) and Havel (Toppel) rivers and the last tide-unaffected Elbe river gauge (Schnackenburg) representing the subcatchments, which were already analysed above. The analysis of NO_3-N and PO_4-P values for the meso-scale Rhin basin (gauge Kietz) based on measurements provided by the LUA is also added (Figure 2.4).

The upper graphs of Figure 2.4 depict the development of the annual average concentrations of nitrate nitrogen, ammonium nitrogen, phosphate phosphorus, and dissolved oxygen for the time period 1991-2010. As one can see, the nutrient concentrations in the Elbe river basin are mainly decreasing with time, whereas the dissolved oxygen is mostly increasing. This indicates on an overall improvement of water quality in the Elbe river.

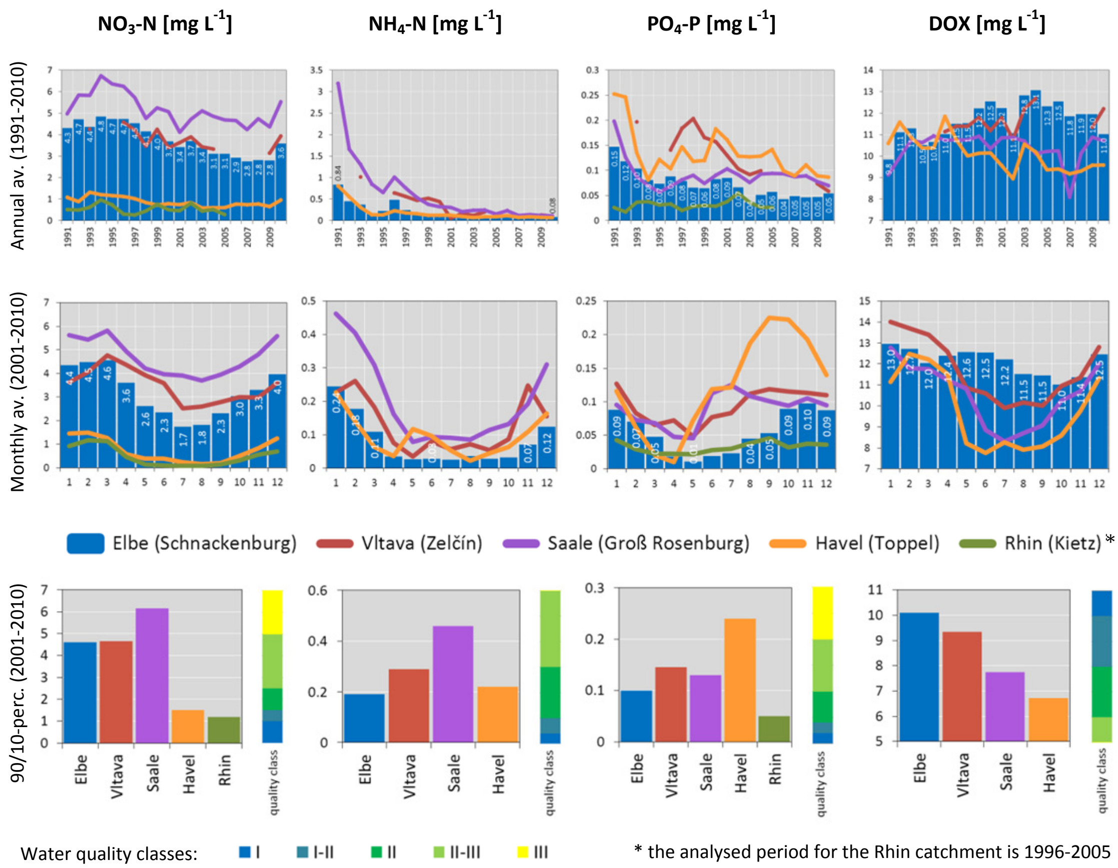

Figure 2.4 Water quality of the Elbe river, its three largest tributaries, and the Rhin (most downstream gauges): annual average concentrations in 1991-2010 (above) and monthly average concentrations in 2001-2010 (middle) of nitrate nitrogen (NO_3-N), ammonium nitrogen (NH_4-N), phosphate phosphorus (PO_4-P) and dissolved oxygen (DOX) and comparison of their 90th percentiles for nutrients and 10th percentiles for dissolved oxygen (below) with the German water quality classes for surface waters according to LAWA (1998) (data sources: FGG Elbe, http://www.fgg-elbe.de/elbe-datenportal.html, December 2012; LUA).

However, some tributaries show a different behaviour and pollution classes for several substances. In subcatchments with dominating agricultural land use (e.g. Saale), the nitrate and ammonium nitrogen concentrations are higher than in the Elbe and in other rivers, resulting probably from a larger fraction of arable land characterised by fertiliser application and leaching. These high nutrient concentrations have also negative effects on the Elbe river. It has been already observed that the ecological status of the Elbe river declines after the confluence of the Saale river, especially due to increase in nitrate nitrogen concentration (Arge-Elbe, 2008).

In contrast, the catchments of the Havel and Rhin rivers are less used for agriculture, and show the lowest nitrogen pollution. The slowly flowing lowland rivers with a lot of lakes and wetlands within their catchments additionally facilitate the retention of nutrients (FGG-Elbe, 2010). Nevertheless, the highest phosphorus level can be observed in the Havel river. Besides phosphate leaching processes in the mainly sandy soils of the catchments, the high phosphate concentrations in the rivers can be additionally explained by desorption from historically polluted sediments (Bronstert & Itzerott, 2006). Such processes mainly occur in times of high temperatures and low oxygen availability, as it can be seen in the monthly average values for the late summer in the Havel river (Figure 2.4, middle).

According to the German classification of water quality (LAWA, 1998), which uses the 90th percentile for nutrients and the 10th percentile for dissolved oxygen to compare with certain water quality thresholds, the highest nitrate level in the Elbe basin results in water quality class III (Saale), the highest ammonium value belongs also to the Saale (class II-III), the maximum phosphate phosphorus level represents water quality class III (Havel), and the lowest dissolved oxygen concentration results in water quality class II (Havel). There are some diversities between the rivers in this respect, and no river exists which has the worst or best status for all components (Figure 2.4, below).

In general, the long-term observations of surface water quality in Germany (1955-2011) show an increase of nutrient pollution with growing industrialisation and intensification of agriculture from the 50^{ies} until the 70^{ies} or 80^{ies}, and then a decrease in nutrient concentrations (or rather 90th percentiles) for PO_4-P and especially NH_4-N, but only slightly for NO_3-N. For the Elbe river the same behaviour could be observed, but only from the beginning of the 90^{ies}, after the German reunification (UBA, https://www.umweltbundesamt.de/en/topics/water/rivers).

Due to former political and socio-economic conditions, until the 90^{ies} the Elbe was one of the most polluted rivers in Europe with a low ecological potential. The improvements in water quality could be recognised after the political change due to closure of industrial enterprises and upgrading of sewage treatment plants in the basin, as well as due to a substantial decrease in fertilisation rates on agricultural land (Lehmann & Rode, 2001; Hussian et al., 2004).

However, nutrient pollution is still an important problem in the Elbe basin, as the availability of nitrogen and phosphorus is the main factor for the riverine primary production, often causing a moderate to bad status of the biological quality components according to the WFD. The main reason for the heightened loads is the still excessive diffuse input of nutrients to rivers, mainly caused by time-delay in leaching from agricultural fields, as well as remobilisation from the heavily nutrient-loaded sediments. The high nutrient pollution loads carried with rivers to the seas are especially dangerous for the coastal ecosystems (FGG-Elbe, 2010).

Therefore, the Elbe river management plan of 2009 requested by the WFD mentions the reduction of diffuse nutrient pollution as one of the most important management points for the national and international water management strategies. It is assumed there that the nitrogen and phosphorus loads have to be reduced within three 6-year periods by 24% (based on the values of 2006 at the gauge Hamburg-Seemannshöft), in order to reach a good ecological status of the coastal waters (FGG-Elbe, 2009). In the actualisation of this management plan published in 2015 target values regarding the average annual nitrogen and phosphorus concentrations are defined (TN: 2.8 mg L^{-1} (Seemannshöft), 3.2 mg L^{-1} (Schmilka); TP: 0.1 mg L^{-1}). These values are still exceeded at the majority of the Elbe river water quality gauges, at some stations by up to 60% (IKSE, 2015).

According to IKSE (2015), a total of 91% of all river waters in the Elbe basin do not reach the good ecological status as requested by the WFD. The main pressures counteracting to reach the aims of the WFD in the intensively used Elbe river catchment can be summarised as follows:

- diffuse sources (42%),
- regulation of discharge and/or morphological changes (35%),
- point sources (20%),
- water abstraction (1%),
- others (2%).

The integrated water quality modelling considering nutrient processes in the Elbe catchment using a model enhanced for that (taking into account nutrient and biological in-stream processes), and the assessment of nutrient concentrations and loads at the outlet of the large-scale Elbe river basin under possible future scenarios of changes in climate and management can help to find suitable measures for the full implementation of the WFD plans in this river basin. The dissertation in hand is aimed to be a step forward in this direction.

2.2 The Soil and Water Integrated Model (SWIM)

The integrated water quality modelling in the Elbe river catchment was performed by using the Soil and Water Integrated Model (SWIM) established and mainly applied at the Potsdam-Institute for Climate Impact Research (PIK) for regional impact studies on water quantity and quality (Krysanova et al., 2000).

SWIM was developed based on the two models SWAT (Arnold et al., 1993) and MATSALU (Krysanova et al., 1989). The model is suited for the integrated modelling of hydrological processes, vegetation, erosion and nutrients (nitrogen and phosphorus) in meso- to macro-scale river basins with areas ranging from 100 km^2 up to 200,000 km^2 using climate, soil and land use conditions as driving forces and considering feedbacks. Hence, SWIM is a suitable tool for the analysis of climate and land use change impacts on hydrological processes, agricultural production and water quality.

The model's ability to adequately simulate hydrological processes, nutrient dynamics, crop yields and erosion has been thoroughly tested and validated in many meso-scale and large river basins in different regions over the last 20 years. The model has been applied firstly in Germany, and later in other European countries, as well as for river basins in Africa, Asia and America. Most of the results in terms of modelling performance were satisfactory or good (Krysanova et al., 2015). SWIM was steadily being developed further in accordance to the particular research needs or specific case characteristics, e.g. by implementing more detailed process description in wetlands and riparian zones (Hattermann et al., 2006), carbon cycles (Post et al., 2007), forest growth (Wattenbach et al., 2005), reservoir control (Koch et al., 2013), glacier dynamics (Wortmann et al., 2016) or – as done for this study – in-stream nutrient transformation and retention (Hesse et al., 2012; Chapter 5).

2.2.1 General model description

SWIM is a process-based and spatially semi-distributed ecohydrological model of intermediate complexity working with the daily time step. The model includes mathematical descriptions of physical, biogeochemical and hydro-chemical processes in river basins, and contains some semi-empirical elements (Krysanova et al., 2005b). Several physically based processes are simplified in a conceptual manner, particularly in cases where physical parameters are difficult to measure.

SWIM simulates hydrological processes, erosion, vegetation, and nutrient cycles using regionally available data (climate, land use and soil) and considering interactions and feedbacks between the different model compartments, such as water and nutrient drivers for plant growth, evapotranspiration by plants, and nutrient transport with water.

To cope with the spatial heterogeneity of a case study catchment, the model uses a three level disaggregation scheme (basin, subbasin, hydrotope), where hydrotopes are sets of elementary units in a subbasin with the same land use class and soil type. It is assumed that hydrotopes behave uniformly regarding hydrological, vegetation and nutrient processes.

The vertical water fluxes, nutrient dynamics and plant growth are calculated at the hydrotope level before the lateral fluxes are simulated. During the lateral movement, nutrients in surface flow, interflow and base flow are subject to retention and decomposition processes, whose rates and intensities are described by special parameters, and can be used for calibration (Hattermann et al., 2006). Finally, the lateral fluxes are aggregated at the subbasin level and routed through the river network to the outlet of the catchment taking transmission losses into account. The original SWIM version did not allow further transformation of nutrients in the river network during the routing process. This option was primarily implemented in SWIM and published in a paper for this thesis (Hesse et al., 2012; Chapter 5).

A general scheme of the SWIM model as applied in this study, including the required spatial and temporal input data used as external drivers, is presented in Figure 2.5. The climate parameters are assumed to be homogeneous at the subbasin level. Usually they are interpolated from data measured at real observation stations (located within and around the river catchment) to the subbasin centroids using the inverse distance method. Like the management data, they are external drivers for the model. More detailed information on data sources and preparation for model setup of the SWIM applications in the Elbe river basin can be found in Chapters 3-7.

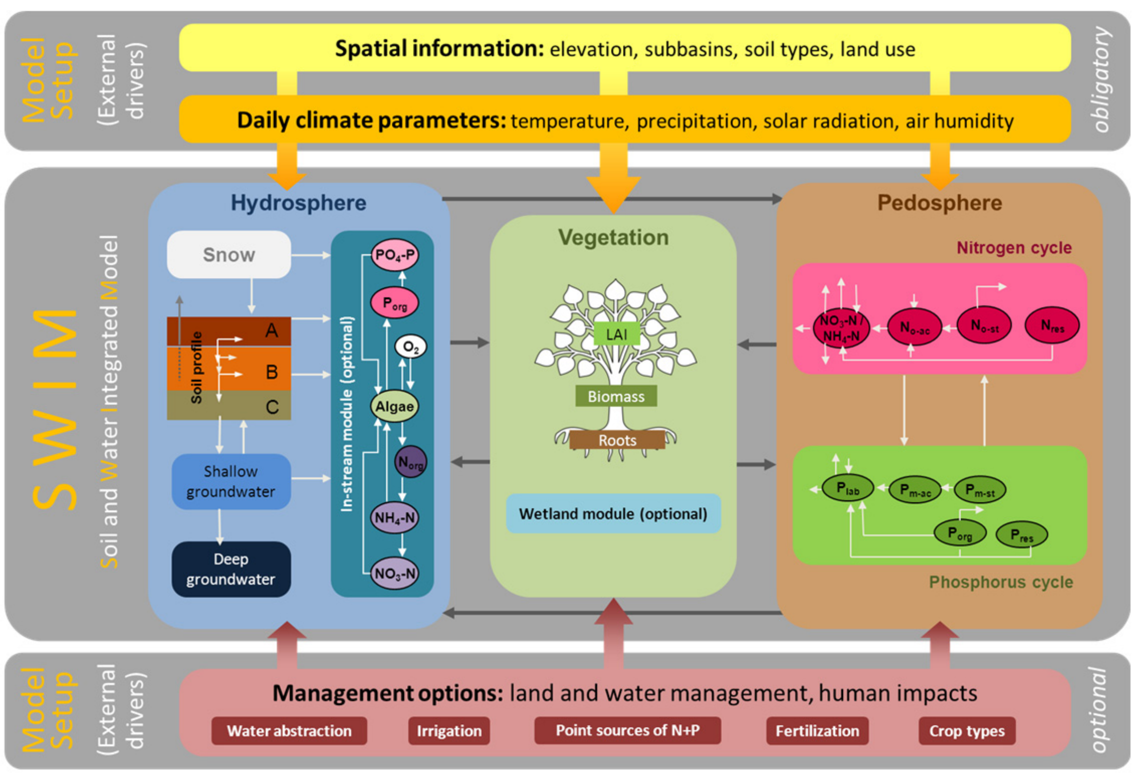

Figure 2.5 Structure of the SWIM model and its external drivers to be prepared during the model setup. All included compartments, processes, modules and management measures were applied and are described in the different chapters of this study, but some of them not always in parallel in every case study (indicated as "optional").

Hydrological processes in SWIM

The hydrological system in SWIM is split into four compartments: soil surface, soil layers, shallow aquifer, and deep aquifer. Hydrological processes in the soil zone are surface runoff, infiltration, evapotranspiration, percolation and interflow, and in the aquifer zone groundwater recharge, capillary rise to the soil profile, lateral flow, and percolation to the deep aquifer.

Hydrological processes in SWIM are based on the water balance equation starting from soil water content:

$$SW_{t+1} = SW_t + P - Q - ET - PERC - SSF$$

where SW_t is the soil water content on the day t, P - precipitation, Q - surface runoff, ET - evapotranspiration, PERC - percolation and SSF - subsurface flow (or interflow). The melted snow (according to the simple degree-day equation) is treated as additional precipitation (Krysanova et al., 2000).

Surface flow is calculated by a non-linear function of precipitation and a retention coefficient which depends on land use and soil type, on management and on the actual soil water content. Subsurface flow and percolation are calculated simultaneously and separately for each soil layer. If in one layer percolation exceeds field capacity, subsurface flow occurs. The number of soil layers is defined depending on available soil parametrisation for the catchment. SWIM is able to consider up to ten different soil layers. Percolation from the bottom soil layer leads to a recharge of the shallow aquifer, from where water can rise again to the soil profile by capillary rise. Other processes in the shallow aquifer are lateral flow and percolation to the deeper aquifer (Krysanova et al., 2015). From the deep aquifer water cannot rise up to soil again.

Potential evapotranspiration is calculated on the basis of solar radiation, daily mean temperature and elevation, using the method of Priestley & Taylor (1972). The actual evaporation is estimated separately for soil and plants as functions of potential evapotranspiration and the Leaf Area Index (LAI), while soil evaporation is reduced when its accumulated amount exceeds 6 mm. The limited soil water content leads to decreased plant transpiration (Krysanova et al., 2000).

Driven by climate conditions, vegetation water demand, soil layering and soil characteristics of the specific hydrotope, water flows through the soil surface and the root zone, and contributes to streamflow as lateral surface, subsurface, or groundwater flow. Water flows in the river network are calculated using the Muskingum flow routing method.

Vegetation processes in SWIM

The crop and vegetation module represents an important interface between hydrological processes and nutrients. The hydrological cycle as well as nutrient dynamics are influenced by vegetation growth and specific plant needs.

SWIM distinguishes the characteristics of 74 different plant types containing crops and natural vegetation. The crops (e.g. summer barley, potatoes, maize, or winter wheat) and natural vegetation (e.g. grass, pasture, or broadleaf forest) are described in a database connected to SWIM by such parameters as maximum leaf area index, maximum plant rooting depth, optimal nutrient content, and harvest index dependent on the accumulated heat units.

The vegetation growth is calculated using a simplified EPIC approach (Williams et al., 1984), where plant development and growth are based on phenological descriptions aimed in enabling the parametrisation of the model at the regional scale. The increase in biomass is calculated as a function of solar radiation, the LAI and a specific plant parameter for converting energy into biomass. The estimation of the LAI increment is based on a function of biomass and daily heat unit accumulation. The latter is calculated from the daily maximum and daily minimum temperatures (Krysanova et al., 2000).

Plant growth in the model can be influenced by the four potential stress factors: temperature, water, nitrogen content and phosphorus content. The degree of discrepancy between potential and actual increase in biomass due to stress factors is calculated as a function of difference between the optimal and actual values of the potential stress factors. Plants grow until the physiological maturity is reached or, in the case of crops, until they are harvested (Krysanova et al., 2000).

Nutrient processes in SWIM

The standard SWIM nitrogen module for the soil layers includes several pools: nitrate nitrogen, active and stable organic nitrogen, and organic nitrogen in plant residues, as well as the flows: fertilisation, mineralisation, denitrification, plant uptake, input with precipitation, wash-off, leaching, and erosion. Two different pools are assumed to be sources for nitrogen mineralisation: crop residues and soil humus. The stable organic nitrogen pool is not subjected to mineralisation. Organic nitrogen flows between the stable and active pools assume that the active pool fraction at equilibrium is 0.15. Nitrogen decomposition rate of residues is a function of the C:N and C:P ratios, soil temperature and water content. Denitrification occurs in periods of oxygen deficit, which usually is associated with high water content in soil, and is a function of soil temperature and carbon content (Krysanova et al., 2000).

The soil phosphorus module is simulated in a similar way and includes the pools: labile phosphorus, active and stable mineral phosphorus, organic phosphorus and phosphorus in plant residues, and the flows: fertilisation, sorption and desorption, mineralisation, plant uptake, erosion, and wash-off. The flows between the different phosphorous pools are governed by equilibrium equations (Krysanova et al., 2000).

Nutrient uptake by plants diminishes nutrient availability; mineralisation of crop residues and soil organic matter increases nutrient amounts in soils. Nutrient uptake is based on a supply and demand approach. Nutrients can be uptaken from all soil layers that have roots, starting from the upper horizon and proceeding downwards until the daily demand is met or until all nutrients are depleted. The daily nutrient demand is calculated as a function of the optimal and the already accumulated nutrient contents in the crop biomass at a specific growth stage.

While passing the soil layers dissolved nitrogen and phosphorus are added to the lateral water flows (surface flow, interflow and base flow) and transported to the river network taking into account retention and decomposition processes. The loads of nitrate nitrogen and soluble phosphorus in surface runoff, subsurface flow and percolation are estimated as the products of the volume of water and the average concentrations. As phosphorus is mostly associated with the sediment phase, the soluble phosphorus loss is estimated as a function of surface runoff and the concentration of labile phosphorus in the top soil layer. After that nutrients are transported through the river reaches to the basin outlet defining the water quality there.

Additional information about the general SWIM model concept, necessary input data, calibration parameters, process equations as well as the GIS interface for model setup can be found in the SWIM User Manual (Krysanova et al., 2000).

2.2.2 Model adjustments for this study

According to the objectives of the studies and to the case specific requirements, some model adjustments had to be implemented in SWIM during the calibration processes for the Elbe basin and subbasins. They are described in details containing all relevant mathematical equations in Chapters 3-7 and in the Appendix. Therefore, the main changes will be only chronologically listed and shortly presented in this section.

1) Simple wetland method: A simple wetland approach (Hattermann et al., 2008a; Chapter 3) was introduced in the model in order to represent specific water and nutrient processes in soils with shallow groundwater tables, where the availability of water and nutrients for vegetation is higher than in the neighbouring upland hillslope areas. The model approach allows increasing the plant uptake of water and nutrients from groundwater in wetland areas in times, when the supply of water and nutrients in soil is limited, while percolation of water and leaching of nutrients to groundwater is decreased to maintain the balances.

2) Water and nutrient inputs: Due to human activities in river catchments (e.g. nutrient emissions from sewage treatment plants or water transfer between catchments) the natural water and nutrient cycles are often strongly affected, which should be considered during the model setup and calibration to enable sufficient model accuracy. Changes in the model code to represent such additional in- or outputs at the subbasin level have been implemented in all model applications presented in Chapters 4-7 depending on the available data.

3) Leaching of phosphorus: In contrast to the standard SWIM version, where soluble phosphorus was assumed only to appear in the first ten millimetres of the soil profile, the soluble phosphorus in the SWIM applications presented in Chapters 4-7 is allowed to leach also vertically through the soil profile as a function of phosphorus concentration, the amount of leaving water and of the ratio between the phosphate phosphorus concentration in the soil to that in soil water (Hesse et al., 2008; Chapter 4). While passing the soil layers, the surplus phosphorus is added to the corresponding lateral water flows (interflow and base flow) to reach the river network. Lateral moving phosphorus is subject to retention and decomposition processes in soils according to the equation introduced in SWIM by Hattermann et al. (2006).

4) Ammonium cycle in soils: To describe nitrogen soil processes in more detail, the ammonium nitrogen pool was added to the nitrogen cycle (Hesse et al., 2012; Chapter 5 and Appendixes A5.1 and A5.2) taking into account decomposition, mineralisation, nitrification, volatilisation, leaching, erosion, and plant uptake processes at the hydrotope level. In contrast to nitrate nitrogen, the ammonium nitrogen leaching is influenced by its high adsorption potential to soil particles. Surplus ammonium is added to the lateral water flows and subject to retention processes before reaching the channel network.

5) Water temperature: Water temperature is one of the driving forces for the in-stream biological and water quality processes, and it is especially important to model the algal growth. To simulate water temperature in SWIM, the approach of the SWAT model (Neitsch et al., 2002a) was used, which is taken from Stefan & Preud'homme (1993) and correlates the water temperature with the average daily air temperature at the subbasin level. This formed a basis for the further implementation of the in-stream processes description in the model.

6) In-stream processes: One of the main tasks of this study related to model development was the implementation of nutrient transformation processes in river reaches in SWIM, in order to come closer to an integrated water quality modelling approach as required for the WFD applications. The SWIM model was extended with the in-stream processes, similar to the method used in SWAT (Neitsch et al., 2002a) based on the algorithms of the QUAL2E model (Brown & Barnwell, 1987). The implemented in-stream processes include algal growth (described by chlorophyll *a*), nitrogen and phosphorus transformation processes and oxygen calculations, mainly driven by water temperature and phytoplankton. Three additional assumptions were implemented in the model code to adequately simulate the case-specific seasonal dynamics of algal growth: temperature stress and photoinhibition limiting the algal growth in summer, as well as predation reducing algal concentration due to consumption (Hesse et al., 2012; Chapter 5 and Appendixes A5.3 and A5.4). This extension of SWIM considerably increased the number of model calibration parameters.

7) In-stream retention experiments: For a first representation of in-stream retention processes, an equation similar to those describing nutrient retention in soils (Hattermann et al., 2006) was applied also for nutrients coming from point sources to the river network (Hesse et al., 2008; Chapter 4). To allow retention and decomposition of the total nutrient loads in river network, the detailed and quite complex in-stream processes were implemented (Hesse et al., 2012; Chapter 5). Chapter 6 deals with the experimental implementation and comparison of different methods to calculate nutrient retention processes in river reaches based on hydromorphology and water temperature. For that several equations and new calibration parameters had to be implemented in addition to the model code, as described in detail in Hesse et al. (2013). They could be selectively switched on or off. This work was aimed in finding the most appropriate model complexity for sufficient accuracy of water quality modelling in river basins. However, only some of the approaches were used in the further SWIM applications.

8) Spatially distributed fertilisation according to expected crop yields: Besides the economic resources of the farms, fertiliser application on agricultural fields is also a function of the soil quality and climatic conditions, as fertilisation rates are recommended to be increased with increased yield expectations (TLL, 2011a). To represent this heterogeneity in the Elbe river basin, the arable land was classified in low, medium and high yield classes based on an exemplarily model run with constant fertilisation amount (Hesse & Krysanova, 2016; Chapter 7). In contrast to the former spatially constant fertiliser usage, the average fertilisation was reduced on acreages with expected lower yields and increased on agricultural areas with higher expectations for ecohydrological model calibration of the large-scale Elbe river basin.

9) Subcatch calibration: As the global calibration was not sufficient to represent the spatial heterogeneity of discharge behaviour and nutrient processes in the entire large-scale Elbe river basin, all subbasins were attributed to the individual main tributary catchments in the model code, and each of them was calibrated with an own set of the main (most sensitive) calibration parameters (Hesse & Krysanova, 2016; Chapter 7).

CHAPTER 3

MODELLING WETLAND PROCESSES IN REGIONAL APPLICATIONS

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Abstract

Wetlands represent an interface between the terrestrial environment and the surface water systems in river basins, functioning as important buffers and filters for water flow, sediments and dissolved nutrients, and pollutants. They mitigate impacts of floods, improve water quality in rivers, and reduce erosion. However, most model applications at the regional scale do not consider hydrological and ecohydrological processes in wetlands. This study describes two approaches which allow integration of the most important wetland processes in hydrological and water quality models for regional applications. Both approaches consider water and nutrient fluxes, but they have different levels of complexity depending on data availability and objectives of the study. They are implemented in the model SWIM (Soil and Water Integrated Model). The first approach is rather simple, and can be introduced in a basin-scale ecohydrological model using two basic assumptions. This method illustrates how a very simple supply/demand approach can help to notably improve the modelling results in terms of seasonal river discharge and nutrient loads in catchments with a notable share of wetlands. The second, more advanced, approach is introduced at the level of hydrological response units (HRU) or hydrotopes, and takes into account fluctuations in groundwater table and hydrotope-related flow distances. This method allows for: (a) improving simulated water discharge in summer; (b) improving validation of nutrient-related processes; (c) estimating the impact of wetlands on water flow and nutrient load; and (d) better identification of areas in the catchment responsible for diffuse source pollution.

3.1 Introduction

Water fluxes with dissolved nutrients and pollutants, as well as sediments from uphill areas, pass wetlands and riparian zones on their way to river networks. By buffering and filtering water and sediment flows, wetlands can mitigate the impacts of floods, reduce erosion, and improve river water quality (Bach et al., 1997; Mander et al., 1997; Maitre et al., 2003; Lane et al., 2003). Wetlands and riparian zones along river courses perform many hydrological, ecological and human service functions "free of charge", such as:

- water storage during wet periods and flood protection;
- water reserve during dry periods;
- retention of sediments and associated pollutants (deposition);
- retention of nutrients (uptake, denitrification) and pollutants on the way to the river network;
- provision of habitat for fisheries;
- conservation of biological diversity; and
- provision of recreational areas.

However, the positive role of wetlands has been underestimated and, therefore, land drainage for agricultural and other purposes has been very extensive in the 20th century worldwide. It is estimated that 1.9×10^6 km^2 of the world's natural wetlands have been lost (Meyer & Turner, 1992). Practically all rivers and their basins in developed countries have been subjected to some channel modification and change of land-use patterns (melioration). Such practices followed extensive land drainage schemes or flow regulation projects (to extend agricultural and settlement areas and to speed up water flow through the channel, etc.). Direct impacts of such actions are: steeper channel slopes, lower roughness, and higher flow velocity. Indirect impacts are: lower self-purification capacity due to lack of wetlands and shortened travel time, bank instability, accumulation of sediments, etc. In many cases these actions resulted in increased frequency and severity of floods, more frequent droughts and higher levels of pollution. Now, negative conesquences are being recognised, and wetlands are increasingly being restored, re-established, rehabilitated and protected worldwide.

In the 21st century, demand on water resources will continue to increase, as will the levels of pollution. The ongoing climate change may increase the severity of problems in relation to hydrological extreme events and pollution. Therefore, the goal of sustainable use of freshwater resources in river basins requires new approaches to water and river basin management, which take the role of wetlands into account.

There are lumped models representing major riparian processes in detail, such as REMM (Riparian Ecosystem Management Model, Lowrance et al., 1997) at the hillslope scale. However, integration of wetlands and riparian zones in the modelling of entire catchments and on the regional scale is still a challenge, due to complex interactions and feedbacks between hydrological processes, vegetation and nutrients in wetlands, and it is still largely restricted to water quantity (see review in Cirmo & McDonnell, 1997). One of the first conceptual approaches to implement riparian zone processes in distributed modelling is the wetland approach of the EGMO (EinzugsGebietMOdel) model (Becker et al., 2003).

This study describes two approaches which allow integration of the most important wetland processes in a river basin model, and use them for regional application. The two approaches have different levels of complexity, which depend on data availability and objectives of the study. They are implemented in the model SWIM (Soil and Water Integrated Model, see Krysanova et al., 1998). The SWIM has been chosen in this study because it simulates the relevant hydrological processes, vegetation growth, erosion and nutrient dynamics at the river basin scale. Both approaches consider water and nutrient fluxes for wetlands. The extended SWIM was applied in two mesoscale catchments located in the Elbe River basin in Germany. The objectives of the study were:

(a) to introduce two approaches with different levels of complexity for implementing wetland processes in SWIM;

(b) to describe their effects on hydrological and water quality modelling; and

(c) to evaluate the usefulness of the approaches for estimating the impact of wetlands on water fluxes and nitrogen load in catchments.

3.2 Methods and study areas

3.2.1 SWIM

The model SWIM (described in Krysanova et al., 1998, 2000) is a continuous-time spatially semi-distributed model, integrating hydrological processes, vegetation growth (agricultural crops and natural vegetation), nutrient cycling (carbon, C, nitrogen, N and phosphorus, P), and sediment transport at the river basin scale. In addition, the model includes an interface to the geographic information system GRASS, which allows extraction of spatially distributed parameters of elevation, land use, soil and vegetation, and creation of the hydrotope structure and the routing structure for the basin under study. SWIM is based on two previously developed tools – SWAT (Arnold et al., 1993) and MATSALU (water quality model of the Estonian Matsalu bay, Krysanova et al., 1989).

A three-level scheme of spatial disaggregation "basin–subbasins–hydrotopes" or "region–climate zones–hydrotopes", plus vertical subdivision of the root zone into a maximum of 10 soil layers are used in SWIM. A hydrotope is a set of elementary units in a subbasin or climate zone with the same land use and soil type. During the simulation, (1) water, nutrients and plant biomass are initially calculated for every hydrotope / every soil layer in a hydrotope, (2) the outputs from hydrotopes are then aggregated to the subbasin outputs, and (3) the routing procedure is applied to the subbasin lateral flows of water, nutrients and sediments taking transmission losses into account.

The following criteria of fit are used to measure the quality of simulated model results: the non-dimensional Nash-and-Sutcliffe-efficiency (E) and the deviation in water/nitrogen balance (B):

$$E = 1 - \frac{\sum(obs - sim)^2}{\sum(obs - obs_{av})^2} \qquad \text{and} \qquad B = \frac{sim_{av} - obs_{av}}{obs_{av}} \times 100$$

where obs defines the observed daily value, sim means the corresponding simulated value, and the variables obs_{av} and sim_{av} describe the mean values of these parameters for the whole simulation period.

3.2.2 First (simple) approach for implementing wetlands in SWIM

Wetlands usually have shallow groundwater, and therefore plant roots in wetlands can reach groundwater and satisfy their demand in water and nutrients if soil water and nutrient supply are insufficient. In other words, the availability of water and nutrients for vegetation in wetlands is higher than in the neighbouring upland hillslope areas. Therefore, water uptake by plants in wetlands is usually higher, and water percolation to the aquifer is lower than in the upland areas. Along with the increased water uptake, the uptake of nitrogen by plants in wetlands is also increased, while leaching to groundwater is decreased.

The following changes in the SWIM code were made to translate these assumptions into the model code. Firstly, the wetlands have to be identified based on available information. Wetlands can be explicitly identified on maps of land use or soils, with an indication on their connection to groundwater. Further, groundwater table maps can be overlaid with land use and/or soil maps to identify riparian areas. In our case the identification was based on soil parametrisation, and wetlands were defined as hydrotopes with soils having connection to groundwater. These are, for example, the heavy organic soils of fens, soils located close to and composed by rivers, or soils influenced by shifting groundwater heights (such as gleys).

How plants are connected to groundwater in wetlands is described in the following. Additional water uptake (and an increased plant transpiration in consequence) is possible if the root depth of the vegetation is greater than two-thirds of the maximum rooting depth, and the actual plant transpiration is lower than the potential value, i.e. the water demand is not satisfied. If these conditions are true, both plant transpiration and water percolation are allowed to change by a certain amount (e.g. 10% of the difference between potential and actual plant transpiration). While transpiration increases, the percolation decreases by the same amount to maintain the water balance.

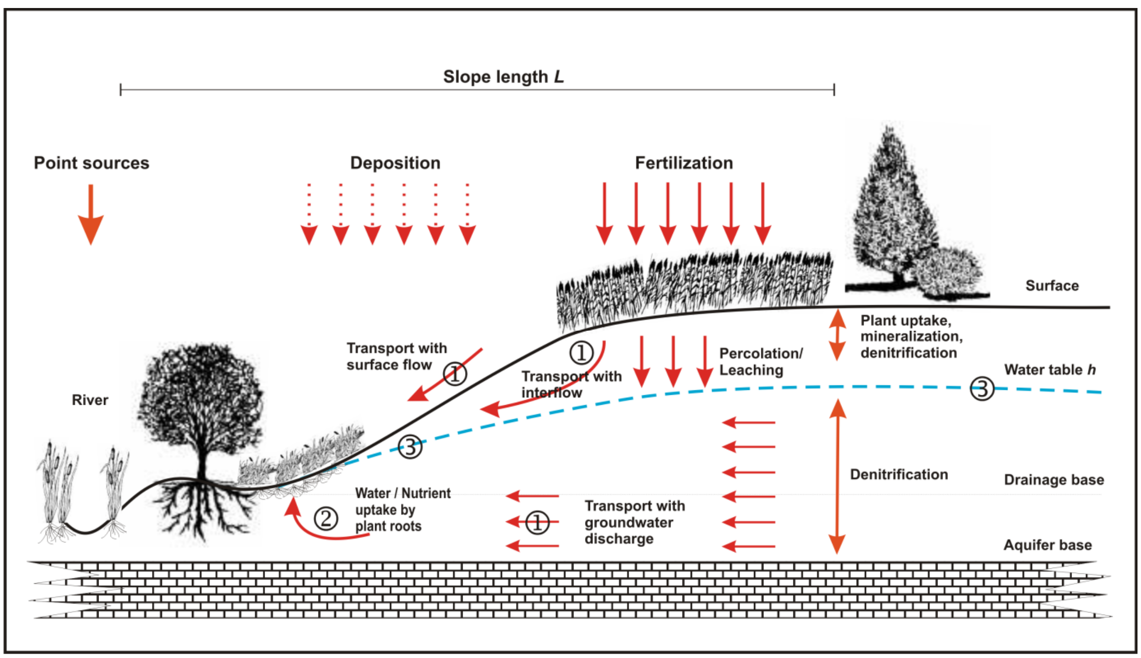

Figure 3.1 Main processes implemented in the second approach: flow path considering the mean residence time of nutrients in the subsurface (①), nitrogen uptake by plants from lateral flow (②), and groundwater dynamics (③) (Hattermann et al., 2006). The simple approach considers only ① and ② (at the subbasin scale), while the advanced approach considers ①, ② and ③ at the hydrotope scale.

Simultaneously, an increased uptake of nitrogen by vegetation is possible in hydrotopes defined as wetlands. The supply and demand approach is used here as well, and the correction is made whenever the demand of nitrogen in soil is higher than supply. The supply and uptake of nitrogen increase by a certain amount as a function of the maximum uptake, whereas the nitrogen leaching to groundwater decreases by the same amount in this case.

Altogether, the following three additional model parameters are needed in the simple version: the mean residence time of nitrogen in a subbasin, the average denitrification rate in a subbasin, and the maximum plant uptake of vegetation in riparian hydrotopes. The first two are subject to calibration (based on measurements or relevant literature), and the third is calculated considering the demand of the riparian vegetation. Figure 3.1 illustrates the main model extensions for this version. The difference between this and the second, more advanced version is that the water and nutrient fluxes are averaged at the subbasin scale in the former.

3.2.3 Second (advanced) approach for implementing wetlands in SWIM

In the second approach the wetlands were identified more precisely compared to the first (lumped) approach, and the specific flow path of water and nutrients to the surface waters was implemented (for more details see Hattermann et al., 2006). The wetland or riparian zone was defined as a hydrotope with a shallow groundwater table wherein plant roots can reach groundwater (see also Hattermann et al., 2004). The riparian zone is a type of wetland located along the river. Groundwater table is simulated daily at the hydrotope level in this model version (in the standard version – at the subbasin level only), and the shallow groundwater is "allowed to enter the soil horizon". Soil depth is variable in this model version, it can decrease if groundwater table is becoming high enough. When this happens, the hydrotope is treated as a wetland or riparian zone. Though there could be "stable" wetlands in the basin, they are usually assumed to be "ephemeral" (depending on the current groundwater table level in the catchment), and the total wetland area in the basin is variable as well.

Besides changes in groundwater dynamics and variable soil depth, the following processes were implemented:

1. in all hydrotopes, nutrients leaving the soil horizon with interflow and leached to groundwater are subjected to retention on their way to the river network, and the retention is a function of the residence time and chemical status of the subsurface on the hydrotope-specific way to the river;
2. in riparian zones and wetlands, plants can satisfy their water and nutrient demands by additional uptake from groundwater in case the demand is not satisfied by the usual supply from soil, whereby
3. the additional uptake of water and nutrients is restricted to the amount of water and nutrients from upland areas passing through the hydrotope.

Denitrification is likely to be the major process leading to loss of nitrogen during subsurface transport to the river (Mander et al., 1997), and the denitrification rate is an important parameter. The second important parameter influencing retention is the residence time of nitrogen in the subsurface, which determines the time period during which nutrients can be subjected to denitrification on the way to the river. Both parameters can be treated in the second version as hydrotope-specific.

Table 3.1 Comparison of the additional parameters used in the simple and advanced approach to reproduce processes in wetlands and riparian zones in SWIM.

Simple approach **(riparian area static)**	**Advanced approach** **(dynamic riparian area)**
Mean residence time of water in a subbasin	Hydrotope (flow path) specific mean residence time
Average denitrification rate in a subbasin	Hydrotope (flow path) specific denitrification rate
Maximum daily plant uptake of water and nutrients per riparian hydrotope	Maximum daily plant uptake of water and nutrients per riparian hydrotope
	Average groundwater table (as initial values) and daily groundwater dynamics per hydrotope for estimating the riparian area per time step
	Hydrotope-specific flow distance to next surface water

Altogether, the following five additional model parameters are needed in the extended version: the average groundwater table (as initial values for the groundwater dynamics), the flow distance from the hydrotope to the river, the hydrotope-specific mean residence time, the flow-specific denitrification rate, and the maximum plant uptake. The first three parameters can be estimated during the data pre-processing using Geographical Information System functions like the flow path method and maps of the geo-hydrology and groundwater contours. The average denitrification rate per geological formation can be taken as an estimate from existing measurements or literature and then calibrated. The maximum plant uptake is calculated by the extended SWIM balancing plant demand and the amount of nutrients flowing through the specific hydrotope. Figure 3.1 illustrates the main model extensions for this version. The difference between this and the first, simpler version is that the water and nutrient fluxes in this version are hydrotope-specific; that is, the actual landscape position determines the retention of nutrients in the subsurface and in the riparian zone. The approach, including the additional model equations, is described in detail in (Hattermann et al., 2006). The additional parameters used in the simple and advanced approaches are summarised in Table 3.1.

3.2.4 Case study areas

The Rhin catchment The first method was tested in the Rhin catchment (drainage area 1716 km^2), located in the lowland part of the Elbe River basin in the north of the German Federal State Brandenburg. Altitudes range from 19 to 116 m a.s.l.. The mean annual precipitation at the climate station Neuruppin in the middle of the catchment is 524 mm year^{-1}, and the mean temperature is 9.4°C (1981–2005). The main land-use categories are: agriculture, forests and pastures, covering 41, 34 and 19% of the area, respectively. The soil map for this catchment includes eight different soil types. Three of them have connections to groundwater and were defined as wetlands in the model. These three soils cover an area of about 683 km^2 (see Figure 3.2(a)).

The river network is influenced by more than 300 dams and weirs; 27 of them located within the main river course. Larger fens and wetland areas are drained. Numerous ditches for irrigation and drainage, along with the weirs, influence the hydrological cycle. There are five hydrological gauges within the Rhin catchment, and none of them shows natural discharge behaviour. Additionally, the water dynamics are heavily influenced by artificial water storage in winter time and by several water exchange points resulting in in- or outflows of water from or to the adjacent catchments.

For the modelling process, the study area and its disaggregation were defined by several raster maps (digital elevation model, soil map, land-use map and subbasin map) with a resolution of 50 m × 50 m as well as by climate data (temperature, precipitation, solar radiation and air humidity), which were interpolated for every subbasin with an inverse distance method. According to subbasin data delivered by the Federal Environment Agency of Brandenburg (LUA), the Rhin catchment was divided into 218 subbasins. Data source for the soil map was the BÜK1000 (Richter et al., 2007), which is the general soil map of the Federal Republic of Germany (scale 1:1 000 000). Land-use data were taken from the European CORINE land-cover map (Dollinger & Strobl, 1996).

Measured water discharge and water quality data of the LUA were used for model calibration: daily measurements of discharge and fortnightly measurements of nitrate nitrogen concentrations at the last Rhin gauge station Kietz (drainage area 1646 km^2). Linear interpolation was applied to nitrogen concentrations in order to estimate daily values and calculate nitrogen loads.

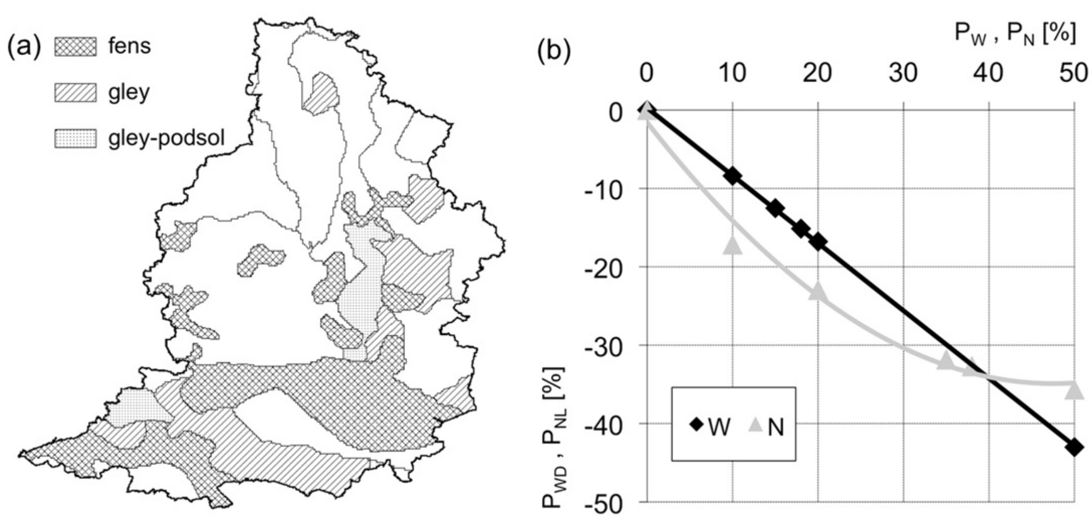

Figure 3.2 (a) Distribution of soils in the Rhin catchment identified as wetlands. (b) Sensitivity analysis of the first approach for water discharge (W) and nitrate nitrogen load (N) in the Rhin catchment for the 5-year period 2001–2005. The black line (W) compares the increase in plant transpiration (as a percentage of the difference between potential and actual plant transpiration, P_W) to the resulting change in total water discharge at the basin outlet (P_{WD}), in %. The grey line (N) compares the increase in soil nitrogen supply (as a percentage of the total amount, P_N) to the resulting change in total nitrogen load at the basin outlet (P_{NL}), in %.

The Nuthe catchment The second method was tested in the Nuthe catchment (drainage area 1938 km^2), which drains into the Havel River, a tributary of the Elbe River. The catchment area is dominated by agricultural land use. The mean annual precipitation is about 600 mm $year^{-1}$. The landscape is rural, dominated by farmland and forest, and the population density is low (although the basin is adjacent to Berlin). The upper areas, with a deeper water table, are covered mainly by sandy, highly permeable soils. The river valley has loamy alluvial soils with riparian grasslands and forests in areas with shallow groundwater, and arable land elsewhere. Approximately 27% of the basin area is covered by wetlands regulated by water management measures. During the last decades many wetlands were drained, and their restoration by river flow regulation measures is now ongoing or planned.

All spatial information necessary for deriving the subbasin and hydrotope structure of the basin includes: the digital elevation model (DEM), the soil map of the State of Brandenburg (LBGR, 2008), the geo-hydrological map (NBL, 1985), the land use map (MLUR, 1998), and the water table contour map, stored on a grid format with 50 m resolution. The groundwater contours were produced by averaging the yearly groundwater level of 226 observation wells and interpolating using External Drift Kriging (Akin & Siemes, 1988), whereby the elevation was taken into account as a second variable. The basin was subdivided into 122 subbasins based on the DEM and the drainage network. The daily meteorological data from six climate stations and 16 precipitation stations had been interpolated for each subbasin using the inverse distance techniques. Information on crop rotations, scheduling and amounts of fertilisers in the basin was taken from regional statistical data.

3.3 Application of the two approaches and results

3.3.1 First approach

Sensitivity analysis The sensitivity analysis of the first approach was performed using data for a 5-year period from 2001 to 2005 (Figure 3.2(b)) for the Rhin catchment described above (Figure 3.2(a)). The approach was tested assuming that all marked areas corresponding to three soil types (fens, gley, gley-podsol) represent wetlands.

The increase in plant transpiration and nitrogen uptake was assumed with different percentages P_W and P_N in relation to the difference between potential and actual plant transpiration and the available soil nitrogen supply, correspondingly. In this sensitivity experiment they were between 0 and 50%. These increases were accompanied by decreases of water percolation and nitrogen leaching with the same amounts to keep the balances. The percentage P_W was compared with the resulting percentage of water discharge decrease P_{WD} at the catchment outlet, and the percentage P_N was compared with the resulting percentage decrease in the total nitrogen load P_{NL} at the outlet. It is apparent (Figure 3.2(a)) that, as expected, the increase in water and nitrogen uptake in wetlands causes decrease in water discharge and nitrogen load at the outlet of the simulated basin. The decrease in water discharge follows a linear trend, while the effect on nitrogen load is nonlinear.

Results The first approach was applied for a three-year period in the Rhin catchment. The following major regulatory measures (see section on case study areas) were taken into account for calibrating the original SWIM model: water and dissolved nitrogen inflow/outflow, water abstraction for agricultural purposes, and point-source pollution for nitrogen. This led to quite satisfactory model results in terms of Nash-and-Sutcliffe-efficiency: E = 0.66 for water discharge and E = 0.68 for nitrogen load. However, visual comparison reveals some obvious discrepancies. In total, the discharge was overestimated by 15%, while nitrogen load was 37% higher. Differences between the measured and simulated values are especially prominent during the summer months. Higher water discharge and some unmeasured small nitrogen peaks were simulated in the summer season. Therefore, it was especially interesting to check whether the problems could be solved and simulations would improve by introducing this simple wetlands approach.

Essentially, the introduction of wetlands in the model using this simple approach by increasing plant transpiration and N uptake, and decreasing percolation and leaching, led to significant improvement of criteria of fit. The efficiency of discharge simulation changed from 0.66 to 0.71, whereas the deviation in water balance changed from 15.3% to 0.01% (see Figure 3.3). The efficiency for nitrogen improved from 0.65 to 0.68, and the deviation in nitrate balance from +37.4% to –0.1% (see Figure 3.4). Especially the observed discharge and concentrations in summer period were reproduced much better using this method. The small peaks in nitrogen load in summer, which were originally simulated, now disappeared, which corresponds much better to the measured data. But the winter peaks decreased as well, making the model results worse in some periods. However, a total account of the simulation period shows that the model results for both water and nitrogen have obviously been upgraded.

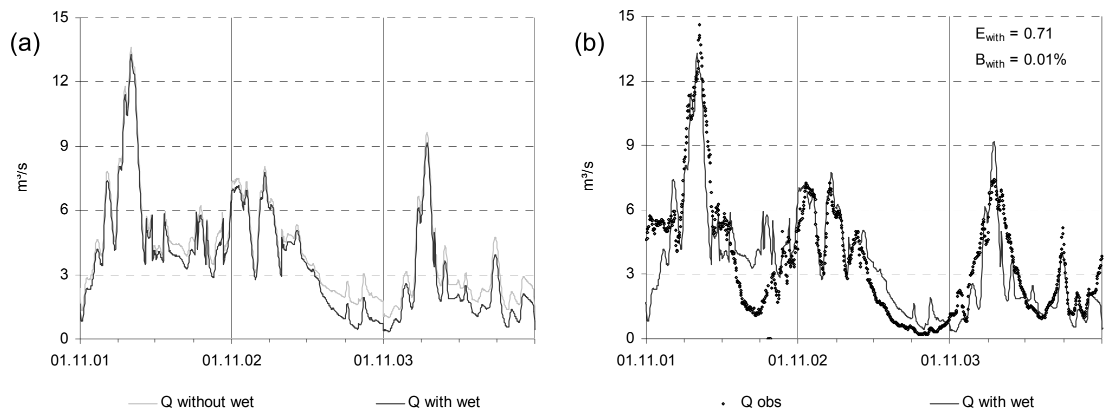

Figure 3.3 (a) Effect of the first approach on the water discharge (*Q*) of the Rhin; and (b) comparison of the simulated water discharge (using the first approach) with the observed water discharge, for the three year period 1 November 2001–31 October 2004.

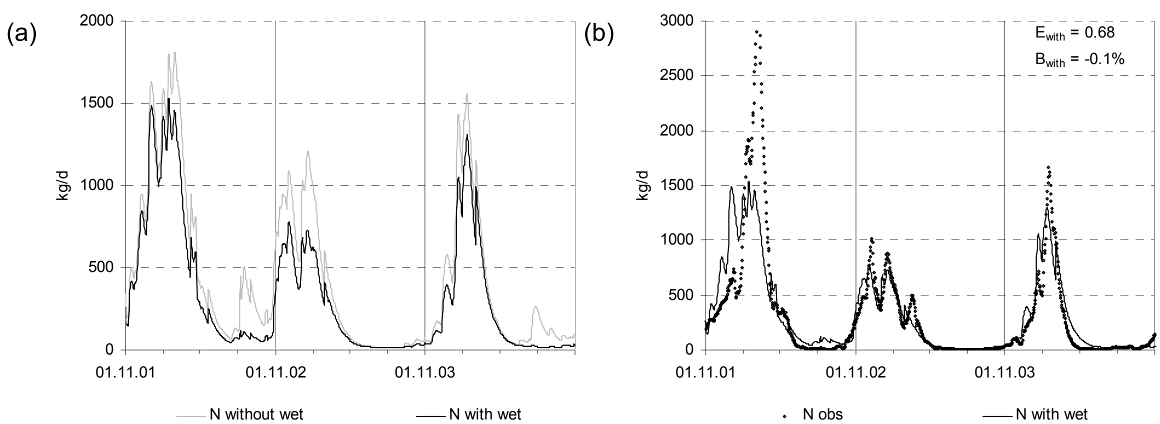

Figure 3.4 (a) Influence of the first approach on nitrate nitrogen load (*N*) in the Rhin River; and (b) comparison of the simulated nitrate nitrogen load (using the first approach) with the observed load, for the hydrological three year period 1 November 2001–31 October 2004.

3.3.2 Second approach

Applying the second approach also enabled notably improved simulation results for water and nutrients in the Nuthe catchment, especially in the summer period. Figure 3.5(a) shows that the seasonal dynamics and amplitude of the observed nitrate concentration are generally reproduced well by the extended SWIM version. A better reproduction is practically impossible due to imprecise information on crop rotations, the fertilisation regime, missing data on flow regulation by dams and weirs, and the influence of drainage systems.

However, the advantage of the second method lies in its consideration of nearly the actual flow path of the nutrients and residence times of substances in the subsurface that are close to reality. It therefore gives a better picture of long lasting processes. The estimated (using GIS) mean residence time of nitrate N fluxes within groundwater for the whole basin is 41 years, with a maximum of about 400 years for hydrotopes located furthest away from the river system. These values agree well with other estimates described in the Report of the Environment Agency (Behrendt et al., 2002). The calibrated rate for N denitrification in groundwater is 0.003 d^{-1}, meaning that the half-life time of nitrate in groundwater is 231 days, agreeing well with estimates from Wendland et al. (1993).

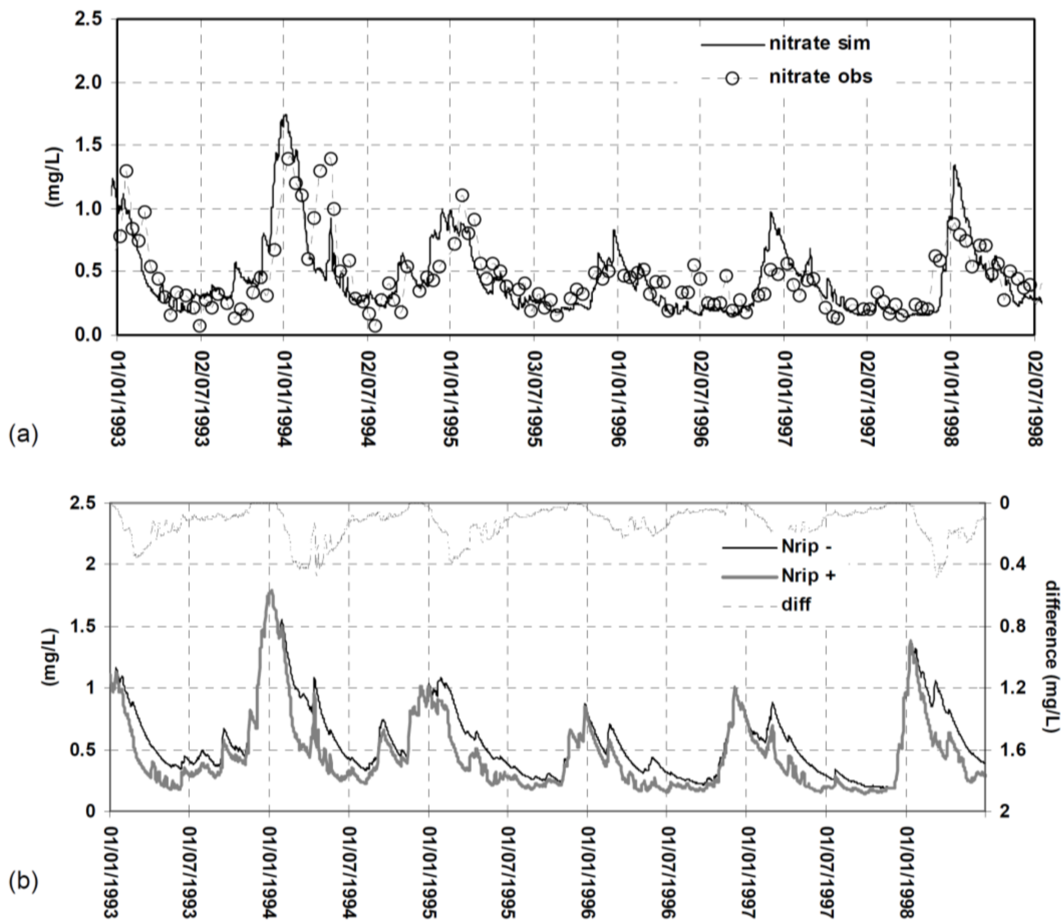

Figure 3.5 Influence of the second approach on nitrogen dynamics: (a) comparison of the observed and simulated nitrate nitrogen concentrations in the Nuthe River, and (b) impact of additional nitrate uptake by plants in wetlands and riparian zones on nitrate nitrogen concentrations in the river (Nrip−: concentration in the Nuthe without the additional uptake, Nrip+: concentration with the additional uptake, Hattermann et al., 2006).

Figure 3.5(b) illustrates the impact of the model extensions (additional nitrate uptake by plants from groundwater in riparian zones and wetlands) on water quality in the River Nuthe. Differences are highest during the summer season when plant nitrogen demand is high and therefore cannot be satisfied by nitrogen in soil. The differences become negligible by late autumn. The long-term decrease in annual river nitrate nitrogen load due to additional plant uptake from groundwater is about 21%.

The second method also allows for detecting areas responsible for groundwater pollution. For example, Fig. 3.6(b) and (c) indicates areas responsible for the pollution of river water for direct flow and base flow separately. It is apparent that the till soils with impermeable clay layers located in the southern part of the catchment generate high amounts of nitrate N transported by surface flow and interflow to the river system, whereas transport by groundwater is negligible in this area. Generally, areas located closer to surface waters contribute more to the total riverine nitrate load than areas in upland areas, due to the shorter transport and denitrification time.

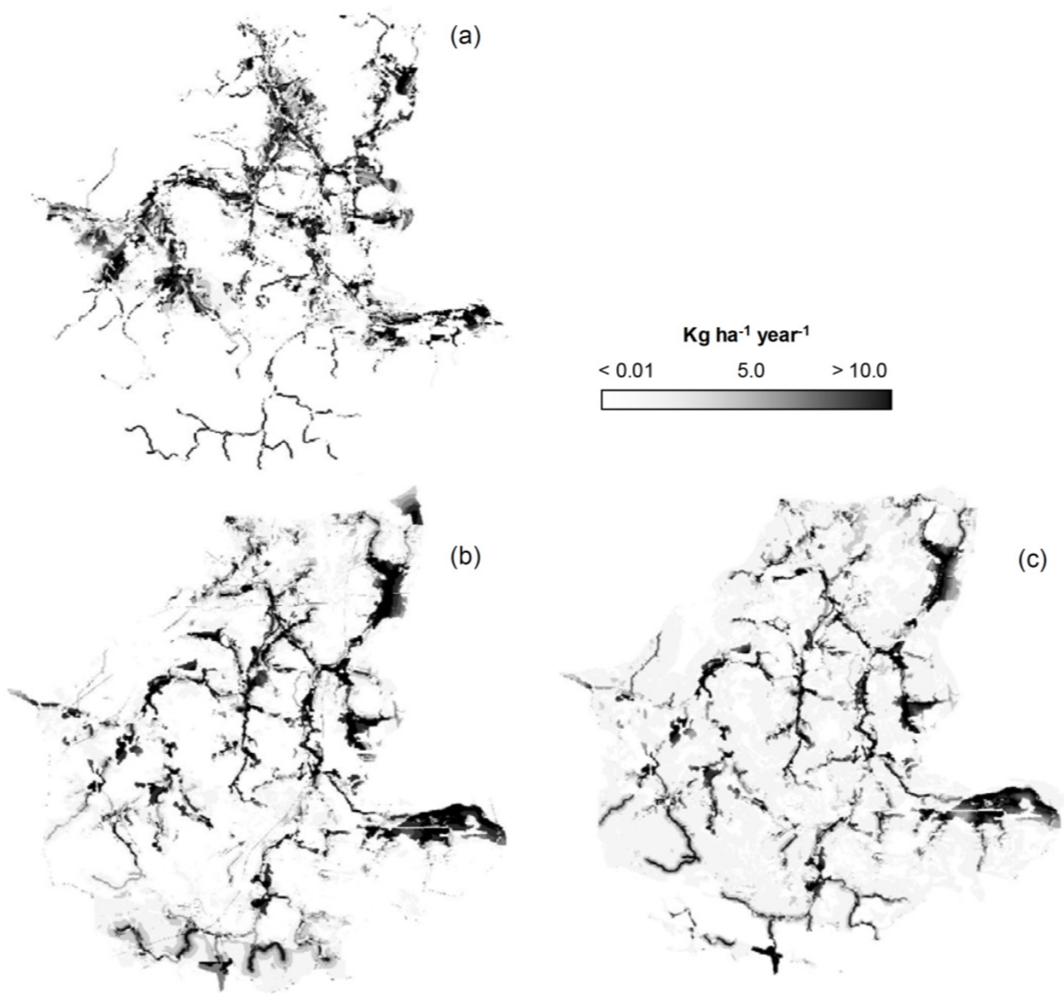

Figure 3.6 (a) Plant uptake of nitrate N from lateral inflow in riparian zones. Nitrate fluxes generated at a specific site that actually reaches the surface water system by (b) direct flow (surface and interflow) and (c) base flow (Hattermann et al., 2006).

3.4 Discussion and summary

Over the past decade the issue of integrated water resources management at the river basin scale has received substantial attention in many parts of the world. However, the integration of wetlands in this process is still not addressed adequately or sufficiently. This is even more the case in regional hydrological modelling, where for many reasons the wetlands processes are not considered or are under-represented. Some reasons for this follow:

- It is difficult to precisely allocate the wetland area within a catchment for the modelled period of time. Maps often do not show the actual area of wetlands in a certain period, mainly due to the fact that river basins were subject to regulation and drainage and therefore wetland areas changed over time.
- By definition, wetlands are influenced by groundwater. However, saturated zone processes are largely unconsidered in meso- and large-scale hydrological modelling, or considered only in a very simple manner, due to the insufficient knowledge and lack of data for regional aquifers.
- Wetlands represent an interface between the upland catchment areas and the surface water system, and they filter water and nutrients coming from upland with lateral inflow. However, for most of the time, lateral flows within subbasins are explicitly left unconsidered in regional-scale hydrological modelling, partly due to data availability, and partly due to additional computation demand.

This study introduces two methods of different complexity to overcome these problems in regional modelling. The first one is a simple but robust method based on a pure supply and demand approach considering the water and nutrient demands of the riparian vegetation. Without knowing the actual connectivity of the riparian wetland to groundwater, it is simply assumed in the model. Therefore, it is easy to apply and implement this method in any semi-distributed hydrological model. The results shown here are promising and demonstrate that the approach improves simulation results, especially during the summer season (because wetland vegetation can satisfy its additional water and nutrient demands from groundwater in this period). This method is helpful if water discharge and nutrient concentrations are overestimated by the model in summer, and there are wetland areas in the studied catchment.

The second method is more advanced and considers additional processes typical for wetlands, like groundwater fluctuations and the amount of water flowing through a specific wetland hydrotope. It allows a better reproduction of effects of riparian zones and buffer strips, because the actual position of a wetland or a riparian zone in the landscape and their connectivity to groundwater are taken into account more comprehensively. Another advantage is that this method considers the residence time and flow path of nutrients with lateral transport via direct and base flow. Thus, it enables to detect areas within a subbasin which are responsible for inadequate water quality. This is especially important for estimating nutrient loads generated by diffuse sources, where the existing knowledge gaps and uncertainties are largest. However, both methods are difficult to validate in terms of their water and nutrient filtering, due to lack of data.

While the first approach does not need any additional information in the basic version of SWIM after the wetland areas are identified, the second method is more data-demanding. The most important additional data refers to information about groundwater (water table, porosity and transmissivity of the aquifer), which has to be known for simulation of the residence time and the water table dynamics. Basic information required is the flow path of water in the subsurface to estimate the amount of water and nutrients flowing through wetland hydrotopes. Therefore, it is recommended to clearly define the goal of a study before choosing the appropriate method. Whenever "only" the better representation of water discharge and nutrient transport in the main river is the goal, one should choose the simple approach. If also the allocation of diffuse sources and hotspots within a basin is the goal, one should choose the more advanced method.

It is possible to develop a third approach of intermediate complexity, e.g. by avoiding complexities related to varying groundwater table, soil depth and variable wetland areas, but having stable wetlands and still describing retention in wetlands following the second approach. The riparian zones can be defined by distance to average groundwater table or still by soil or vegetation information, and should be located adjacent to the river network. The additional water and nutrient uptake can then be calculated from available flows coming from upland to these stable wetland areas.

CHAPTER 4

ECOHYDROLOGICAL MODELLING IN A HIGHLY REGULATED LOWLAND CATCHMENT

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Eco-hydrological modelling in a highly regulated lowland catchment
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Abstract

Water quality modelling in the meso-scale Rhin catchment in the German federal state Brandenburg was done 1) to answer some specific questions concerning identification of point and diffuse sources of nutrient pollution in the catchment, 2) to assess the influences of possible climate and land use changes on water quantity and quality and 3) to evaluate potential measures to be done in order to achieve a "good ecological status" of the river and its lakes as required by the Water Framework Directive (WFD).

The Rhin catchment is a typical highly regulated lowland river basin in Northern Germany. The regulations complicate water quantity and quality modelling in the catchment. The research was done by using the ecohydrological model SWIM (Soil and Water Integrated Model), which simulates water and nutrient fluxes in soil and vegetation, as well as transport of water and nutrients to and within the river network. The modelling period was from 1981 until 2005. After calibrating the hydrological processes at different gauges within the basin with satisfactory results, water quality (nitrogen and phosphorus) modelling was done taking into account the emissions of different point sources (sewage treatment plants etc.) and identifying the amount of diffuse pollution caused mainly by agriculture.

For suggesting some feasible measures to improve water quality and to reduce diffuse pollution considering possible climate and land use changes, different reasonable scenarios were applied in consultation with the Environmental Agency of Brandenburg (LUA). The study revealed that the amount of water discharge has significant influence on the concentration of nutrients in the river network, and that nitrogen pollution, caused mainly by diffuse sources, could be notably reduced by application of agricultural measures, whereas the pollution by phosphorus could be diminished most effective by reduction of point source emissions.

4.1 Introduction

Lowland river systems and their catchments are typical ecosystems with small amplitude in altitude, low flow velocity, high groundwater table and a substantial share of typical organic soils, e.g. fens (Krause et al., 2007a; Müller et al., 2004). In former centuries different melioration measures were applied in order to provide areas for agriculture. Therefore the lowland areas are often heavily regulated. This led to a reduction of retention time of water and nutrients, which contributed to eutrophication problems in the river network and coupled lakes. Nitrogen, and to some extent phosphorus, introduced to the system by fertilisation and not uptaken by plants, have not enough time to be decomposed (N - mainly by denitrification (Trepel & Palmeri, 2002)) or uptaken by vegetation during their pathway to the river network. Mineralisation of drained wetlands results in higher nutrient outputs with negative effects on water quality, too (Kieckbusch & Schrautzer, 2007; Tiemeyer et al., 2008). On the other hand, these areas are also influenced by additional human interferences (e.g. water management activities and point source emissions), which also have relevant effects on water amount, nutrient (mainly phosphorus) loads and concentrations in the basin (Krause et al., 2007b; Wriedt et al., 2007).

Knowing these problems and being interested in finding solutions to get a better ecological status of such a lowland river, the Environmental Agency of Brandenburg (LUA) requested a modelling study to support implementation of the European Water Framework Directive (WFD) in Brandenburg, where the Rhin catchment is considered as a representative example. The WFD requires that all European water systems should achieve a "good ecological status" until 2015 (EC, 2000). This "good ecological status" should be as near to the reference status of the water body as possible. In general, future water management decisions should be more adaptive, as we are living in a rapidly changing world. It can not be expected that the former conditions will stay unchanged. Some changes in temperature, precipitation and/or intensity and frequency of extreme events have already been observed in the region (Gerstengarbe & Werner, 2005; Krysanova et al., 2008). For this reason, scenarios as different options for a possible future should be taken into account by implementing the WFD. Model scenarios can be helpful in order to find reasonable measures for achieving a better ecological status taking into account possible changes of land and water use, management practices and climate conditions (Højberg et al., 2007; Jørgensen et al., 2007; Krysanova et al., 2005a).

Starting with modelling conservative substances in the 1970ies, models to solve eco-hydrological problems became more and more complex by taking into consideration also transport and transformation processes for reactive substances. According to the aims of model application as well as to availability of measured data, models of different complexity can be used nowadays: 1) conceptual models using statistical relations which allow only a limited reproduction of the landscapes heterogeneity but are easily transferable to different scales and need a restricted amount of measured data (e.g. Palmeri et al., 2005; Biondi et al., 2008); 2) physically based models derived from physicochemical laws and using detailed process description, which require a high amount of data and computation time and are used especially at the point and small scale (e.g. Vanclooster et al., 1995b, Arhonditsis et al., 2007); and 3) process-oriented models of average complexity, which combine the advantages an try to minimise the disadvantages of 1) and 2) by simplification of physicochemical process description and using also empirical approaches (e.g. Bouraoui & Grizetti, 2008; Jackson et al., 2007). As the most complex model is not necessarily the most "useful" one at the meso- and macro-scale (Lindenschmidt, 2006) a model of type 3) was used for this study. The dynamical process-based ecohydrological model SWIM (Krysanova et al., 1998) was extensively tested in advance regarding its ability to simulate nutrient leaching in meso-scale river basins (Krysanova et al., 2002; Hattermann et al., 2006). The dynamical process-based modelling has many advantages compared to statistical ecohydrological modelling, and the ability to provide projections for scenario conditions based on preliminary calibration and validation is one of the most important.

However, experiences of different European and national projects dealing with the model-supported implementation of the WFD revealed as well that the available models and model systems are still far from being suitable for operational applications. This is especially the case for modelling of water quality, like simulation of nutrient transport and nutrient turnover processes, where the results of different models for nutrient concentrations in rivers differ often by more than 100% and are sometimes even contradictory (Euroharp-Project, 2007). There are different possible reasons for such a problematic result as for example deficits in model structure, spatial distribution and process description, uncertainties in model parametrisation, insufficient data support, or inexperienced model users.

To overcome these problems not only more intensive research in improving the model systems is necessary but also a closer cooperation between model developers with model users and experts knowing the specific problems of the study areas. A close cooperation of the research institutes and the executive agencies responsible for implementing the WFD can help to find suitable operational application measures. In this respect the stakeholders of the LUA were strongly asked to participate in the modelling process and to claim for desired results. For the study presented here the LUA was especially interested in answering the following questions, which became the research subjects:

- What are the shares of point and diffuse sources of pollution, and where are the main areas of diffuse pollution located?
- What is the reference status of the Rhin river?
- Which consequences could possible changes in management, land use and climate have for the river system in the future?
- What are the most appropriate measures to reach the “good ecological status” as required by the WFD?

4.2 Materials and methods

4.2.1 Study area and data preparation

Study area The study area was the Rhin catchment (drainage area 1716 km^2) in the north of the German federal state Brandenburg. The Rhin river drains into the Havel river, a tributary of the Elbe river. The catchment belongs to the lowland part of the Elbe basin with an altitude between 19 and 116 meters above sea level. Main average climate and water characteristics measured in the Rhin catchment are listed in Table 4.1. The location of the basin, discharge gauges and the analysed climate station Neuruppin are shown in Figure 4.1.

There are a lot of lakes within the river network (3% of the area is covered by surface water bodies), 41% of the area is used for agriculture (mainly winter crops and maize), 34% is covered by forest (mainly evergreen) and 19% by intensively used pastures. The pasture area practically coincides with the fen soil type area (ca. 23% of all soils), which can only be used as pasture due to the intensive water regulation system.

variable		unit	period	value
P	precipitation	mm a^{-1}	01/1981-12/2005	524.4
T	temperature	°C	01/1981-12/2005	9.4
Q	discharge	$m^3 s^{-1}$	11/2001-10/2005	3.73
N	NO_3-N	mg l^{-1}	01/1981-12/2005	0.62
P	PO_4-P	mg l^{-1}	01/1981-12/2005	0.04

Table 4.1 Average climate characteristics of the Rhin catchment (P, T; station Neuruppin), and mean water discharge, NO_3-N and PO_4-P concentrations in the outlet (Q, N, P; gauge Kietz).

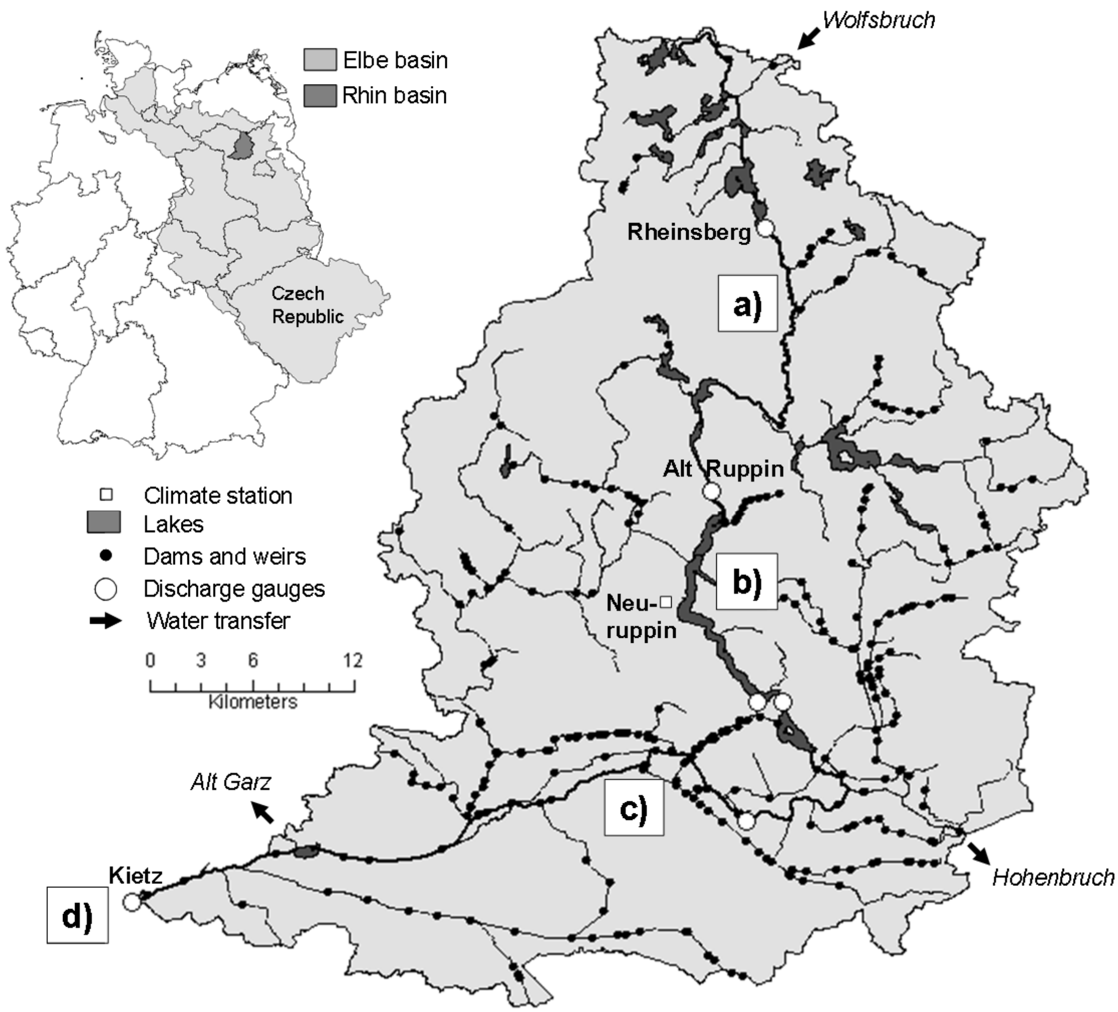

Figure 4.1 Location of the Rhin catchment within the Elbe basin (one-third of which belongs to the Czech Republic) together with borders of the federal states of Germany (small map) and location of rivers, lakes, discharge gauges, the climate station Neuruppin, water transfer points and dams and weirs within the Rhin catchment (large map); the numeration a) to d) shows the approximate location of four parts in the river network used for an Input-Output-Analysis (see Figure 4.2).

The Rhin river network is influenced by more than 300 small dams and weirs (see Figure 4.1). 27 of them are located within the main river course. The large fens and wetland areas near the middle course of the river are strongly meliorated. A lot of ditches for irrigation and drainage together with the barrages influence the hydrological cycle. Natural discharge behaviour at the five observation gauges within the Rhin catchment can not be recognised. Additionally, the water dynamics is strongly influenced by storage of water in winter time (mainly in the upper course of the Rhin river), which is later used for irrigation during dry periods in summer, and several in- or outflows of water from or to the adjacent catchments (see Figure 4.1). These water transfer points have significant effects on water discharge in the basin. Especially the lower course of the Rhin river is influenced by an important water loss, as in winter nearly half of the Rhin discharge is transferred to the adjacent Dosse catchment (transfer point Alt Garz) and does not reach the basin outlet in Kietz.

Regarding water quality the river network can be clearly distinguished as less polluted in the upper part and higher polluted in the lower part of the catchment. Particularly the ditches draining agricultural areas are heavy loaded with nutrients and often exceed the target value for a “good ecological status” (90-percentile NO_3-N: 2.5 mg/l, o-PO_4-P: 0.1 mg/l (LAWA, 1998)). To analyse the amount and behaviour of nitrogen and phosphorus within the Rhin basin a special Input-Output-Analysis was done for two parts of the river stream and two lakes (for location see Figure 4.1, for results see Figure 4.2). The aim was to find typical patterns of nutrient behaviour (e.g. areas, river parts or lakes predominantly or seasonally acting as sink or source), which could be interpreted by the model later. But no universally valid behaviour could be observed. However, some conclusions could be drawn: 1) an increase of concentration along the course is obvious for the substances NO_3-N, NH_4-N and PO_4-P with occasional exceeding the target values, especially in the lower course, 2) a difference between lakes and river courses can be seen looking at total and particulate phosphorus amounts (lakes have higher concentrations and behave temporary as sources), 3) a lake can behave in different ways and predominantly be a source for some substances in winter time probably due to mixing of a temporary stratified water body (e.g. Ruppiner See) or in summer time probably due to intense eutrophication processes and algae growth or release of nutrients from sediments (e.g. Gülper See), and 4) phosphorus seems to be more problematic for water quality than nitrate nitrogen. But it should be kept in mind that the comparison in Figure 4.2 is shown for the measured input and output substances of one day, without taking into account flowing distances and/or transformation processes. Besides, a similar input-output analysis was done taking into account time delay from 1 to 6 months with a monthly time step. However, this analysis did not reveal more dependencies.

Measures to improve water quality and to reach the aims of the WFD are necessary especially in the lower part of the basin, which is classified as an endangered water body (also due to its trophic status and oxygen demand). Looking at the actual status, one can ask whether it is possible at all for the lower part of the river to reach the “good ecological status” and the “good chemical status” as required by the WFD. However, the modelling could help to clarify these questions.

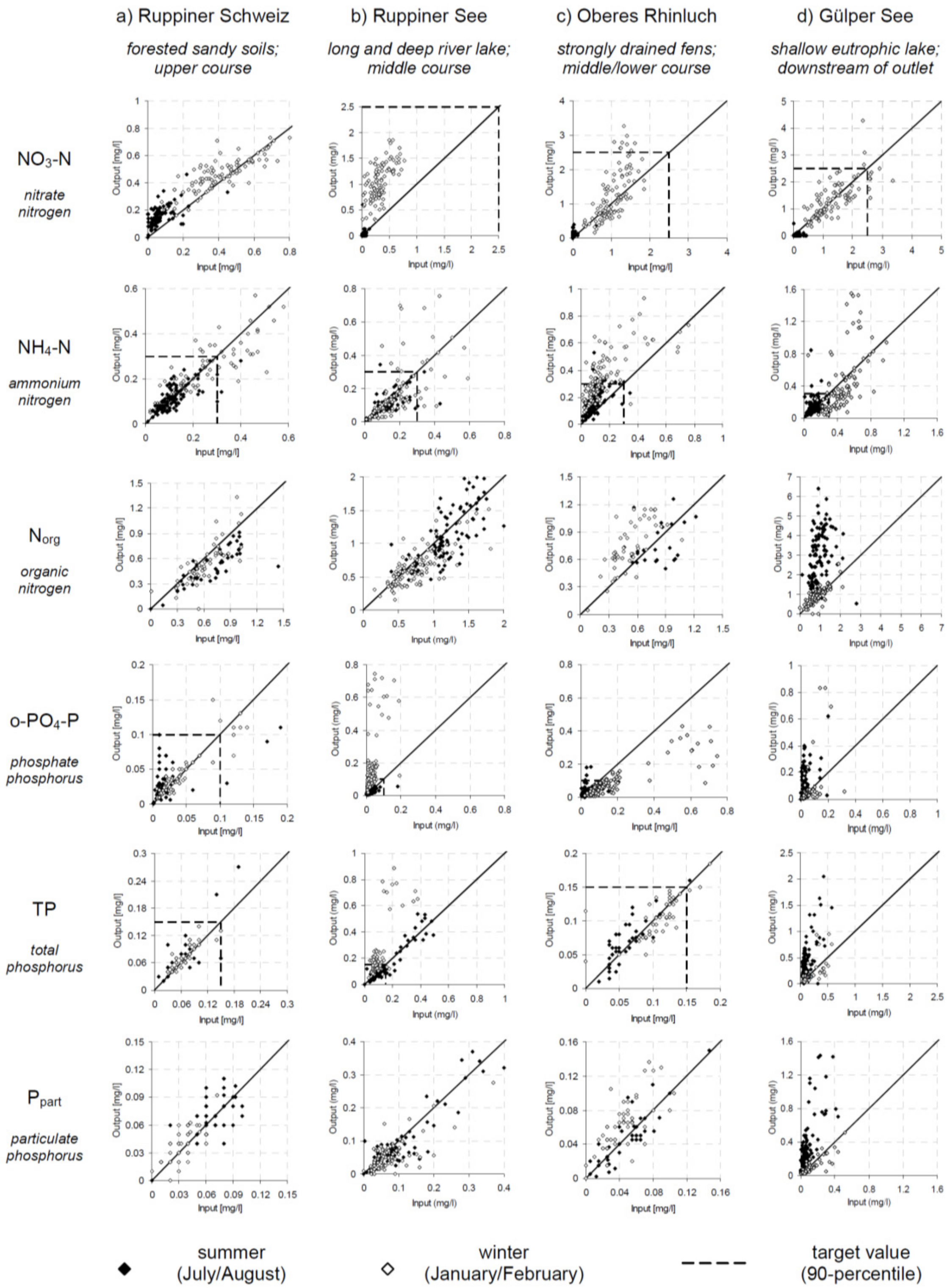

Figure 4.2 Input-Output-Analysis of different nitrogen and phosphorus forms for selected river parts and lakes of the Rhin river network aimed in defining river sections with predominant sink (points below the diagonal) or source functions (points above the diagonal) for the time period from 1981 to 2005 distinguished into summer (July/August) and winter (January/February) sub-periods and compared with the target values of a "good ecological status" (LAWA, 1998).

Data preparation To setup the model the study area was defined by several raster maps (digital elevation model (DEM), soil (BÜK 1000), land use (Corine2000) and subbasin) with a resolution of 50 m x 50 m. Climate data (temperature, precipitation, solar radiation and air humidity) provided by the German Weather Service were interpolated to the centroids of every subbasin by an inverse distance method using 37 climate stations in and around the Rhin catchment and 11 additional precipitation stations within the basin. According to the subbasin map delivered by the LUA the Rhin basin was divided into 218 subbasins.

For model calibration the following measured data provided by the LUA were used: daily measurements of water discharge at the three gauges Rheinsberg, Alt Ruppin and Kietz (Figure 4.1), and fortnightly measurements of nitrate nitrogen and phosphate phosphorus concentrations at the last Rhin gauge Kietz for different long time periods between 1981 and 2005. To validate the model also some intermediate water quality observation points with fortnightly measurements of nutrient concentrations have been taken into account. Linear interpolation was necessary for calculating the daily nitrogen loads. The LUA provided one detailed and two general data sets about water transfer points from or to the adjacent catchments (Wolfsbruch, Hohenbruch and Alt Garz) as well as information about 56 sewage treatment plants in the Rhin basin and groundwater quality measurements for 19 observation gauges within and around the catchment.

Fertilisation data for eight different crop types (winter wheat, maize, potatoes, summer barley, winter barley, winter rape, winter rye and sugar beet) and intensively used grassland were taken from the Havel management project (Voß, 2007). Information about needed fertilisation amounts for oil flax was taken from the literature (Umweltlexikon, 2007).

4.2.2 Model SWIM

Model description The dynamic ecohydrological model SWIM (Soil and Water Integrated Model) was developed on the basis of the models SWAT (Arnold et al., 1994) and MATSALU (Krysanova et al., 1989). SWIM simulates hydrological processes, vegetation and nutrient cycles at the river basin scale (Krysanova et al., 1998, 2000) by disaggregating the basins to subbasins and hydrotopes, where the hydrotopes are the highest disaggregated units (sets of elementary units in a subbasin with the same soil and land use types). Up to ten vertical soil layers can be considered for hydrotopes. It is assumed that a hydrotope behaves uniformly regarding hydrological processes and nutrient cycles.

Water fluxes, nutrient dynamics and plant growth are calculated for every hydrotope and then lateral fluxes of water and nutrients to the river network are simulated taking into account retention processes in the subbasins (see below). After reaching the river system, water and nutrients are routed along the river network to the outlet of the simulated basin.

The hydrological system is split into four compartments in the model: the soil surface, the soil layers, the shallow aquifer and the deep aquifer. Processes taken into account for the soil zone are surface runoff, infiltration, evapotranspiration, percolation and interflow. Hydrological processes in the aquifer zone are groundwater recharge, capillary rise to the soil profile, lateral flow and percolation to the deep aquifer.

The nutrient modules include pools of active and stable phases, inorganic and organic phases and nutrients in the plant residue for nitrogen and for phosphorus. The following processes are taken into account: mineral and organic fertilisation, input with precipitation, mineralisation, denitrification, plant uptake, leaching to groundwater, and losses with surface runoff, interflow and erosion.

The nitrogen and phosphorus mineralisation considers two sources a) fresh organic pool associated with crop residue, and b) active organic pool associated with the soil humus. Organic nutrient flows between the active and stable organic pools are governed by the equilibrium equations and depend on the C:N ratio, C:P ratio, soil temperature, and soil water content. Mineral phosphorus is distributed between three pools: labile phosphorus (LP), active mineral phosphorus (AMP), and stabile mineral phosphorus (SMP), and the flows between AMP and SMP and the AMP and LP pools are governed by the equilibrium equations.

The denitrification in soil occurs only in the conditions of oxygen deficit, which usually takes place when soil is wet. The denitrification rate is estimated as a function of soil water content, soil temperature, organic matter, a coefficient of soil wetness, and mineral nitrogen content. The soil water factor is an exponential function of soil moisture with an increasing trend when soil becomes wet.

Crop uptake of nitrogen and phosphorus is estimated using a supply and demand approach. The optimal crop N and P concentrations are calculated as functions of growth stage. The daily crop demand of nutrients is estimated as the product of biomass growth and optimal concentration in the plants. Actual nitrogen and phosphorus uptake is the minimum of supply and demand. Uptake starts at the upper soil layer and proceeds downward until the daily demand is met or until all nutrient content has been depleted.

Amounts of NO_3-N and soluble P in surface runoff, lateral subsurface flow and percolation are estimated as the products of the volume of water and the average concentration. Because phosphorus is mostly associated with the sediment phase, the soluble phosphorus loss is estimated as a function of surface runoff and the concentration of labile phosphorus in the top soil layer.

While passing the soil and groundwater by flowing to the river system the nutrients within surface flow, interflow and base flow are subject to retention and decomposition processes, whose rate and intensity are described by special parameters using the equation

$$N_{t,out} = N_{t,in} \times \frac{1}{1+K\lambda} \times \left(1 - e^{-\left(\frac{1}{K}+\lambda\right)\Delta t}\right) + N_{t-1,out} \times e^{-\left(\frac{1}{K}+\lambda\right)\Delta t},$$

where $N_{t,out}$ means the nutrient output and $N_{t,in}$ the nutrient input at time t, the parameter K represents the retention time and λ the decomposition rate of the nutrients. The term Δt is the time step. Within ranges specified from literature the retention parameters can be used for calibration. Under the term "decomposition" mainly denitrification in soil and groundwater is meant. This approach was developed and validated previously for the SWIM model in another German lowland catchment in the Elbe basin (Hattermann et al., 2006).

Model adjustments For simulating the Rhin catchment some additional model assumptions had to be set. Firstly, it was necessary to define subbasins with additional in- or output of water (and dissolved nutrients) from or to adjacent catchments according to the information delivered by the LUA. The water transfer point Wolfsbruch (inflow) was defined by adding daily measurements of water discharge and the corresponding calculated nutrient load. The outflow point Hohenbruch was introduced by using long time mean values of the outflow discharge and load. Alt Garz was defined by the constraint that in winter time and in times with discharge higher than 5 m^3/s, the outflow and nutrient load of the corresponding subbasin are nearly halved.

Secondly, the LUA delivered information on location and output of point sources (sewage treatment plants), which were added to the daily nutrient amount of the corresponding subbasins. Unfortunately, these data have a high uncertainty, as they are annual values estimated from one or two measurements per year. As there were no better data on point sources available, they were still used for simulation of the nitrogen and phosphorus loads.

Thirdly, it was assumed in this study that nutrient retention in SWIM represents retention in subbasin and retention in streams for both nitrogen and phosphorus. Therefore the introduced retention equation above with the parameters K and λ was used not only for nutrient transport with surface flow, interflow and groundwater flow but also for transport of nutrients coming from point sources (meaning in-stream retention processes). The retention parameters were taken as ranges from literature (Voß, 2007) and then subjected to calibration.

Fourthly, a simple wetland approach (Hattermann et al., 2008a) was introduced in the model in order to represent specific wetland processes, as about 40% of the catchment belongs to fens or groundwater influenced soils with shallow groundwater tables. These conditions justify the model approach, which allows increasing the plant uptake of water and nutrients from groundwater in wetland areas in times, when the supply of water and nutrients in soil is limited.

Fifthly, according to the natural conditions in the basin it was necessary to change parts of the original SWIM phosphorus module (where soluble phosphorus was assumed only to appear in the first ten centimetres of the soil profile) and to allow the soluble phosphorus to leach also vertically through the soil profile. Phosphorus leaching to groundwater in the Rhin catchment is justified by the fact that measured phosphate phosphorus concentrations at some groundwater observation gauges within and around the Rhin basin have quite high amounts (0.08 mg/l on average) and achieve almost the target value for surface water (0.1 mg/l). While passing the soil profile the phosphorus is added to the corresponding water flows (interflow and base flow) and then is subjected to retention. The leaching is a function of the concentration of soluble phosphorus in the soil layer, the amount of water leaving the layer and the ratio between the phosphate phosphorus concentration within the soil and within the soil water using the equation of Voß (2007)

$$P_i = \frac{0.01 \times P_{lab,i} \times W_{tot}}{RP_{s,w}}$$

with P_i meaning the total amount of phosphate phosphorous leaving the soil layer i, $P_{lab,i}$ being the concentration of labile phosphate within layer i, W_{tot} meaning the total amount of leaving water and $RP_{s,w}$ being the ratio between phosphate concentration in the soil to that in the soil water.

4.2.3 Evaluation of model results

To evaluate the quality of simulated model results different criteria of fit can be taken into account. In this study the non-dimensional efficiency criteria of Nash & Sutcliffe (1970) (E) and the relative difference in balance (B) were used.

E is a measure to describe the squared differences between the observed and the simulated values on a daily time step using the following equation:

$$E = 1 - \frac{\sum(obs - sim)^2}{\sum(obs - obs_{av})^2} ,$$

whereas B shows the long-term differences of the observed values against the simulated ones in percent for the whole modelling period:

$$B = \frac{sim_{av} - obs_{av}}{obs_{av}} \times 100 .$$

In these equations *obs* defines the observed daily value, *sim* means the corresponding simulated value, and the variables obs_{av} and sim_{av} describe the mean values of these parameters for the whole simulation period.

The efficiency can vary from minus infinity to 1 and should be as near as possible to 1, while the deviation in balance has its best values near 0. The Nash-and-Sutcliffe-Efficiency and deviation in balance were used for discharge as well as for nutrient loads.

4.3 Results and Discussion

4.3.1 Calibration of water discharge

The discharge gauge Kietz as the outlet of the Rhin basin is partly influenced by the Havel and/or Elbe river and reasonable gauging is very difficult. Therefore discharge measurements are available only for short time periods: two years in the 20th and four years in the 21st century. The latter one was used for calibration.

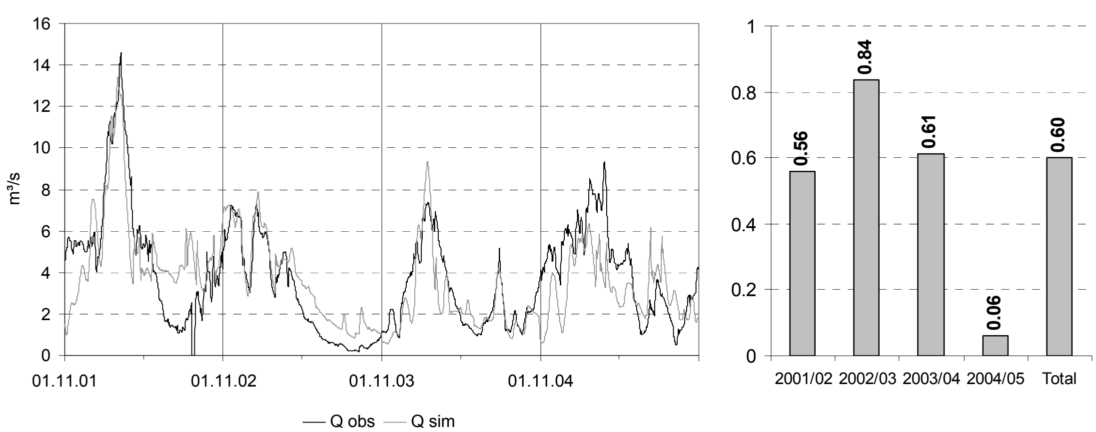

Figure 4.3 Comparison of the daily observed and simulated discharges at the gauge Kietz (left), and corresponding Nash-and-Sutcliffe-efficiencies for the hydrological years and the whole period (right).

For the period from November 2001 to October 2005 the best model efficiency obtained was 0.6 with large differences between the single years (0.06 to 0.84) as shown in Figure 4.3. The corresponding deviation in water balance was -2.5%. Problems are more pronounced during the summer months. Most probably this results from the complex water regulation and management system in the Rhin river. Water is stored in the upper part of the basin and then used for irrigation (artificially increased evapotranspiration), which can lead to lower discharge in summer than expected according to the precipitation amount. Exact data about this measure are not available and therefore were not represented in the model. Besides, when in August 2002 the extreme Elbe flood occurred, the lower parts of the Havel and partly Rhin lowlands were used to cut the flood peak of the Elbe river by opening some polder areas for flooding to protect downstream Elbe regions. During this time the Rhin discharge was strongly influenced and for some days even interrupted. But the next year had very dry conditions, and here another factor should be taken into account: an underestimation of evapotranspiration in the lower part of the Rhin catchment with high groundwater table.

In general, it seems that actual evapotranspiration should have different intensities in the upper and the lower parts of the basin due to natural conditions and human interventions described above. Calibrating the three gauges Rheinsberg, Alt Ruppin and Kietz (for their location see Figure 4.1) and comparing their best parameter settings a continuous spatial decrease of the evapotranspiration correction parameter thc (meaning an increase in evapotranspiration) was necessary to get the results shown in Figure 4.4, which compares the mean monthly average discharges for these three gauges along the Rhin river. Quite good efficiencies and typical seasonal dynamics could be achieved (Rheinsberg: maximum flow in summer; Alt Ruppin: more or less continuous decline in discharge during the year; Kietz: maximum flow in winter, minimum in summer). But still the question is, whether the different evapotranspiration parameters were needed due to different locations within the basin, or due to different time periods compared as result of data availability (time periods of different political and water management regimes). Anyway, different locations and water management schemes described above play a very important role in this lowland catchment.

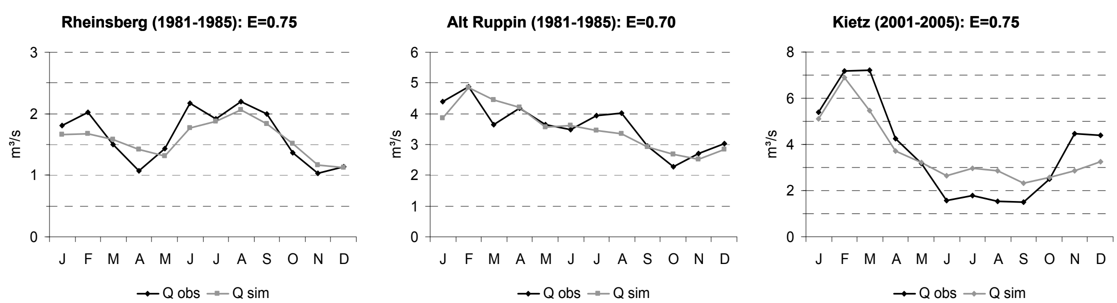

Figure 4.4 Comparison of the observed and simulated monthly average discharges for three discharge gauges of the Rhin basin (different periods due to data availability).

4.3.2 Nitrogen calibration

Nitrate nitrogen calibration was done for the gauge Kietz by taking into account all known point sources in the Rhin basin as well as diffuse pollution (coming mainly from fertilised fields). The nutrient transformation processes on the fields and in the underlying soil profile are highly influenced by soil conditions (water content and temperature). The amount of nutrients reaching the river system and the basin outlet is also controlled by special characteristics of vegetation (leaf area index, optimal temperature, nutrient uptake parameters, rooting depth etc.) and the type of growing crops on agricultural land.

Figure 4.5 shows model results for the calibration period from November 2001 to October 2005. The two years in the middle of the period are very well reproduced, whereas the peak in the first year is underestimated, and concentrations in the last year are overestimated. The characteristic nitrogen behaviour with high concentrations and loads in winter months and low nitrogen loads in drier summer months (as a result of the high influence of diffuse pollution) is reproduced quite well. But it seems that it is difficult to reproduce better nutrient dynamics during extreme events (like the high flood in the beginning of 2002 or the winter following an extremely dry period in 2003), probably due to unusual system behaviour and unexpected interruption or intensification of some nutrient transformation processes with extreme events.

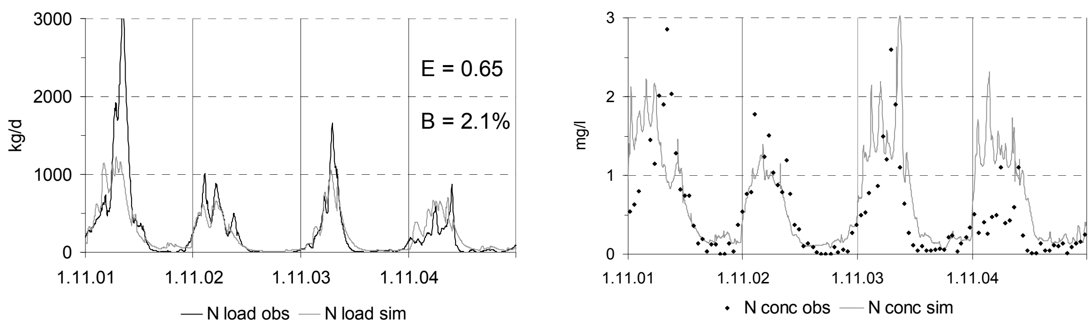

Figure 4.5 Observed and simulated nitrate nitrogen loads with the efficiency E and deviation in balance B (left) and NO_3-N-concentrations (right) for the gauge Kietz in the calibration period from November 2001 to October 2005.

The nitrogen calibration was done assuming winter wheat on all agricultural areas (because of insufficient information about crop rotations), which is not realistic but acceptable as winter wheat behaves like an average of all crop types usually grown in the Rhin basin, which was seen during a sensitivity analysis of the model results against the growing crop. The results of this analysis were later also used for scenarios dealing with effects of different crop type composition on water amount and water quality.

4.3.3 Phosphorus calibration

Calibrating phosphorus processes within the Rhin basin required considerable change in the SWIM code regarding vertical phosphorus leaching processes through the soil profile as described in section 4.2.2. Only with this method the calibration results shown in Figure 4.6 could be achieved. Apart from that, the resulting load and concentration of phosphorus at the basin outlet in Kietz are heavily influenced by emissions from point sources. As the fraction of point-borne loading is much higher for phosphorus than for nitrogen, the phosphorus concentrations in the river remain relative constant throughout the year and do not show such a clear seasonal behaviour as the concentration of nitrogen.

Looking at the graphs of the calibration period from November 2001 until October 2005 (Figure 4.6) one can see acceptable results for these four years at the outlet Kietz. The simulated loads correspond quite good to the interpolated ones. Especially the higher loads in winter/spring time (caused by vertical leaching of phosphorus during humid season) are reproduced well. But in the very dry summer 2003 the phosphorus loads are overestimated due to a more or less constant basis of point source emissions used in the model.

The influence of the cultivated crops on phosphorus concentration can be explained above all by the amount of crop specific discharge. Crop types causing the highest discharge lead to the lowest phosphorus concentrations due to dilution processes.

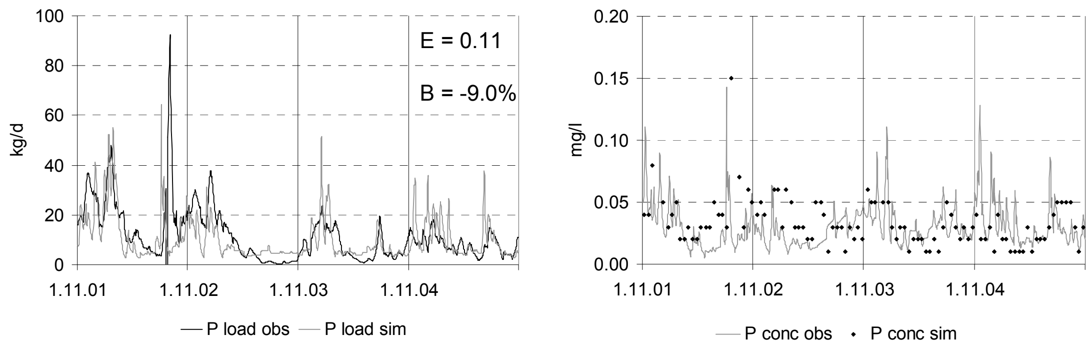

Figure 4.6 Observed and simulated phosphate phosphorus loads with the efficiency E and deviation in balance B (left) and PO_4-P-concentrations (right) for the gauge Kietz in the calibration period from November 2001 to October 2005.

4.3.4 Model test for a long-term period

After finding the best parameter combination for the four-years-calibration-period, the model was tested for a 25-years-period from 1981 until 2005. Due to lack of discharge data at the gauge Kietz for almost 20 years, the test was done by comparing the measured nitrate nitrogen and phosphate phosphorus concentrations for these 25 years with the simulated ones. Figure 4.7 shows nitrogen concentrations and phosphorus concentrations as well as water discharge to facilitate interpretation of the results for concentrations.

In general, the seasonal dynamics of the measured nitrate nitrogen concentration is simulated satisfactorily. Usually there are peaks in winter time and low amounts of nitrogen in summer months. No trends can be observed. But it can be seen that in two years of low winter discharge (1989 and 1996) the measured nitrogen concentration is reproduced quite well, whereas in each case in the following two years the concentration peaks are overestimated.

It is not quite clear why the model behaves in such a way, and it is not easy to explain without knowing whether the simulated discharge is correct or not. Perhaps the reason for the overestimation of nitrogen can be a wrong assumption of a threshold parameter of water content for denitrification (globally set to 0.7, which delivered the best results on average). It is known that in soils with easy available carbon (as in the fens of the Rhin catchment) denitrification is also possible with water contents lower than 60-70% because of the high activity of micro-organisms (Scheffer & Schachtschabel, 2002). Another possibility is different water management in years with lower discharge than assumed (e.g. no water transfer out of the basin in the lower course or more water input from the storages and transfer points in the upper course during dry winter times), and as a result more water than expected by the model with the consequence of lower measured concentrations at the outflow Kietz.

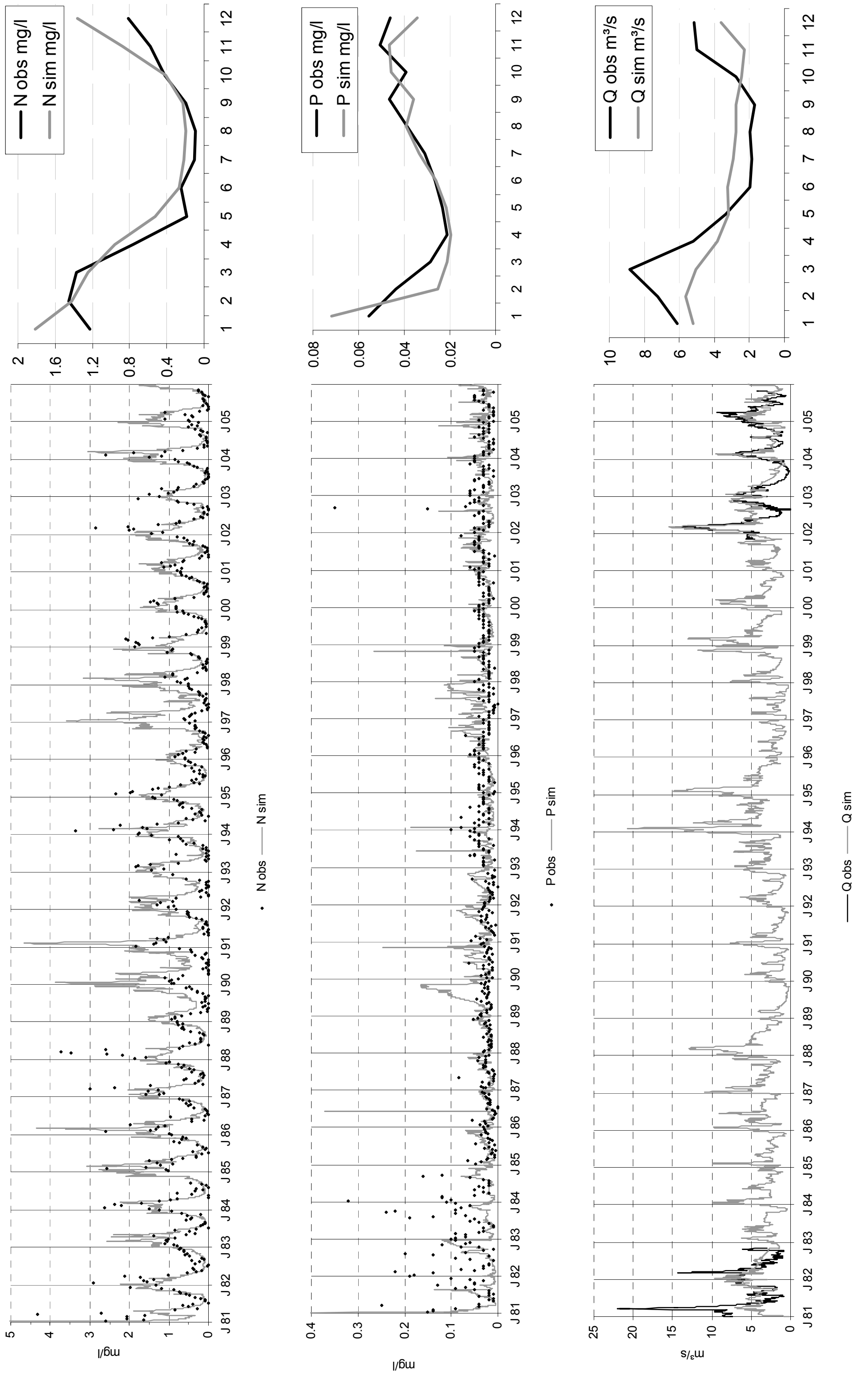

Figure 4.7 Long-term modelling: nitrate nitrogen concentrations (upper graphs), phosphate phosphorus concentrations (middle graphs) and water discharge (lower graphs) in Kietz for the period 1981-2005 as a comparison of available measured data with the simulated ones (left) and the corresponding monthly averages for the whole test period (right).

Unlike for nitrogen, higher concentrations of phosphate phosphorus were measured in 1981 to 1985 probably due to higher contribution of sewage treatment plants at this time, whose capacities were improved after that. In general, the simulated phosphorus concentration values of the test period from 1981 until 2005 meet the range of measured ones although some deviations can be noticed, too. Especially in the first five years an underestimation can be seen whereas in the probably drier years explained above an overestimation of the measured values takes place. The first problem can most probably be explained by the fact that in the 1980th the negative effects of too high phosphorus concentrations in surface water bodies (e.g. eutrophication processes) became known and great efforts were undertaken to avoid these pollution (UBA, 2006; Metzner, 2006). As data about point source emissions in the catchment were available only for the last five years and their average was used for the whole test period it is very likely that the point source emissions (as well as fertilisation data) used for the first years in the 1980th are underestimated. The problems in phosphorus concentration model results during dry years can supposable be explained in the same way as for nitrogen, namely via not exact assumptions regarding nutrient transformation processes and/or water management measures in extremely dry seasons.

Comparison of measured and simulated nutrient concentrations for some observation gauges located within the basin results in a similar model accuracy although there are some differences in the upper part of the Rhin catchment. The polluted ditches with their higher nutrient concentrations than on average are reproduced quite well.

4.3.5 Sources of nitrogen and phosphorus load

A special interest of the study was to identify contribution of diffuse sources of nutrients to the total loads in the Rhin river and to define the reference status of the catchment. For this purpose different simulation experiments were done paying attention on the different nutrient flows coupled to the three water flows: surface flow, interflow and base flow. To identify the sources of nutrient concentrations, the percental composition of the simulated nutrient loads at the basin outlet was analysed. The results for nitrate nitrogen and phosphate phosphorus for the total calibration period as well as differentiated for summer (April – September) and winter seasons (October – March) are shown in Figure 4.8.

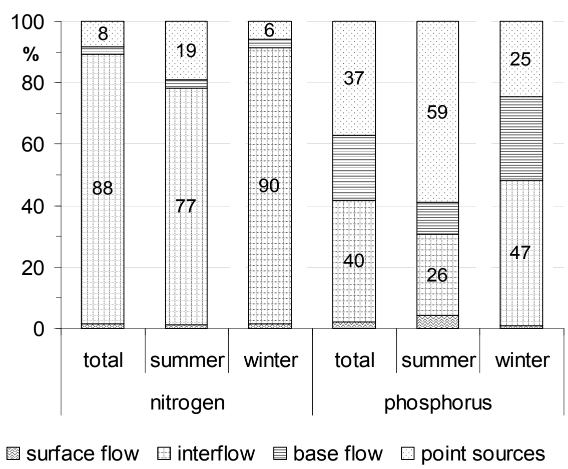

Figure 4.8 Composition of nitrate nitrogen and phosphate phosphorus loads coming with surface flow, interflow, base flow and from point sources at the gauge Kietz for the period 2001-2005 in total and for summer (Apr – Sept) and winter (Oct – Mar) subperiods.

Differences between nitrogen and phosphorus and a clear seasonality are obvious. The amounts of nutrients originating from point sources are highest in summer whereas in winter months the influence of interflow-based nutrients is at maximum. This can be seen for both nitrogen and phosphorus.

For the whole five years period 88% of the nitrogen load comes with interflow, 2% with base flow, 2% with surface flow, and 8% from point sources. These percentages differ slightly between the years mainly due to differences in precipitation amount and occurrence of dry and wet conditions. The very dry year 2003 with rare precipitation and low water level in the river has the highest percentage of point sources; whereas in the very wet year 2002 the fraction of point sources is lower than on average. The contribution of diffuse pollution from arable land is highest in winter due to “washing” soils by precipitation. In summer the larger part of soil nitrate nitrogen on agricultural land and areas covered by vegetation is uptaken by plants. Additionally, there is lower discharge, so that the proportion of point sources is higher. A quite high share of nitrogen coming with interflow can be explained by a) a relatively high share of wetland-type soils in the catchment, and b) an extensive network of drainage ditches, which speed up the transportation of nutrients to the river and is responsible for higher concentrations in time of high water flow. Though the drainage ditches are not implemented “directly” in the model, the model is calibrated for the current conditions, and the calibrated retention times and decomposition rates reflect these conditions indirectly.

For phosphorus the influence of point sources is noticeable higher than for nitrogen. For the whole simulation period 37% of the phosphorus load originates in point emissions, 40% comes from interflow, 21% from base flow and 2% from surface flow. Interannual and seasonal variations can be explained in the same way as for nitrogen. The high percentage of phosphate phosphorus loads coming from groundwater at the basin outlet (with a mean concentration of 0.02 mg/l at the gauge Kietz) matches the real measured data in and around the basin, where high phosphorus concentrations in the groundwater (between 0.01 and 0.61 mg/l with an average of 0.08 mg/l) are observed.

Analysis of map outputs of the SWIM model shows that denitrification and mineralisation of nitrogen are maximal in areas with organic soils and high groundwater table, whereas the loss of nitrogen with interflow reaches its maximum on agricultural areas with parabrown soils. Transformation and leaching processes of phosphorus are more intensive on grassland on organic soils and not as much on agricultural areas.

For defining the reference status of the river (not influenced by human nutrient inputs) a model experiment was done with no fertilisation and no point sources but the same land use and climate data for the period 1981 to 2005. The resulting mean nitrogen load at the gauge Kietz was reduced by about 58% and that of phosphorus by about 53%. Although this can be assumed as a kind of potential natural conditions and used to define the reference status, it is not realistic to postulate these conditions in an inhabited area with agricultural use. However, the “good agricultural practices”, aimed in reduction of nutrient losses from arable land, should be applied in order to reduce diffuse pollution as much as possible. Scenario simulations in this respect will be explained beside others in the following section.

4.3.6 Measures to reduce nutrient concentrations

This study was aimed in finding measures to reduce nutrient concentrations in the Rhin river and its tributaries. For this purpose some model experiments have been done which were expected to decrease nutrient loads in the basin. An explanation of these experiments together with their implementation in SWIM can be found in Table 4.2; the scenario results are presented in Figure 4.9.

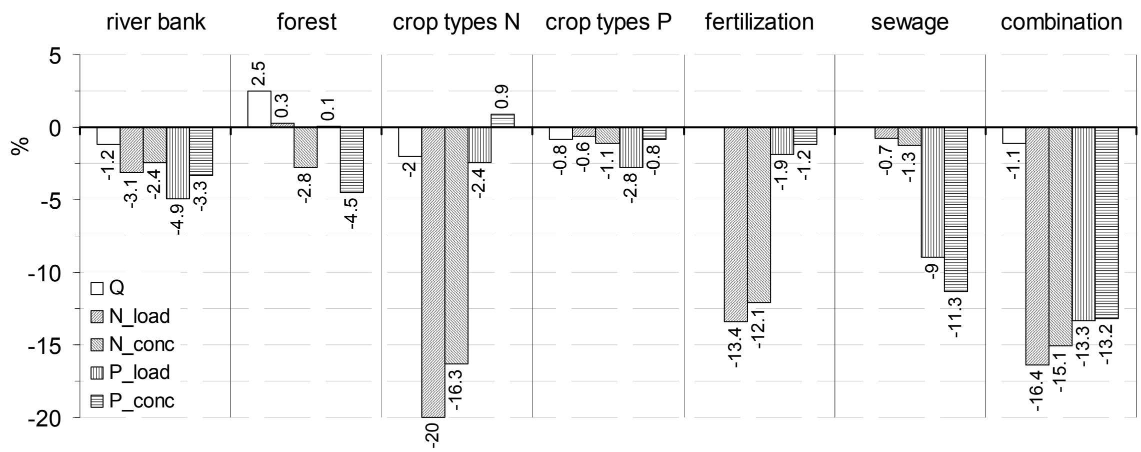

Figure 4.9 Results of seven different scenarios for measures aimed in reduction of nutrient pollution (for detailed explanations see Table 2): percental change of the mean model outcome for the gauge Kietz under scenario conditions compared to the reference conditions (Q – water discharge, N_load – nitrate nitrogen load, N_conc – nitrate nitrogen concentration, P_load – phosphate phosphorus load, P_conc – phosphate phosphorus concentration).

The first six scenarios led to nutrient reduction with different results for nitrate nitrogen and phosphate phosphorus. Nitrogen seems to be more sensitive against changes in fertilisation regime and crop type composition, whereas phosphorus can be reduced most effective by decreasing point source emissions, due to the relative influence of point and diffuse pollution on the total loads of nitrogen and phosphorus. Noticeable changes in phosphorus concentration via crop type variances and agricultural land use changes could only be achieved by growing crops (or rather no crops) causing higher discharges at the basin outlet (e.g. increase of the amount of set-aside) as a result of dilution processes.

Measure	**Description**
river bank	conversion of agricultural land with fertilisation within 50 m around rivers and lakes to extensive grassland without fertilisation
forest	conversion of all forested areas (34% of the whole catchment, thereof 80% evergreen) to deciduous forests
crop types N	change of the three crop types causing the highest nitrogen concentrations (winter wheat, sugar beet and winter rape) to winter rye
crop types P	change of the three crop types causing the highest phosphorus concentrations (winter barley, sugar beet and oil flax) to winter rye
fertilisation	maintaining the reference situation for crop types composition but reducing crop specific N and P fertilisation by 20%
sewage	reducing the N emissions of all sewage treatment plants within the catchment by 10% and the P emissions by 20%
combination	combination of the scenarios “river bank”, “fertilisation” and “sewage”

Table 4.2 Example measures to reduce nutrient pollution and description of their realisation during SWIM modelling.

The decrease of point source pollution was assumed for nitrogen and phosphorus with different percentages as a consequence of the actual status of treatment plant equipment in the basin, where phosphorus reduction possibilities for small treatment plants are more often missing than that for nitrogen. Therefore it was assumed that phosphorus reduction of point source pollution could have a higher amount after upgrading the facilities.

Two tested measures were dealing with possible changes in landscape composition: the installation of buffer zones without agricultural use around surface water bodies and the conversion of all evergreen and mixed forests to deciduous ones. Both methods result in decreasing nutrient concentrations in the Rhin river; the first one due to decreased nutrient loads (caused by a smaller fertilised area in the catchment) and the second one due to a higher discharge at the outlet (caused by reduced plant transpiration of deciduous trees in winter months) and dilution processes. But in general, the effects of a changed land use on nutrient concentrations do not exceed five percent. Changes in fertilisation regime and point source emissions can have a much higher influence on nutrient concentrations.

As no single scenario results in considerable decrease of nutrient loads and concentration for both nitrogen and phosphorus, a combination of some measures was tested, which would allow notable improvement of water quality. In this respect combinations of different measures are possible, but only one will be presented here: buffer zones around surface water bodies combined with a reduction of point source pollution and fertilisation by 20%. Simulating this scenario, nitrogen as well as phosphorus loads and concentrations are minimised by about 15%, which would allow pushing the system closer to the “good ecological status” as required by the WFD.

4.3.7 Climate sensitivity and climate scenarios

To investigate the influence of a changing climate on the water quality of the Rhin river two different approaches were applied. Firstly a simple climate sensitivity analysis was performed followed by two different scenarios based on real climate data for the Elbe region.

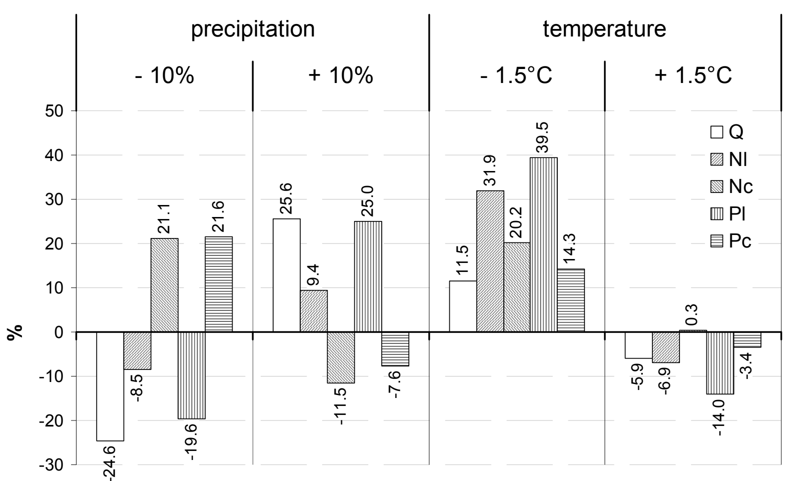

Figure 4.10
Climate sensitivity of the SWIM results: percental change of the mean model outcome (Q – water discharge, Nl – nitrogen load, Nc – nitrogen conc., Pl – phosphorus load, Pc – phosphorus conc.) at the gauge Kietz for the period 2001-2005 after changing precipitation or temperature.

Climate sensitivity For the climate sensitivity analysis the precipitation was first reduced and increased by 10% with the same temperature, and then temperature was reduced and increased by 1.5°C with unchanged precipitation. The results and effects on discharge, nutrient loads and nutrient concentrations are shown in Figure 4.10. A reduced precipitation leads to reduced discharge and nutrient loads (less diffuse pollution as a result of less washing out) but increased nutrient concentrations as the reduction of discharge is much higher than the reduction of loads; and an increase of precipitation behaves in the opposite way (higher discharge and higher nutrient loads but decreased concentrations at the gauge Kietz). Lower temperatures cause higher discharge and more leaching (as a consequence of lower evapotranspiration and inhibited denitrification processes) and result in higher nutrient loads and concentrations in the Rhin river. With higher temperatures a decrease in discharge and loads can be observed because of higher evapotranspiration and decreased leaching.

Climate scenario This simple climate sensitivity experiment was completed by testing a real climate scenario based on data for the period 1951-2003 provided by the statistical climate model STAR (Gerstengarbe & Werner, 2005) for 831 stations within the whole Elbe region. Using these data a climate scenario for the period 2004-2055 consisting of 100 realisations (which all have the same probability) were produced statistically (Orlowsky, 2006). 37 of these 831 stations are located within or around the Rhin catchment and were used to find the driest (S 36) and wettest realisation (S 82) for modelling by ranking the mean precipitation and climatic water balance (difference between precipitation and potential evapotranspiration calculated using the equation of Haude (1955)) for the scenario period 2016-2025. The climate variables for the two realisations in this period compared with these of a reference period for one of the 37 stations can be found in Table 4.3. The results of the two climate scenario model runs are shown in Figure 4.11.

		Reference	S 36 (dry)	S 82 (wet)
time period		1991 - 2000	2016 - 2025	2016 - 2025
temperature	°C	9.4	10.0	10.3
precipitation	mm a^{-1}	535	477	589
climatic water balance	mm d^{-1}	0.32	0.12	0.39

Table 4.3 Mean climate parameters for two simulated scenarios in comparison with the reference period (climate station Neuruppin in the middle of the catchment).

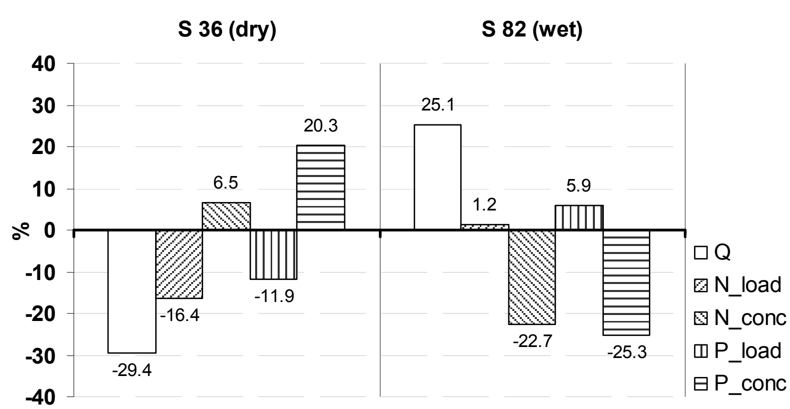

Figure 4.11 Results of two climate scenario model runs: Percental change in mean water discharge (Q), nitrate nitrogen loads (N_load) and concentrations (N_conc), phosphate phosphorus loads (P_load) and concentrations (P_conc) by comparing the scenario time period 2016-2025 with the reference period 1991-2000 at the gauge Kietz for the drier scenario S 36, and wetter scenario S 82.

In general, the outcomes of these two realisations resemble the climate sensitivity analysis with changed precipitations: drier climate causes lower loads but higher nutrient concentrations, whereas wetter climate leads to reduced concentrations mainly due to increased discharge. It seems that the changed precipitation of the scenario runs has much more influence on water and nutrient flows in the region than the changed temperatures, but it should be recognised, that the increase in precipitation corresponds quite well to the expected change in the sensitivity analysis, whereas the change in temperature is not as high as assumed there.

4.4 Conclusions

Simulation of the discharge behaviour and water quality with ecohydrological catchment models is much more difficult for regulated lowland rivers than for rivers in mountainous areas due to the special characteristics of the former ones (e.g. water management and melioration activities or high percentage of wetland areas). This leads to problems in reproducing water amount and water quality by models. In our case study these problems were partly solved by introducing available information about water management, which allowed achieving satisfactory results of model calibration.

However, further improvement of the model results can not be achieved without a better knowledge of human impacts and management activities. But also some special landscape processes (especially during extreme events like floods or droughts) need a more detailed analysis in future.

Nevertheless such modelling experiments help to understand the river system behaviour better. Especially for identifying the fractions of point and diffuse sources at the outlet of the river system and the areas of highest diffuse pollution the model can be very useful. Knowing these sources and hotspot areas, it is easier to identify useful measures for reducing actual nutrient loads in the river network and for achieving the “good ecological status” as required by the WFD. A dynamic catchment model taking into account water and nutrient processes as a function of vegetation, land use and human impacts, driven by climate conditions, can provide a very functional tool for creating a river basin management plan taking into account possible changes, which the basin could be confronted with in future.

This Rhin study was a pilot project with a close cooperation of researchers and representatives of the decision-making government to support implementation of WFD with research results. The stakeholders of the Environmental Agency of Brandenburg can benefit from the model results as well as the researchers benefit from their special knowledge of the basin and the available data. Such participatory approach allows providing results, which are requested and will be used by water managers and politicians to improve the adaptability of river systems to changing conditions in future.

CHAPTER 5

IMPLEMENTING IN-STREAM NUTRIENT PROCESSES

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Abstract

For a long time watershed models focused on the transport of chemicals from the terrestrial part of the watershed to the surface water bodies by leaching and erosion. After the substances had reached the surface water, they were routed through the channel network often without any further transformation. Today, there is a need to extend watershed models with in-stream processes to bring them closer to natural conditions and to enhance their usability as support tools for water management and water quality policies. This paper presents experience with implementing in-stream processes in the ecohydrological dynamic watershed model SWIM (Soil and Water Integrated Model) and its application on the large-scale in the Saale river basin in Germany. Results demonstrate that new implemented water quality parameters like chlorophyll *a* concentrations or oxygen amount in the reach can be reproduced quite well, although the model results, compared with results achieved without taking into account algal and transformation processes in the river, show obvious improvement only for some of the examined nutrients. Finally, some climate and water management scenarios expected to impact in-stream processes in the Saale basin were run. Their results illustrate the relative importance of physical boundary conditions on the amount and concentration of the phytoplankton, which leads to the conclusion that measures to improve water quality should not only take nutrient inputs into account, but also climate influences and river morphology.

5.1 Introduction

5.1.1 In-stream water quality and modelling in river basins

Ecohydrological modelling in river catchments has a long history. Computer models dealing with water quality issues were developed and used in several studies since almost 40 years (Horn et al., 2004; Thorsen et al., 1996). Starting in the 1970ies with conservative substances (Refsgaard et al., 1999), models to solve ecohydrological problems in landscapes and rivers became more and more complex by incorporating also transport and transformation processes of different reactive substances. In order to simulate water quality usually two types of models were used: (1) watershed models with a focus on terrestrial processes and management options, but simple routing of the different substances in the river itself; or (2) river water quality models with detailed description of the riverine processes, but without any processes or management options in the corresponding catchment areas, or considering input from them only in a simplified form (Horn et al., 2004). Nowadays, a tendency can be seen to combine these two different model approaches in order to build a more realistic scheme of the ecohydrological processes in a watershed. This is particularly necessary in meso- to large-scale landscape modelling, as number and intensity of riverine processes increase in downstream direction.

Additionally, there is an increasing demand on integrated catchment and water quality modelling due to political water protection measures, e.g. Water Framework Directive of the European Commission (WFD) (EC, 2000). Watershed models can be a good supporting instrument in these processes, but should be adapted to the new requirements. Watershed modellers have to develop tools capable of linking physico-chemical variables already predicted by existing watershed models with additional hydromorphological and biological quality elements demanded by policy programs, especially regarding possible future developments and for finding feasible adaptation measures.

According to the European WFD a “good ecological status” should be achieved for all water bodies. Numerous measures could be implemented to get closer to it. Besides influencing the chemical composition by controlling the emissions of point or diffuse sources, the status of a water body is characterised to a large extent by its morphology. Water courses close to nature have a high self-purification capacity and capability to improve their water quality. Several measures could be implemented to improve river morphology after centuries of river regulation and hydraulic construction measures, for example rechanneling the river course by giving back meanders and extending floodplains, or enlargement of the rivers cross section.

While management changes can be realised as certain actions by humans to improve the quality of a water body, climate change cannot be directly influenced by the regional authorities and inhabitants. However, model experiments taking possible climate change into account can show a probable future direction of the water system development in order to be aware of it and to aid in finding adaptation possibilities.

A realistic simulation of future water quality developments in large catchments includes the processes occurring in the rivers itself. Several processes can be observed in the flowing water. Apart from input from point sources and diffuse pollution, the main factors affecting the chemical composition within a river are dilution processes, evaporation and deposition, adsorption and desorption to sediments and suspended solids, and transformation processes in the river water (Schwoerbel, 1999), the latter to a large extend influenced by algal growth and death.

Although riverine plankton organisms (potamoplankton) are almost undetectable in rivers with catchments smaller than 1000 km^2 due to little residence time of water (Mischke et al., 2005), they can achieve population densities comparable to that of lakes in larger and slowly flowing waters. Chlorophyll *a* concentrations between 100 and 250 µg L^{-1} are not a rarity (Nixdorf et al., 2002), and algae can have a noticeable influence on nutrient amounts and water quality in such cases.

Algae ingest soluble nitrogen and phosphorous substances, use and produce dissolved oxygen during respiration and photosynthesis and provide organic nitrogen and phosphorous compounds by their decomposition after death. Apart from algal caused substance conversions, bacteria induced transformation processes in the river itself, such as nitrification, oxidation or mineralisation, influence the substance composition in the water body, too (Horn et al., 2004; Ji, 2008; Neitsch et al., 2002a). All these processes mentioned should be taken into consideration simulating the processes in river basins.

Considering processes in surface water bodies during watershed simulations could be done either by linking two separate models (Debele et al., 2008; Ennet et al., 2008), or by integrating special equations of a hydrologic water quality model in the watershed model itself, as done for this study. A detailed description and comparison of numerous available river and watershed models (partly with incorporated in-stream processes) can be found in Horn et al. (2004), also in comparison with SWIM (Soil and Water Integrated Model) (Krysanova et al., 2000), which is used for the research study in hand. Although an increasing demand in models with integrated in-stream processes could be noticed, the authors detected only "limited attempts to integrate river water quality issues in watershed models so far". And those modellers, who tried to update their model codes with specific river water quality routines, ran only few test applications with these features (Horn et al., 2004), so that additional tests and experiences are necessary in the future.

This also applies to the SWAT model (Soil and Water Assessment Tool) (Neitsch et al., 2002a), which is a river basin scale model developed to quantify the impact of land management practices in large, complex watersheds and was once one of the bases to develop the SWIM model. The SWAT model does already contain equations to simulate riverine processes. However, several authors stated that all aspects of stream routing in SWAT need further testing and refinements (Arnold & Fohrer, 2005; Gassmann et al., 2007; Migliaccio et al., 2007). To go forward in this direction, van Griensven developed ESWAT (Extended SWAT) and achieved good results for nutrients in the studied areas (van Griensven, 2002; van Griensven & Bauwens, 2005). But further research and application of in-stream procedures in large-scale watershed modelling is still required. Hopefully, the approach and model application described in this paper will contribute to this development as well.

5.1.2 Motivation and objectives

Objective of the study presented here is the integration and testing of an in-stream process module in the existing watershed model SWIM in order to get a realistic tool for climate and land use change assessments in future applications. Keeping in mind the state of the art in modelling watersheds and the new requirements for catchment models described above, the aim of this study is to update the original SWIM model (which was developed especially to investigate climate and land use change impacts at the regional scale) with in-stream processes in order to improve the model's usability for future ecohydrological scenario simulations in meso- to macro-scale basins. The improved SWIM model will allow simulating impacts on riverine processes, especially regarding climate change assessments, better than other models (either focusing only on catchment processes and ignoring river processes, or modelling only riverine processes with prescribed inputs from the catchment) due to its special development objectives, spatial distribution and process description.

The SWIM model in its basic form is a watershed model with a simple river routing of nutrients. All water substances under investigation (nitrogen and phosphorus) introduced to the river network by erosion, leaching and/or point source emissions are added within the water body and then routed through the river network without any further transformations. Former model application in the meso-scale (Hesse et al., 2008) led to the conclusion that such simple assumption does not provide sufficiently good water quality results for all seasons, and that the model would benefit from adding retention or rather transformation processes in the river water body, especially in summer time. Apart from that, the original SWIM model does not take biological water components into consideration, which are increasingly often asked for by policy makers and stakeholders. Hence, to improve the model's applicability, a new in-stream module has been implemented, in which algal and bacterial induced nutrient processes in the river as well as the population dynamics of the algae themselves are simulated.

The following detailed steps are planned for this study:

- implementing in-stream processes for nitrogen and phosphorous in the model SWIM based on the approach used in the Model SWAT;
- application of the new SWIM code in the Saale catchment and evaluation of its importance for water quality modelling in meso-scale and large rivers and streams;
- modelling various water quality scenarios in consideration of possible management/environmental changes influencing riverine processes to estimate possible future changes.

5.2 Study area and data preparation

5.2.1 The Saale case study

The implementation of in-stream processes was tested for a large-scale river system, the Saale river catchment in Germany. The location of the study area and the water quality monitoring stations used for calibrating and validating model results, as well as maps of DEM, land use and location of point sources can be found in Figure 5.1. General and detailed characteristics of the catchment are listed in Table 5.1.

The Saale river is the second largest tributary of the Elbe river (Reimann & Seiert, 2001) flowing to the North Sea, and its catchment has a population of about 4.2 million people. Both relief and precipitation are heterogeneous. Strongly depending on the relief and location of the observation point, the average annual precipitation amount varies between 450 and 1600 mm yr^{-1} (FGG-Elbe, 2004b). Wide loess areas and low mountain ranges characterise the Saale catchment. Due to very fertile loess soils, almost two thirds of the catchment area are used for agriculture. A detailed water quality monitoring network was established along the Saale river in the last decades (compare Figure 5.1), whose data can be used for evaluation of water quality.

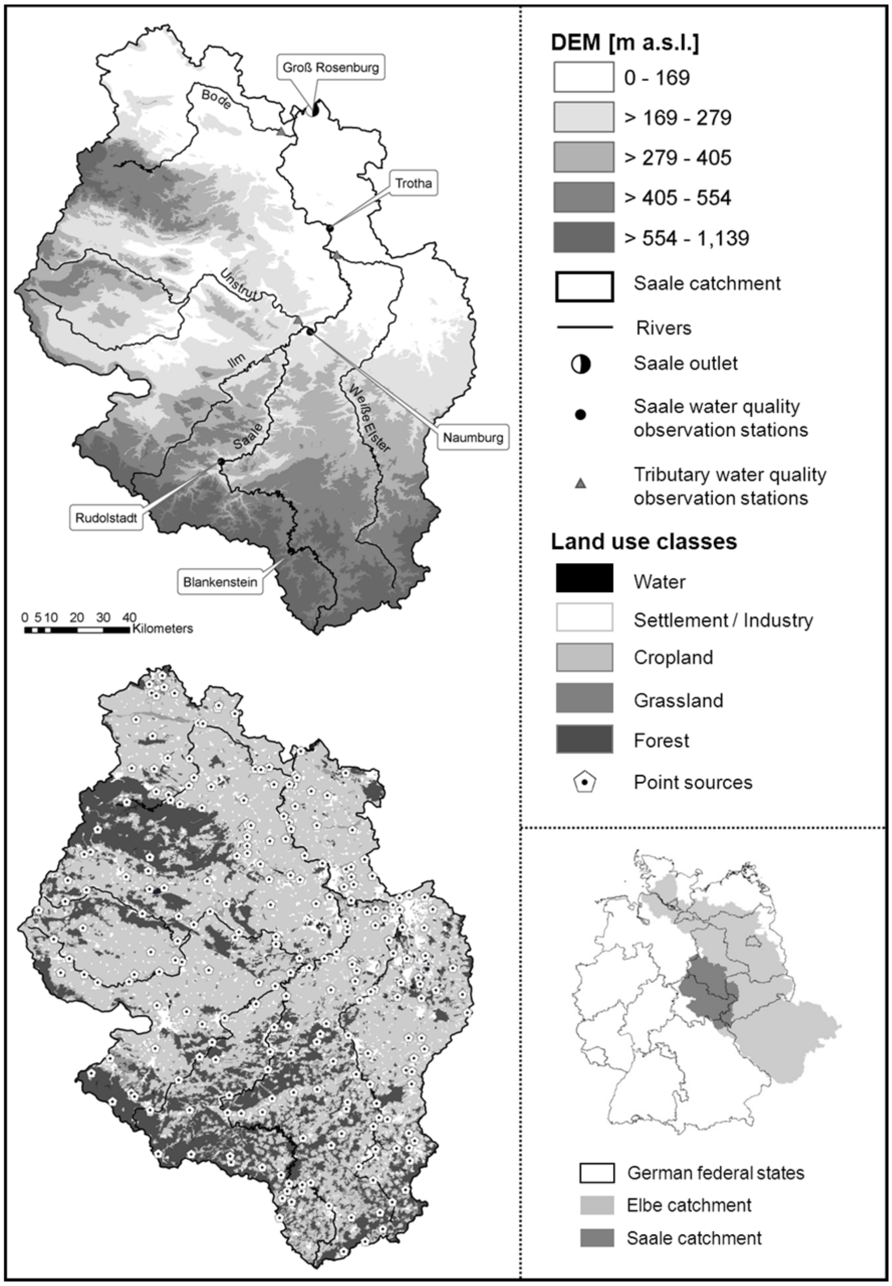

Figure 5.1 The area under study: Digital elevation model (DEM) of the Saale catchment with location of main rivers, basin outlet and intermediate observation stations (top left); land use classes and location of point sources (bottom left); and the location of the Saale catchment within the total Elbe basin and in Germany (bottom right).

At time of the German reunification the Saale river was a very eutrophicated and polluted water body. Although the water quality in the Saale river has been progressively improved after the German reunification due to improvement of sewage treatment, closure of some industries and changes in agricultural practices, the river is still heavily loaded with nutrients, mainly coming from diffuse sources (Behrendt et al., 2001). As a result of the long retention time of nutrients in some lower parts of the catchment and the high proportion of agricultural areas in the basin (FGG-Elbe, 2004b), the total nitrogen concentration at gauges of the lower Saale river is not expected to decrease significantly in the near future (Theile, 2001), even though there are some studies available, which show comparably short residence time of nitrate nitrogen in small catchments within the hard rock and sandstone lower mountain ranges of the upper Saale basin (Hesser et al., 2010; Rode et al., 2009).

Table 5.1 Characteristics of the Saale catchment and water quality observations at its last gauge Groß Rosenburg averaged for the simulation period 1996-2003.

Description		unit	value
Catchment area		km^2	24130
River length		km	427
Discharge		$m^3\ s^{-1}$	113.2
Altitude		m a.s.l.	14 - 1139
Precipitation		mm y^{-1}	643
Land use			
	agriculture	%	62.79
	grassland	%	4.52
	forest	%	23.30
	settlement	%	8.47
Soils			
	brown soils	%	47.58
	pseudogley	%	15.81
	chernozem	%	19.93
	floodplain soils	%	9.22
N point sources			
	total input	kg d^{-1}	9947
	contribution to total N load	%	14.1
P point sources			
	total input	kg d^{-1}	715
	contribution to total P load	%	30.2
Water quality parameters			
	average / 90 percentile		
	nitrate nitrogen	mg L^{-1}	5.2 / 6.8
	ammonium nitrogen	mg L^{-1}	0.5 / 1.01
	phosphate phosphorus	mg L^{-1}	0.08 / 0.13
	dissolved oxygen	mg L^{-1}	10.7 / 12.9
	chlorophyll a	µg L^{-1}	33.2 / 88.1

Regarding phytoplankton abundance and chlorophyll *a* content, most stations of the lower Saale river show a decreasing trend of this pigment since the beginning of the 90-ies, confirming the improved water quality in the Saale river (Lindenschmidt, 2005). However, the maximum concentration of chlorophyll *a* at the Saale's outlet still exceeds 100 µg L^{-1} in the growing season, so that the river can definitely be classified as a planktonic river. In the lower reach, weirs and locks have been constructed to store the water and to make the river navigable in the drier summer months. Additionally, the river's morphology is modified by a series of five reservoirs in the upper course for water harvest, flood protection, and a salt-load control system. All these water engineering measures lower the rivers flow velocity and strengthen the planktonic behavior of the Saale. Therefore, together with its relative good availability of water quality data, the Saale river is an perfect study area to test a large-scale watershed model with implemented in-stream processes.

5.2.2 Data preparation

Setting up the model requires four different raster datasets: elevation, land use, soil types and subbasins. They are used to generate the hydrotope classes, basin structure and routing structure, as well as the attributes of subbasins and rivers. The following datasets with a resolution of 100 x 100 m were used for the Saale basin: the digital elevation model (DEM) provided by the NASA Shuttle Radar Topographic Mission (SRTM), the general soil map of the Federal Republic of Germany (BÜK 1000) originating from the Federal Institute for Geosciences and Natural Resources (BGR), the land use map CORINE Land Cover 2000 prepared by order of the German Federal Environment Agency (UBA) by the German Aerospace Center (DLR), and the Elbe subbasin map provided by the UBA.

The daily climate data (minimum, maximum and mean temperature, precipitation, solar radiation, and air humidity) is the main driver of the simulation. Real climate data provided by the German Weather Service (DWD) were interpolated to the centroids of every subbasin by an inverse distance method.

The model results regarding water discharge and water quality were calibrated and validated using daily discharge and fortnightly to monthly water quality data of the gauge Groß Rosenburg at the Saale basin outlet provided by the State Office of Flood Protection and Water Management Saxony-Anhalt (LHW). Linear interpolation was necessary for calculating the daily loads of the different water components of interest. In case the concentration data for some days were named as “below the threshold of measurement”, they were assumed to be the half of this quantification limit.

Data for location and averaged output of point sources within the Saale basin were taken from the River Basin Community Elbe (FGG-Elbe, 2004b) and added to the daily water and nutrient amounts of the corresponding subbasins. Unfortunately, these data have a high uncertainty. There were only averaged values of total nitrogen and phosphorus amounts available, which had to be used as a constant for the whole simulation period. In addition, the total nitrogen and phosphorus emissions were subdivided into the different nutrient phases by a constant assumption due to a lack of more detailed data and knowledge about the real composition of the sewage waters (in terms of nitrogen the organic nitrogen pool, nitrate nitrogen pool, as well as the ammonium nitrogen pool were each added with one third of the total nitrogen emissions of the point sources, whereas the phosphate phosphorus as well as the organic phosphorus loads were each added with half of the total phosphorus emissions of the point sources).

The parameters for different crop types and their corresponding fertilisation regimes are of importance, especially in case of water quality modelling. Fertilisation dates and amounts for the crops were taken from Voß (2007), adjusted to recommendations regarding a “good practice” given by regional authorities of the studied area (TLL, 2007; LUFA, 1999).

5.3 Material and methods

5.3.1 The original model SWIM

The dynamic ecohydrological model SWIM is a model of intermediate complexity for the river basin and regional scale. It simulates hydrological processes, erosion, vegetation, and nutrient cycles at daily time steps using regionally available data (climate, land use and soil) and considering interactions and feedbacks between the different model compartments, such as water and nutrient drivers for plant growth, evapotranspiration by plants, and nutrient transport with water.

The Model was developed on the basis of the models SWAT93 (Arnold et al., 1994) and MATSALU (Krysanova et al., 1989) to investigate climate and land use change impacts in Germany and Europe at the regional scale. Simulation is based on a three-level disaggregation scheme from the basin to subbasins and hydrotopes, where hydrotopes are the highest disaggregated units (sets of elementary units in a subbasin with the same soil and land use types). It is assumed that a hydrotope behaves uniformly regarding hydrological processes and nutrient cycles.

The hydrological system is split into four compartments: soil surface, soil layers, shallow aquifer, and deep aquifer. Hydrological processes in the soil zone are surface runoff, infiltration, evapotranspiration, percolation and interflow, and in the aquifer zone groundwater recharge, capillary rise to the soil profile, lateral flow, and percolation to the deep aquifer.

The nutrient modules include pools of active and stable phases, inorganic and organic phases, and nutrients in the plant residue. The following processes are considered: mineral and organic fertilisation, input with precipitation, mineralisation, denitrification, plant uptake, leaching to groundwater, and losses from soil profile with surface runoff, interflow and erosion.

The module representing crops and natural vegetation is an important interface between hydrology and nutrients. Arable crops (like winter wheat, summer barley or maize) and aggregated vegetation types (like pasture, evergreen forest or mixed forest) are simulated using specific parameter values for each of 74 crop/vegetation types specified in a database attached to the model. Vegetation in the model affects the hydrological cycle (e.g. cover-specific retention coefficient for surface runoff, leaf area index for transpiration) as well as the nutrient processes (e.g. loss by plant uptake, origin in plant residue).

Loads of nitrate nitrogen and soluble phosphorus in surface runoff, lateral subsurface flow and percolation are estimated as the products of the volume of water and the average concentration. Because phosphorus is mostly associated with the sediment phase, the soluble phosphorus loss is estimated as a function of surface runoff and the concentration of labile phosphorus in the top soil layer.

Water fluxes, nutrient dynamics and plant growth are calculated for every hydrotope. Then lateral fluxes of water and nutrients to the river network are simulated. The nutrients within surface flow, interflow, and base flow are subject to retention and decomposition processes, whose rate and intensity are described by special parameters (Hattermann et al., 2006). In the original model version water and nutrients are routed along the river network to the outlet of the simulated basin without any further transformation or retention after reaching the river system.

Additional information about model concept, input and output data, parameters, equations, as well as the GIS interface can be found in Krysanova et al. (2000).

5.3.2 SWIM model adaptation for in-stream processes

Modelling in-stream processes required several changes of the original SWIM code. Apart from implementing point source discharges to the river system or leaching and retention of soluble phosphorus through or inside soil layers as already described in Hesse et al. (2008), two major changes were required: 1) introducing an ammonium nitrogen phase in the model and 2) implementing riverine processes. These changes were done on the basis of newer versions of SWAT (Neitsch et al., 2002a) (as SWAT93 was the base for the SWIM model), adjusted by some individual equations, and will be explained in detail in the following sections.

Implementing ammonium cycle in soils The original SWIM model does not take ammonium into account. However, for simulating in-stream processes it was necessary to incorporate ammonium processes in the catchment as the ammonium pool is an important component in the in-stream nutrient cycle. Implementation of ammonium in soils was achieved using the approach of the SWAT model (Neitsch et al., 2002a) and the experiences and adjustments for the SWIM model developed by Voß (2007). An illustration of this new cycle in soils is given in Figure 5.2 (thick black lines are the new implemented parts), the mathematical descriptions of the different processes can be found in the Appendix (Table A5.1 and Table A5.2).

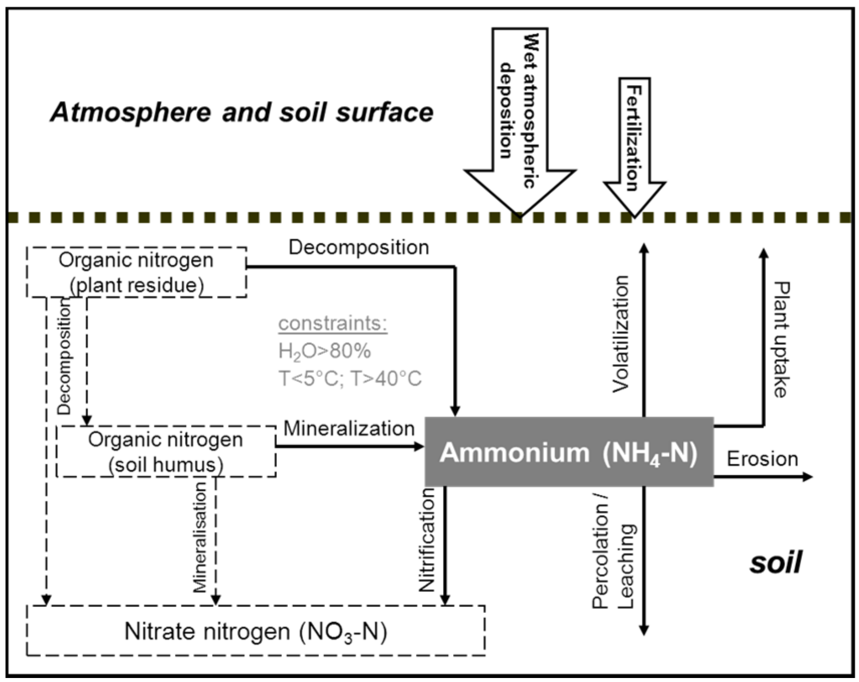

Figure 5.2 The new implemented ammonium cycle and influencing processes in the soils of the watershed (thick black lines) in connection with model variables and processes, already existing in the original SWIM code (thin dashed lines).

The ammonium nitrogen in soil is assumed to be originated in mineralisation and decomposition of organic nitrogen components such as plant residue or soil humus. In times when the water content is higher than 80% (close to anaerobic conditions) and the soil temperatures are outside of the interval between 5 and 40°C, ammonium emergence is expected (Scheffer & Schachtschabel, 2002; Werner, 1997). In this case 60% of the mineralised nitrogen from soil humus and 60% of the decomposed nitrogen from plant residue are added to the ammonium pool, whereas in cases of aerobic conditions and moderate temperatures no ammonium is accumulated. Apart from that, ammonium is added to the soil by fertilisation and wet atmospheric deposition (Werner & Wodsack, 1994).

The amount of ammonium in soil is reduced by several biological, chemical and/or physical processes. It is taken up by plants according to a demand and supply approach, whereas the demand is calculated by multiplication of the biomass increase with the optimal nitrogen concentration of the species. The crop is allowed to take nitrogen from all soil layers that have roots. Uptake starts at the upper layer and proceeds downward until the daily demand is met or until all nitrogen has been depleted (Krysanova et al., 2000). In this study it is assumed that the ammonium nitrogen demand is half of the total nitrogen demand. Uptake of nitrogen proceeds with nitrate and ammonium, and in case one of the pools is exhausted, the other one will be used.

Ammonium reduction can also take place as a result of erosion or leaching with soil water through the soil layers (Scheffer & Schachtschabel, 2002). But while leaching of nitrate nitrogen is coupled to the total amount of soil water flowing from a soil layer, the ammonium nitrogen behaves in a different way, as it is much less mobile due to its high bonding capacity to soil particles. To calculate leaching of ammonium, the ratio of the ammonium nitrogen concentration in the soil to that in soil water is considered. Due to its high ability of sorption to soil particles ammonium nitrogen in the upper soil layer is also subject to erosion processes, which can reduce the ammonium amount in the soils of the basin. The equation to calculate the loss of ammonium caused by erosion is based on a function of McElroy (1976) modified by Williams & Hann (1978).

The most important ammonium transformation processes in soils are nitrification (transformation to nitrate) and volatilisation of ammonium (transformation to gaseous ammonia), which firstly are simulated together, and then separated into the two processes. These processes are dependent of three soil characteristics: temperature, water content and depth represented by special coefficients (Neitsch et al., 2002a).

After simulating the ammonium cycle in a catchment the rest amount of accumulated ammonium, which is not taken up by plants or decomposed by transformation processes to nitrate nitrogen or ammonia gas, is added to the soil water flows and, after reaching the river, routed through the channel network and transformed by in-stream processes as described in the following section. The same as for nitrate nitrogen, it was assumed and implemented in the model that, while transporting with the different water flows (surface flow, subsurface flow and groundwater flow), the ammonium is subject to retention and/or decomposition processes, whose dimension can be customised within ranges by calibration of retention time and decomposition rate according to the equation presented in Hattermann et al. (2006).

Implementing in-stream processes The SWIM model (Krysanova et al., 2000) was extended with in-stream processes using the approach implemented in SWAT (Neitsch et al., 2002a) as well, in order to improve how river processes are reproduced. The algorithm used for the description of constituent interactions is based on that of the QUAL2E model (Brown & Barnwell, 1987). Now, the SWIM model takes several in-stream processes in the water body into account, driven by water temperature (as a function of mean air temperature of every subbasin according to the equation introduced in Stefan & Preud'homme (1993)) and light, and controlled by the concentration of algae (described by chlorophyll *a*) in the stream water body. Chlorophyll *a* is assumed to be directly proportional to the concentration of phytoplanctonic algal biomass and is calculated using the ratio of chlorophyll *a* to algal biomass. The new implemented in-stream transformation processes are graphically shown in Figure 5.3 and described mathematically in the Appendix (Table A5.3 and Table A5.4).

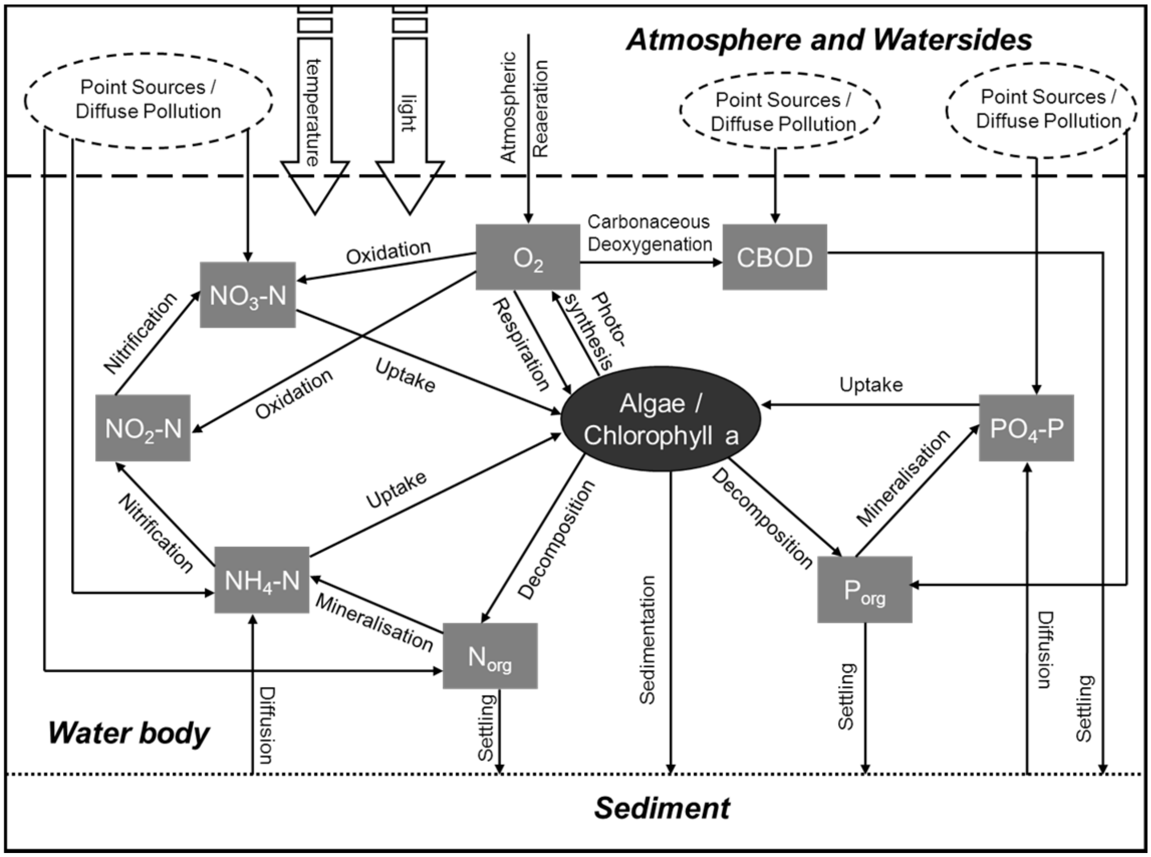

Figure 5.3 Scheme of the new implemented in-stream processes to the SWIM model.

Two different code versions to simulate in-stream processes are provided with the SWAT2005 code (http://www.brc.tamus.edu/swat/): the original one and a modification of it by van Griensven (2002), both based on the QUAL2E concept. We used the adapted version. The modification considered the closure of the mass balance equations in comparison to the original SWAT approach in order to close nutrient cycles, and to correct inconsistencies in the mass balance, which were criticised earlier by some water quality modellers (Horn et al., 2004).

Using the equations provided with the SWAT code and manual to simulate algal processes with SWIM returned quite good model outputs, but the Saale river's characteristic algal concentration peak in spring time could never be achieved, as all algal processes are coupled to temperature, which is highest in later summer. Hence, three additional assumptions were implemented in the model code: temperature stress (above a certain optimum temperature) and photoinhibition (above a certain optimum solar radiation) limiting algal growth in summer, as well as algal predation reducing algal concentration due to consumption (e.g. by zooplankton or benthic filterers).

Regarding the influence of temperatures on algal populations, Garnier et al. (1995) pointed out for the Seine river and its tributaries that growth may be inhibited when temperatures exceed a certain optimum. Similar behavior with an exponential increase in algal loss rate at temperatures higher than 20°C can be assumed for the Elbe river basin (Scharfe et al., 2009). Hence a slightly modified growth constraint was used for taking temperature stress into consideration, which is also implemented in SWIM for terrestrial vegetation (Krysanova et al, 2000). The temperature stress factor for algal growth TS_{alg} is calculated as an asymmetrical function, differently for temperatures below or equal to the optimal temperature T_{opt} in °C (no inhibition), and above it:

$$TS_{alg} = exp\begin{cases} 1 & \text{if } T_{wat} \leq T_{opt} \\ \left(ln(0.01) \times \left(\frac{T_{opt} - T_{wat}}{2 \times T_{opt} - T_{wat} - T_{bas} + 1 \times 10^{-6}} \right)^2 \right) & \text{if } T_{wat} > T_{opt} \end{cases}$$

where T_{wat} is the water temperature of the modelled subbasin channel in °C and T_{bas} the base temperature for algae population growth in °C. These temperature stress equations for algal population allow an unhindered growth of the algae for temperatures below the optimal temperature, but a very rapid decrease in algal growth rate with temperatures above it.

Another possible mechanism reducing algal growth and photosynthesis could be photoinhibition, which can be often observed in large rivers (Mischke et al., 2005). Very intensive radiation can harm the photosynthetic reaction center of the photosystem II, which leads to a light-induced reduction in the photosynthetic capacity of the algae, especially in shallower, slowly flowing rivers. Consequently, impoundments of rivers are negative for these effects and photoinhibitoring conditions occur similar to those in lakes (BfG, 1996), as one could also expect for the heavily dammed Saale river. The photoinhibition factor PI_{alg} was represented by a growth constraint according to temperature stress equations explained above, but replacing T_{opt} and T_{bas} with Rad_{opt} and Rad_{bas} (meaning the optimal and base radiation for algal population growth in ly) compared to the daily radiation of the subbasin (Rad_{sub}):

$$PI_{alg} = exp\begin{cases} 1 & \text{if } Rad_{sub} \leq Rad_{opt} \\ \left(ln(0.4) \times \left(\frac{Rad_{opt} - Rad_{sub}}{2 \times Rad_{opt} - Rad_{sub} - Rad_{bas} + 1 \times 10^{-6}} \right)^2 \right) & \text{if } Rad_{sub} > Rad_{opt} \end{cases}$$

Regarding the consumption of algae in large rivers, several papers point out that grazing can have significant effects on algal biomass in rivers, even though it is less pronounced than in lakes (Garnier et al., 1995; Scharfe et al., 2009; Viroux, 1997). Several effects can impact the phytoplankton and zooplankton interactions (e.g. rotifers and benthic filter feeders) and complicate their interpretation (Gosselain et al., 1998). Nevertheless, when simulating phytoplankton composition and biomass, zooplankton (or other consumers) grazing can not be neglected: This can be a key factor involved in the “summer decline” of phytoplankton biomass in rivers, as long as phytoplankton consists mostly of small, edible algae (Everbecq et al., 2001), and rotifer reproduction in the main channel of large rivers were able to generate abundances comparable to those reported in stagnant water bodies (Holst et al., 2002). Because zooplankton and filter feeder data was not available, a detailed formulation of consumer population as a model variable was excluded. However, there is a possibility to describe algal predation rate without directly modelling zooplankton and filterers by linking the predation rate of the algae PR_{alg} with water temperature and algal biomass (Ji, 2008):

$$PR_{alg} = PR_{20} \times 1.24^{(T_{wat}-20)} \times \left(\frac{algcon}{aconc_{PR}} \right)^{0.1}$$

where PR_{alg} means the predation rate of the day in day^{-1}, PR_{20} being the predation rate in the water body at 20°C in day^{-1}, T_{wat} meaning the water temperature in °C, algcon being the algal biomass concentration at the beginning of the day in mg L^{-1}, and $aconc_{PR}$ representing the reference algal concentration for predation in mg L^{-1}.

Hence, the equation to calculate the amount of algae in a river taken from the SWAT code (see Table A5.3 in the Appendix) was adjusted for the Saale river as follows:

$$algae = algcon + \begin{pmatrix} \left(PI_{alg} \times TS_{alg} \times \mu_a \times algcon\right) - \left(\rho_a \times algcon\right) - \\ \left(\frac{\sigma_1}{depth} \times algcon\right) - \left(PR_{alg} \times algcon\right) \end{pmatrix} \times TT$$

where the first term is representing algal growth limited by light and temperature inhibition, the second term being the algal death component, the third term calculating algal settling, and the last term representing algal loss by grazing. The abbreviations are described above or can be found in Table A5.4.

All in-stream processes are controlled by a large amount of global or subbasin-specific variables and constants, which can be used within predefined ranges for calibration of the model (compare with Table 5.3).

5.3.3 Method used for sensitivity analysis

The sensitivity analysis was performed to find a measure for the influence of the different model parameters on the model variables to facilitate calibration of the SWIM model with implemented in-stream processes. Model parameters with a high sensitivity on the model results have to be calibrated very carefully, whereas other parameters with low or even no sensitivity can be used without calibration. This could help to reduce the amount of necessary model runs for calibration.

The local sensitivity S was calculated with a method found in Lindenschmidt (2005) using the equation

$$S = \frac{\partial O}{\partial P} \times \frac{P}{O} = \frac{(O_x - O_{base})}{(P_x - P_{base})} \times \frac{P_{base}}{O_{base}}$$

where P means the input parameter values and O the model output values. A base run with the parameter settings P_{base} gives the output O_{base} which can be used to calculate the sensitivity after increasing or decreasing a parameter by a certain fraction x (designated as P_x) to return the resulting O_x.

Since $P_x = (1 + x) \times P_{base}$ the equation above reduces to

$$S = \frac{1}{x} \times \left(\frac{O_x - O_{base}}{O_{base}}\right)$$

The sensitivity analysis in the Saale catchment was performed for the time period 1991 to 2003 for each of the 36 new model parameters with four different x values (+/-0.1 and +/-0.2 to be consistent with +/-10% difference and +/-20% difference) using the limiting nutrient option to calculate algal growth. Sensitivity was then calculated four times by comparing the basic model output with the average model output of a certain substance at the model outlet after changing the parameter. In the last step the four (slightly) different sensitivities per substance and parameter were averaged to receive the resulting sensitivity of the different model output substances against the new SWIM model parameters. These positive or negative sensitivities were visualised in a matrix diagram by drawing circles with areas representing the sensitivity value (Figure 5.4).

5.3.4 Criteria of fit used for evaluation of model results

To determine the quality of achieved model results different measures of accuracy can be used. Three of them were chosen for this study: the Nash-and-Sutcliffe-efficiency (NSE), the coefficient of determination (R^2), and the RMSE-observations standard deviation ratio (RSR).

The non-dimensional NSE (Nash & Sutcliffe, 1970) is a measure to describe the squared differences between the observed and the simulated values and is based on the dispersion of variates around the line of equal values. R^2 specifies the degree of collinearity between simulated and measured data (Moriasi et al., 2007). It describes the total variance in the measured data that can be explained by the model (Legated & McCabe, 1999). The RSR was developed by Moriasi et al. (2007) based on the recommendation of Singh et al. (2004). In order to develop a performance rating for the RMSE (Root Mean Square Error) value, this measure is divided by the standard deviation of all observed values.

Detailed equations describing the different model evaluation statistics can be found in the literature cited. Their general performance rating is listed in Table 5.2.

Table 5.2 Possible ranges and general performance ratings for the different model evaluation parameters including references.

	range	optimum	very good	good	satisfactory	unsatisfactory	reference
NSE	- ∞ to 1	1.0	> 0.75	> 0.65 to ≤ 0.75	> 0.5 to ≤ 0.65	≤ 0.5	Moriasi et al., 2007
R^2	0 to 1	1.0	≥ 0.75	≥ 0.5 to < 0.75	≥ 0.25 to < 0.5	< 0.25	Parajuli et al., 2009
RSR	0 to ∞	0.0	≤ 0.5	> 0.5 to ≤ 0.6	> 0.6 to ≤ 0.7	> 0.7	Moriasi et al., 2007

5.3.5 Scenario development and analysis

Keeping in mind the actual status of the Saale catchment regarding nutrient emissions and river morphology, as well as probable directions of climate changes in this region projected in scientific literature (Wechsung et al., 2005) and discussed by regional authorities (TMLNU, 2009), seven model experiments were elaborated to model the effects of possible management or future climate changes on the Saale water quality (see Table 5.4). Four scenarios are dealing with management changes (two of them assuming reduced emissions and two modified river morphology) by changing the corresponding input data for the reference period 1996-2003 and running the model again. The same was done regarding the climate change experiments. The climate inputs (precipitation, temperature and solar radiation) for this 8-years-period were each modified by a certain percentage or, respectively, by some degrees Celsius, the model was run, and the resulting model outputs were analysed. Hence, these model runs were not truly "future scenarios", but rather management and climate sensitivity experiments. Analysis of the results of the seven experiments was done by comparing the averaged model outputs for the reference period with the averaged model outputs after changing the corresponding input parameters. The differences are graphically shown in bar diagrams for each model experiment visualising the percental discharge and concentration changes.

5.4. Results and discussion

5.4.1 Sensitivity analysis

Figure 5.4 shows results of the sensitivity analysis as a matrix diagram. Here, the estimated sensitivities of the observed model output concentrations of nitrate nitrogen (NO_3-N), ammonium nitrogen (NH_4-N), phosphate phosphorus (PO_4-P), chlorophyll *a* (Chl-a) and dissolved oxygen (O_2) against the different model calibration parameters are presented by circles of different area: the larger the circle, the higher the sensitivity. The type of circles distinguishes a positive (solid line) and negative sensitivity (dashed line). A positive sensitivity means an increase of model output with increasing parameter value, whereas a negative sensitivity shows an increase in model output with decreasing parameter value.

It is apparent that the most sensitive parameters are the maximum specific algal growth rate μ_{max}, the optimal temperature for algal growth T_{opt}, the optimal radiation for algal growth Rad_{opt}, the algal respiration or death rate $\rho_{a,20}$, and the linear algal self-shading coefficient $k_{l,1}$. All these parameters have the largest influence on algal biomass (represented in the model by chlorophyll *a* concentration), and, in consequence, on the mean nutrient concentrations needed for algal growth as well. In accordance to the definition in the model on how the phytoplankton community is limited by phosphorus availability and prefers ammonium nitrogen as nitrogen source, these nutrients are most influenced by a change in biomass and, accordingly, show their highest sensitivity against the same parameters as chlorophyll *a*. Nitrate nitrogen, in contrast, is only marginally influenced by changes in new parameter composition.

The dissolved oxygen concentration is most influenced by processes producing (like photosynthesis or reaeration) or consuming oxygen (like respiration or nitrification), but the reaction rate is not as high as described before for other model outputs. A few parameters have no influence on model results and can be neglected during the model calibration.

5.4.2 Model calibration and validation

The model was calibrated and validated for the Saale catchment with data from its last water quality observation gauge Groß Rosenburg for the time periods 1996-1999 (calibration) and 2000-2003 (validation). After implementing in-stream process modules, the SWIM model produced quite good results with sufficient performances for the new introduced model variables (water temperature, dissolved oxygen and chlorophyll *a*) as well as for the nutrient loads and (partly) concentrations.

Along with their accuracy of fit, Figure 5.5 exemplifies model results in comparison with the measured data for the whole Saale basin at its last water quality gauge Groß Rosenburg. The monthly averaged observed and simulated values are shown for eight years of calibration and validation. The seasonal dynamics of water discharge, water temperature and water component loads are reproduced quite well, meeting the “peaks” and “valleys” in the majority of cases. These very sufficient results are described also by the three values for modelling performance calculated for the different substances and time periods. Concentrations are reproduced with less quality than loads. However, the simulated dynamics and levels reflect the observed values comparatively well.

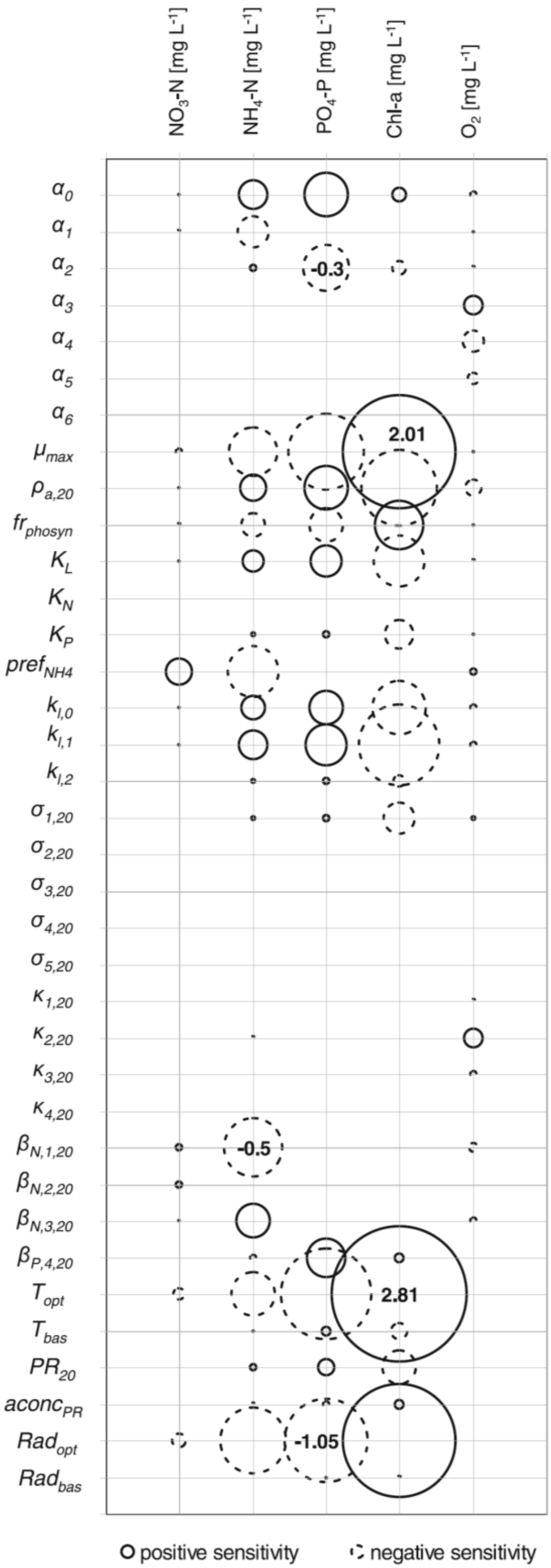

Figure 5.4 Sensitivity matrix of the different observed model output substances against the introduced new SWIM model parameters (the area of the circles represent the sensitivity value; for parameter descriptions see Table 5.3).

Very good results were achieved for water temperature, which is only a physical process taking into account measured mean air temperature per subbasin. The occurrence and amount of dissolved oxygen and chlorophyll *a* is influenced by many more processes and shows some discrepancies between measured and simulated values. Oxygen concentrations seem to be slightly overestimated in summer time, due to a big amount of biological and chemical processes taking place with higher temperatures, but showing a good reproduction of the seasonal dynamic. This dynamic is also simulated quite well for algae (chlorophyll *a*), but showing some differences between years. There is no clear seasonality in the phytoplankton growth, but one can always find a decrease in biomass between a spring and an autumn algal peak, which was also simulated by the model after taking into account possible influences by temperature, light and grazers.

As the measured data of nitrate and phosphate concentrations do not show a clear seasonality, it is difficult to reproduce the observations with the model. In terms of nitrate nitrogen, it seems that the concentrations are partly overestimated in years or winters with lower discharge, whereas the simulated concentrations are lower than the measurements in times of very high discharge (leaching and/or dilution processes are overestimated by the model). The ammonium loads and concentrations show a clear decreasing trend during the calibration period, which could be partly reproduced by the model assuming a higher amount and influence of point sources on ammonium occurrence in the 90-ies. This assumption seems to be quite realistic when looking at data from water treatment plants before and after upgrading the facilities, where a reduction to one hundredth of the emitted ammonium loads to the discharge system were observed (Ziemann, 2001). The lowest phosphate loads and concentrations can be observed in times with high algal biomass in summer (due to phosphate being the most important nutrient for phytoplankton). Times with phosphate concentrations close zero, often very short, were reproduced quite well by the model.

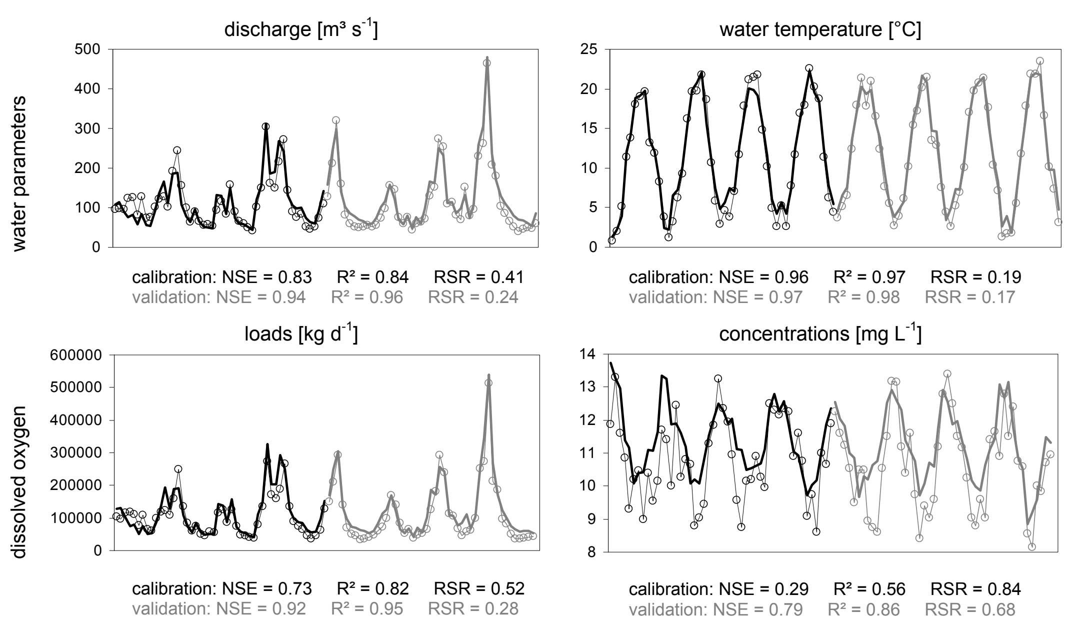

Figure 5.5 (start) for description see below

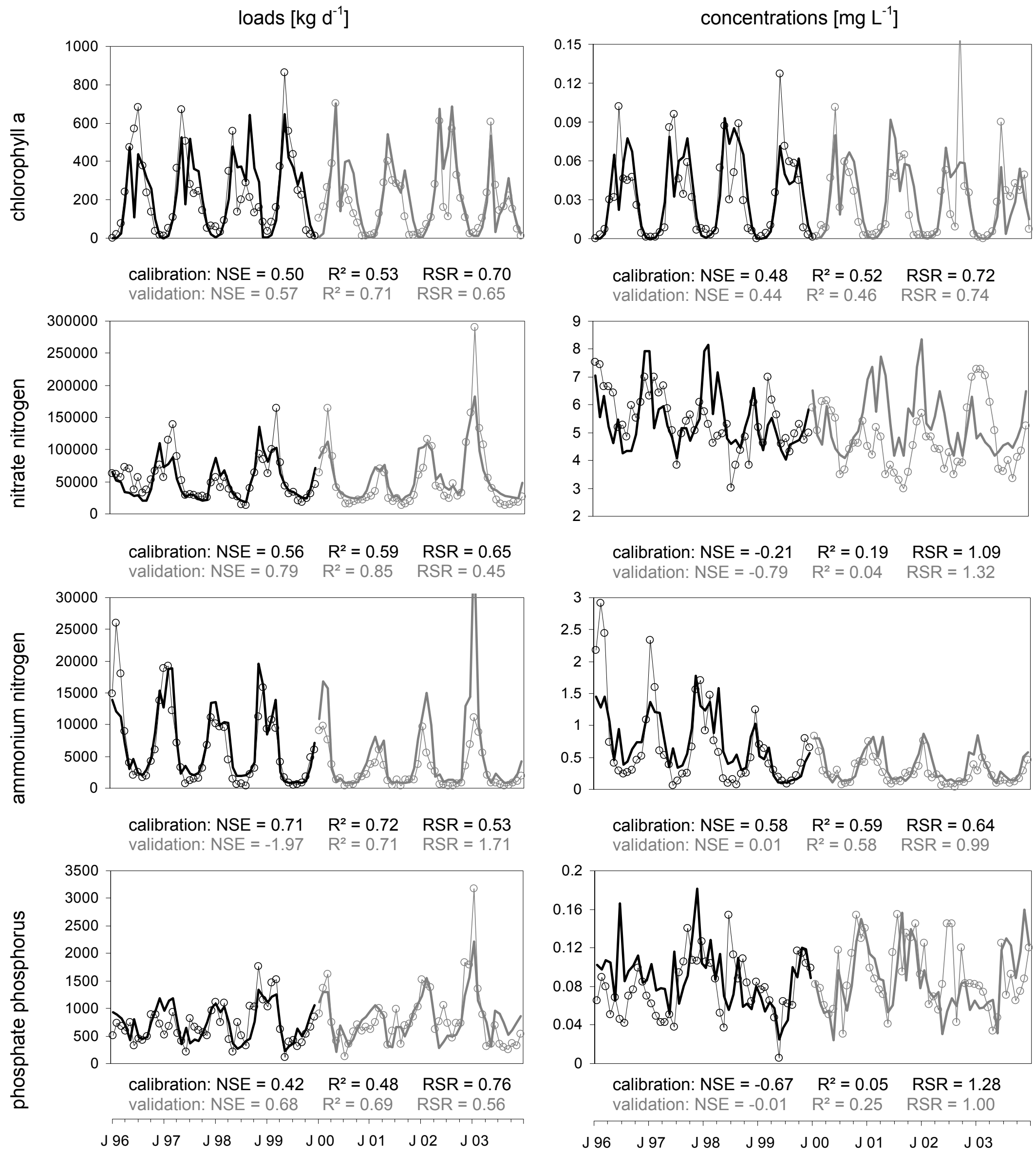

Figure 5.5 (continuation) Model results for the whole Saale basin (gauge Groß Rosenburg) for the calibration period 1996-1999 (black) and the validation period 2000-2003 (grey): monthly averaged measured values (thin lines with points) and simulation results (thick lines) together with their accuracy of fit for discharge, water temperature and the loads and concentrations of the different water quality components under observation.

Figure 5.6 shows the same water and water quality parameters as illustrated in Figure 5.5, but now averaged per month for the whole simulation period of eight years together with their standard deviation of these monthly averages. Nitrate nitrogen, ammonium nitrogen and phosphate phosphorus are also plotted in comparison to model results, which were achieved with the same model code and parameter set, but with switching-off in-stream processes. Chlorophyll *a*, dissolved oxygen, and water temperature as new model components are compared only with the measured data.

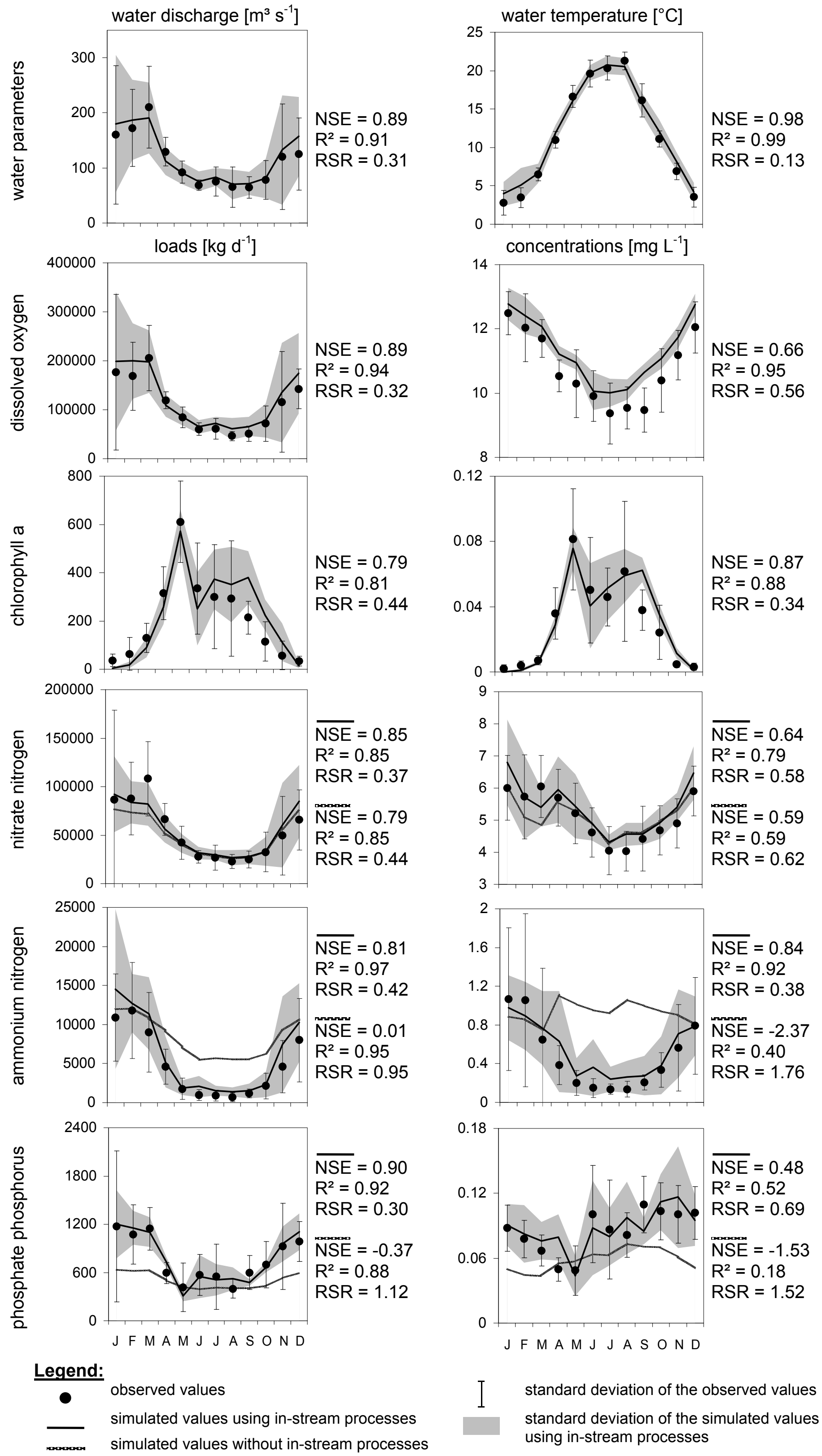

Figure 5.6 Monthly averages of the observed (points) and simulated (lines) water discharge, water temperature, and loads and concentrations of the different water components under observation for the 8-years-simulation period 1996-2003 (with a daily time step) at the Saale gauge Groß Rosenburg together with their accuracy of fit and standard deviation intervals; NO_3-N, NH_4-N and PO_4-P in comparison with model results achieved with in-stream processes switched off.

Looking at the graphs and the parameters for accuracy of fit, water discharge, temperature, and loads consistently show very good model performances. The seasonality of the substances and parameters under observation were reproduced in all cases. The spring peak of chlorophyll *a* and the corresponding sharp decrease of phosphate phosphorus have been simulated especially well. To achieve such results the three new implemented growth constraints additional to the original SWAT code were necessary. Only assuming temperature stress and photoinhibition after the spring peak, enabled the model creating a chlorophyll curve representing the measured data. Looking at the concentrations, a slight overestimation of dissolved oxygen during the year and of ammonium nitrogen in summer time is discernible. But the curve progression of all substances meets the observed curves very well with good or at least satisfactory performance.

When comparing model results with and without in-stream processes, the highest influences of algal growth on the nutrients composition in the water body can be seen for ammonium nitrogen and phosphate phosphorus. The seasonal dynamics of these main foodstuffs of phytoplankton were achieved very well with the new parameter set for calibration, whereas the “original” model results did not reflect the real situation. The very high ammonium concentrations in summer months modelled without riverine processes are the result of a constant assumption of point source emissions to the river network, influenced only by dilution processes. Although these emissions really have the highest influence on the total amount of ammonium in the river itself, the ammonium concentrations in surface water bodies clearly show higher variations than can be explained by discharge dynamics alone (Schröder & Matthies, 2002). Therefore, biological processes such as nitrification or uptake by plants cannot be neglected during ammonium simulation. In terms of phosphate phosphorus, in-stream processes can especially influence the sharp decrease in spring time very well, but they also lead to higher loads and concentrations during the winter months than modelled without riverine processes. This complies with the measured data and can be explained most likely by diffusion of soluble phosphorus from the sediments or mineralisation of organic material in the river, which lead to an increase of phosphate phosphorus. The higher amount of nitrate nitrogen in the river during the winter months can be explained by nitrification processes in time periods without ammonium consumption by algae, whereas ammonium is mostly ingested by algae before transforming to nitrate in summer months. Additional source of ammonium to be nitrified to nitrate nitrogen is provided by diffusion from the sediments (was not considered in the former model version without the in-stream module).

Although the model was calibrated looking only at the results and measurements at the outlet of the Saale basin, a comparisons of the simulated and observed values for nutrient and chlorophyll *a* concentrations at several intermediate gauge stations of the catchment shows sufficiently good results as well. This can be seen in Figure 5.7 presenting the comparison of average results in longitudinal direction of the Saale river and for its main tributaries, as well as the comparison of seasonal dynamics for selected gauges and components.

Table 5.3 lists all new implemented calibration parameters together with their ranges/values recommended by SWAT (Neitsch et al., 2002b), and the final used values for the Saale basin in this study. Some deviations have to be stated, where the calibrated parameters did not fit to the suggested ranges, mainly with regard to the benthic source rates of ammonium and phosphate, the nitrification and mineralisation rates, the algal growth rate, and fraction of nitrogen in algal biomass. However, the calibration results for the two last-mentioned parameters correspond to other model experiences for the lower Saale reach (Lindenschmidt, 2005), where some measured values of nutrient concentrations could only be achieved by increasing growth rate of phytoplankton to 4 d^{-1}, and where nitrogen-to-carbon ratio was calibrated to a similar value of 0.293 mg mg^{-1}. The organic nitrogen mineralisation rate at 20°C is similar for both model approaches as well (0.075 and 0.057 d^{-1}) notwithstanding the recommended SWAT ranges. Nevertheless, some differences can be seen for a couple of values, which require additional tests, not only virtual by a model but also physical by measurements in the study area, maybe also correcting the recommended ranges.

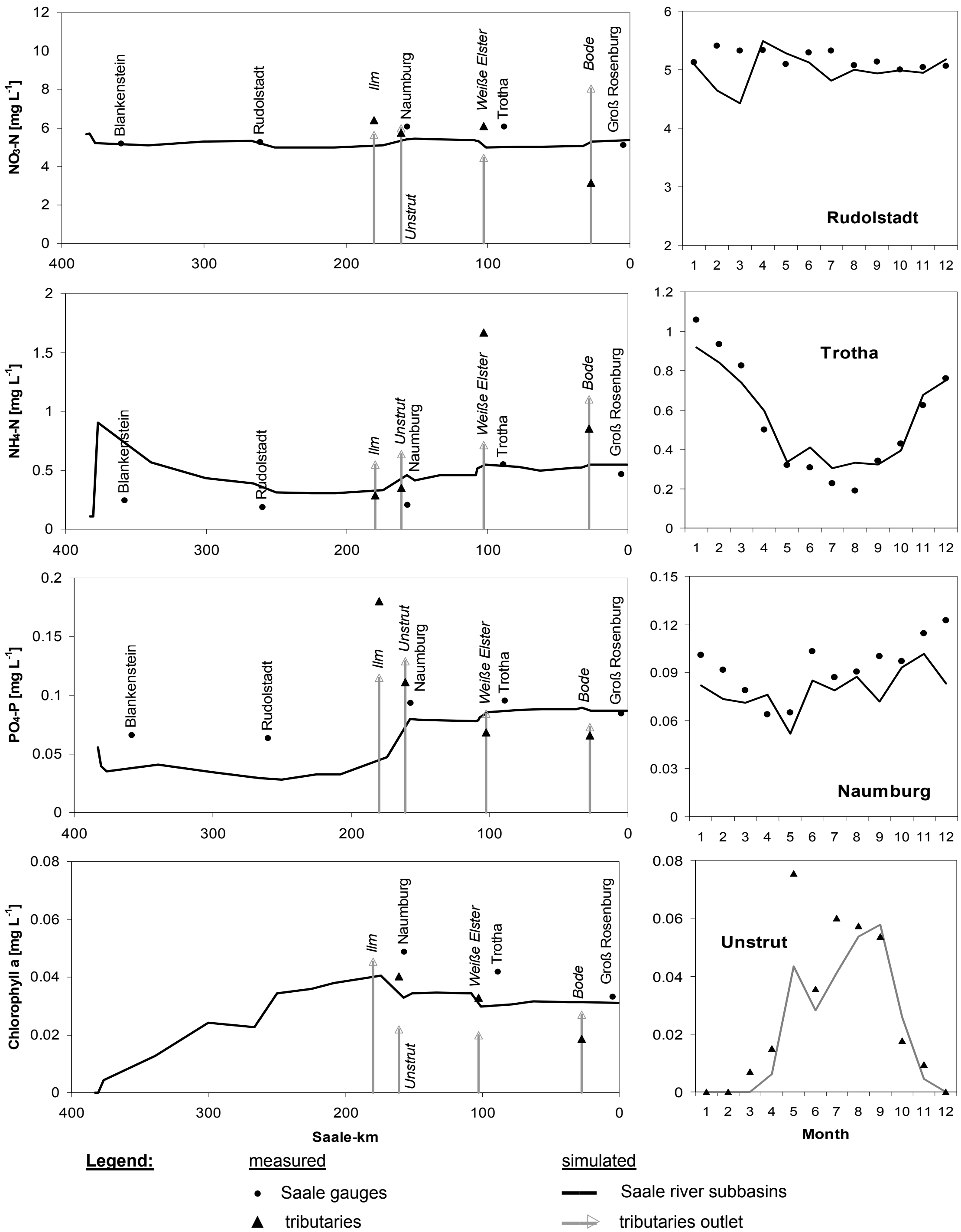

Figure 5.7 Longitudinal model results in comparison with measurements at intermediate observation stations of the Saale river and at the outlets of main tributaries averaged for the simulation period 1996-2003 (left); as well as the monthly averages for the simulation period 1996-2003 showing seasonal dynamics at selected stations/rivers (right).

Table 5.3 Calibration parameters of the in-stream submodel, their ranges suggested by the SWAT manual (Neitsch et al., 2002b), and the final values chosen during the calibration process.

parameter	unit	definition	SWAT range	value
α_0	µg mg^{-1}	ratio of chlorophyll *a* to algal biomass	10 - 100	10
α_1	mg mg^{-1}	fraction of algal biomass that is nitrogen	0.07 - 0.09	0.2
α_2	mg mg^{-1}	fraction of algal biomass that is phosphorus	0.01 - 0.02	0.01
α_3	mg mg^{-1}	oxygen production rate per algal photosynthesis	1.4 - 1.6	1.2
α_4	mg mg^{-1}	rate of oxygen uptake per unit of algal respiration	1.6 - 2.3	2.3
α_5	mg mg^{-1}	rate of oxygen uptake per unit of NH_4-N oxidation	3.0 - 4.0	4.0
α_6	mg mg^{-1}	rate of oxygen uptake per unit of NO_2-N oxidation	1.0 - 1.14	1.1
μ_{max}	day^{-1}	maximum specific algal growth rate	1.0 - 3.0	4.0
$\rho_{a,20}$	day^{-1}	algal respiration or death rate at 20°C	0.05 - 0.5	0.05
fr_{phosyn}	-	photosynthetically active fraction of solar radiation	0.01 - 1.0	0.8
K_L	kJ (m^2 · min)$^{-1}$	half-saturation coefficient for light	0.2227 - 1.135	0.2227
K_N	mg L^{-1}	half-saturation constant for nitrogen	0.01 - 0.3	0.01
K_P	mg L^{-1}	half-saturation constant for phosphorus	0.001 - 0.05	0.001
$pref_{NH4}$	-	algal preference factor for ammonia	0.01 - 1.0	0.999
$k_{l,0}$	m^{-1}	non-algal portion of the light extinction coefficient	1	1.0
$k_{l,1}$	m^{-1} (µg L^{-1})$^{-1}$	linear algal self-shading coefficient	0.0065 - 0.065	0.034
$k_{l,2}$	m^{-1} (µg L^{-1})$^{-2/3}$	nonlinear algal self-shading coefficient	0.054 or 0	0.054
$\sigma_{1,20}$	m day^{-1}	local algal settling rate in the reach at 20°C	0.15 - 1.82	0.15
$\sigma_{2,20}$	mg (m^2 day)$^{-1}$	benthic source rate for PO_4-P in the reach at 20°C	0.05	0.3
$\sigma_{3,20}$	mg (m^2 day)$^{-1}$	benthic source rate for NH_4-N in the reach at 20°C	0.5	0.05
$\sigma_{4,20}$	day^{-1}	rate coefficient for organic N settling at 20°C	0.001 - 0.1	0.001
$\sigma_{5,20}$	day^{-1}	organic phosphorus settling rate at 20°C	0.001 - 0.1	0.001
$\kappa_{1,20}$	day^{-1}	CBOD deoxygenation rate in the reach at 20°C	0.02 - 3.4	0.1
$\kappa_{2,20}$	day^{-1}	oxygen reaeration rate in the reach at 20°C	0.01 - 100	2.3
$\kappa_{3,20}$	day^{-1}	CBOD loss rate due to settling in the reach at 20°C	-0.36 - 0.36	-0.26
$\kappa_{4,20}$	mg (m^2 day)$^{-1}$	benthic oxygen demand rate in the reach at 20°C	2.0	2
$\beta_{N,1,20}$	day^{-1}	biological oxidation rate of NH_4 to NO_2 at 20°C	0.1 - 1	0.001
$\beta_{N,2,20}$	day^{-1}	biological oxidation rate of NO_2 to NO_3 at 20°C	0.2 - 2	0.002
$\beta_{N,3,20}$	day^{-1}	hydrolysis rate of organic N to NH_4 at 20°C	0.2 - 0.4	0.075
$\beta_{P,4,20}$	day^{-1}	mineralisation rate of organic P to PO_4 at 20°C	0.01 - 0.7	2.5
T_{opt}	°C	optimal temperature for algal growth	–	18
T_{bas}	°C	base temperature for algal growth	–	0.0
PR_{20}	day^{-1}	predation rate in the reach at 20°C	–	0.14
$aconc_{PR}$	mg L^{-1}	reference algal concentration for predation	–	0.06
Rad_{opt}	ly	optimal radiation for algal growth	–	360
Rad_{bas}	ly	base radiation for algal growth	–	0.0

5.4.3 River future: simulation experiments

The results of seven model experiments dealing with possible management and climate changes for the entire Saale basin can be seen in Figure 5.8, and a description of the experiments is listed in Table 5.4.

On the one hand, the management scenarios aim at reducing point and diffuse sources by minimising emissions from water treatment plants and industries, or from agricultural fields. In our study, a reduction of fertiliser rates by 20% was considered as a measure to reduce diffuse source emissions. Both options lead to a reduction of nutrient concentrations, but with different amounts. While the reduction of point sources has the highest influence on phosphate phosphorus concentrations in the river, the fertilisation reduction influences mainly nitrate nitrogen concentrations. This can be explained looking at the percentages of the three nutrients coming from point or diffuse sources (Figure 5.9). For nitrate, a reduction of point source emission has only little influence on the total resulting nitrate loads in the river, due to its predominant diffuse origin. Phosphate phosphorous loads, having on a contrary a high point source fraction, are more sensitive to changes in point source emissions and less sensitive to fertilisation variation. In general, a reduction of point sources seems to have a more direct and straightforward effect on the river system. A 20% decrease of phosphorus from point sources results in up to 20% reduction of phosphate phosphorus concentration in the river, whereas a 20% reduction of fertiliser decreases nutrient concentrations by no more than five percent. As a result of the decreased concentrations of nitrogen and phosphorus in the river water and the lowered food supply the chlorophyll *a* concentrations also decreased slightly, if only by about two percent.

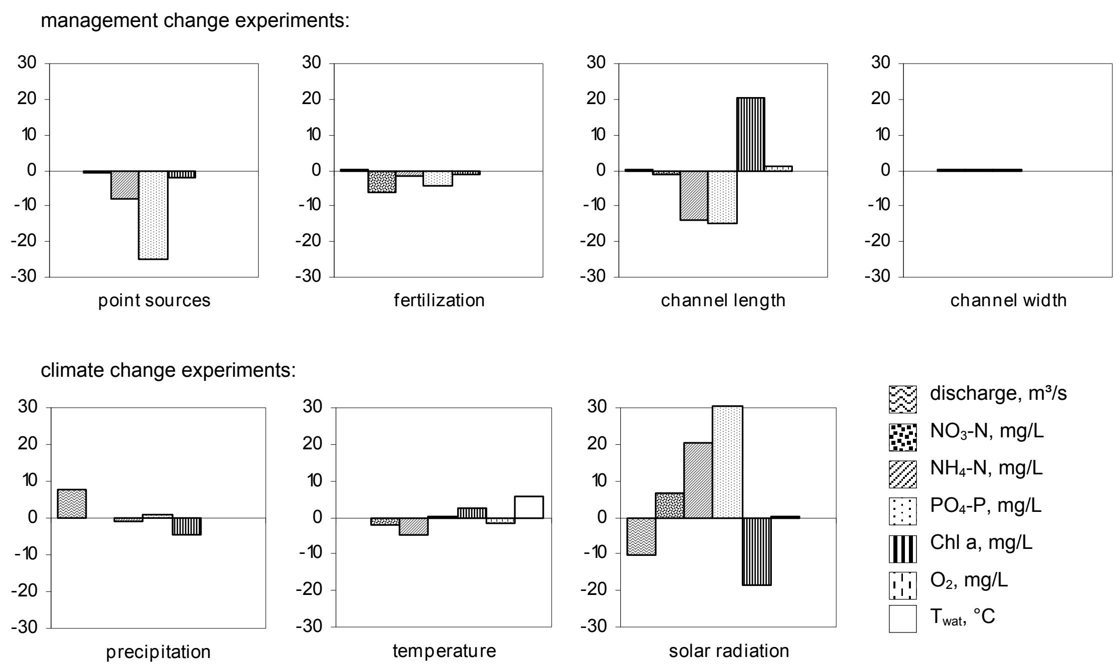

Figure 5.8 Influence of possible changes in management and climate on the model results with new implemented in-stream processes: Percental change of the averaged model outcome for the simulation period 1996-2003 assuming different possible future changes.

On the other hand, two other management experiments had aimed at improve river's morphology bringing it closer to the natural status: enlargement of the channel length and channel width was assumed. The results were different. An increase of all channel lengths by 20% resulted in a decrease of nutrient concentrations but in an increase of phytoplankton biomass. A possible explanation is that the algae has more time to grow in longer channels, as the water retention time rises and water velocity declines, and the growing algal biomass consumes more nutrients. In general, water flow velocity has a large influence on in-stream processes and biotic interactions, as it affects most of the primary factors influencing stream ecosystems (Horn et al., 2004). Thus, the model outcome is very sensitive to the changing channel length. The change in channel width, in contrast, had almost no influence on the observed concentrations of nutrients and phytoplankton. The detected changes are all lower than 0.1% with a tendency of declining chlorophyll *a* concentrations and increasing nutrient concentrations (due to lower consumption).

Table 5.4 Description of the seven different future experiments for the Saale river.

scenario name	description
point sources	reduction of all point source emissions (nitrogen by 10% and phosphorus by 20%)
fertilisation	reduction of all fertiliser amounts by 20%
channel length	extension of all channel lengthes per subbasin by 20%
channel width	enlargement of all channel widths per subbasin by 20%
precipitation	precipitation increase in winter times (October – March) and decrease in summer times (April – September) by 15%
temperature	temperature increase in winter/spring (January – June) by 1.5°C and in summer/autumn (July – December) by 0.5°C
solar radiation	solar radiation increase in summer times by 15%

The climate change experiments are based on research results for the Elbe basin, which project several changes in water balance, environment and society; partly due to changed climate conditions (Wechsung et al., 2005). Generally, the precipitation trends and projections show a high diversity. Jacob & Bülow (2005) expect an increase by 10% on average for the entire Elbe basin, with high spatial differences and a general increase in extreme events. Negative mean trends are expected for the eastern German part of the Elbe basin, with some increase in winter time and a strong decrease in spring and autumn (Reimer et al., 2005). In accordance with its location, an increase of precipitation in winter and a decrease in summer (each by 15%) were assumed for the Saale basin for the simulation experiments, which correspond to expected regional trends (TMLNU, 2009). On average, this assumption leads to an increase of water discharge (following the precipitation change due to higher absolute increase of winter precipitation than the absolute decrease in summer precipitation), while the chlorophyll *a* concentration declines and the nutrients show only very minor changes without a clear trend (as dilution and diminished uptake by algae are compensating each other).

As a result of assumed temperature stress and photoinhibition influencing algal growth, the phytoplankton population is very sensitive against changes in temperature and solar radiation. According to literature, a general increase in annual mean temperature by about 1°C for the Elbe basin can be expected, but the increase in winter/spring is higher than that in summer/autumn (Jacob & Bülow, 2005). Therefore, the increase of mean air temperature for the simulation experiment was distinguished into 1.5°C in winter and 0.5°C in summer. These assumptions resulted in an increase of water temperature by almost 6% (corresponding to +0.7°C). The phytoplankton biomass increases as well, as its growth rate is augmented with a rising temperature, and the optimum temperature is not exceeded on average. In contrast, ammonium nitrogen and nitrate nitrogen concentrations decline due to higher consumption by an increasing algae biomass in summer and to influenced ammonium emergence in the soils of the basin in winter (which will be more often within the temperature interval of 5-40°C and restricting mineralisation of organic nitrogen to ammonium).

Regarding solar radiation in the Elbe basin Gerstengarbe & Werner (2005) suppose an increase in summer time due to enlarged sun-shine duration and diminished cloudiness. A model experiment assuming an increase by 15% in summer leads to a clear decrease of chlorophyll *a* concentration (due to photoinhibition) and reduced water discharge (due to increased evapotranspiration), and results in higher nutrient concentrations (summation effect of lower dilution and lower algal uptake).

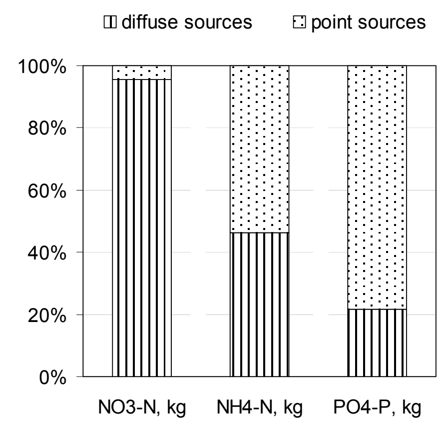

Figure 5.9 Origin of the nutrients from point or diffuse sources - Percental composition of nitrate, ammonium and phosphate loads at the Saale river outlet calculated by the model for the period 1996-2003.

The results of the river future experiments demonstrated here show the relative importance of physical boundary conditions on the amount and concentration of the phytoplankton. Mostly, river plankton is not nutrient limited, but rather strongly influenced by physical conditions, such as light, water residence time, flow velocity or temperature (Nixdorf et al., 2002). Mischke et al. (2005) rank the residence time of water among the most important control factors for algal growth. This can also be seen looking at the results of our simulation experiments. Changing solely the amount of nutrients in the river by influencing the point or diffuse emissions has only some effect on the chlorophyll *a* concentrations, whereas altered channel length, temperature or solar radiation changes this concentration more distinctly. Therefore, measures to improve water quality should always not only consider the nutrient input amounts and composition, but also the river morphology. Unfortunately, changing the river shape and boundary conditions are those measures, which are almost impossible for the local agencies (as for climate variations), or require application of complex and costly intervention measures. Taking this into account, it is recommended to focus on reduction of emissions, namely: lower rates of fertilisers adjusted to the plant requirements to reduce nitrate concentrations, and lower input from point sources to reduce phosphate and ammonium contamination.

5.5 Conclusion and outlook

Model results after implementing in-stream processes in SWIM show the high influence of riverine processes on the final model outputs at the basin outlet. The effect is pronounced especially looking at ammonium and phosphate concentrations, as these substances are supposed to be the favored or most limiting nutrients for the algae in the river. In time periods with a high algal population, these nutrients are diminished almost to zero, which is also partly reflected by observational data. Especially the ammonium nitrogen concentrations were simulated much better now, as the typical seasonal dynamic (peaks in winter and low amounts in summer time) was reproduced quite well now.

Our results differ from those of Migliaccio et al. (2007), who tested the usability of the in-stream kinetic functions of the SWAT model by switching them on/off or, respectively, loosely coupling the former SWAT with the stand-alone QUAL2E model, and found no significant statistical difference in the results generated. Possibly due to the additional assumptions regarding the algal growth equation implemented to the model code (which have a considerable influence on the model output), or even due to special characteristics of the modelled catchment (high amount of unfortunately constant point sources), the nutrient loads and concentrations in the study presented here show a different behavior using the new approach in contrast to the original SWIM version. The seasonal dynamics were reproduced much better than before, especially for substances whose absolute amounts are highly influenced by point source emissions.

Future modelling tasks regarding riverine nutrient processes should concentrate on including possible transformation processes in the river sediments, which were omitted up to now (e.g. denitrification has been identified as an important sink for nitrate nitrogen in parts of Saale tributaries (Wagenschein & Rode, 2008)). Furthermore, it could be helpful to use some of the calibration parameters with a spatial distribution to get better results for intermediate stations and to better represent the special behavior of nutrients in reservoirs or in lock and weir systems. Nevertheless, although it is indisputable that further investigations of the in-stream kinetic functions of the SWAT (and SWIM) model are necessary, as also expressed by different authors (Gassmann et al., 2007; Horn et al., 2004; Migliaccio et al., 2007), the new implemented in-stream processes already helped to improve the model results.

However, the question remains whether similar model results could also be achieved by simply using a riverine retention approach for nutrients introduced to the river network (as it is done in SWIM for all nutrient flows within the landscape), and/or by extended calibration of retention times and decomposition rates in the landscape. Additionally, more detailed data about amount and date of substances delivered by point sources to the surface water system, as well as their composition, would be very helpful.

One possible objection must be treated particularly seriously: the high amount of in their real dimension mostly unknown calibration parameters influencing each other. Several combinations could likely be used to achieve similar results at the end. So, it would be desirable to set realistic limits for these parameters based on real measured data in the river basin under study.

However, a higher amount of biological processes taken into account by a model may increase the number of influencing parameters rapidly, and this would complicate the calibration process. Therefore, it should always be well chosen, which processes and model versions are really necessary to answer the research questions. For example, an assessment of diffuse emission from agricultural fields in meso-scale river basins can also be performed successfully with the original SWIM version using the simple routing approach in the river. Nevertheless, for evaluating the resulting ecological status of the waterway, in-stream processes must not be neglected, especially for large, slow-flowing and phytoplankton dominated rivers.

The benefit of this new created model version is its ability to consider biological processes (also in the future). Only by knowing the perspectives of a river basin development, feasible measures can be evaluated and suggested to improve its ecological status and relevance. But algal growth and phytoplankton biomass are not the only aspects used to evaluate the status of flowing waters. Zooplankton, macrophytes and -invertebrates, fishes, river morphology, as well as flowing velocity are also important components. In case other indicators have to be considered in addition, some further steps in the model development should follow to extend the model predictability regarding biological processes.

CHAPTER 6

MODELLING NUTRIENT RETENTION PROCESSES IN WATERSHEDS

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Comparison of several approaches representing terrestrial and in-stream nutrient retention and decomposition in watershed modelling.
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Abstract

Retention and transformation of nutrients within a river catchment are important mechanisms influencing water quality measured at the watershed outlet. Nutrient storage and reduction can occur in soils as well as in the river and should be considered in water quality modelling. Consideration is possible using various methods at several points during modelling cascade. The study compares the effects of five different equation sets implemented into the Soil and Water Integrated Model (SWIM), one describing terrestrial and four in-stream retention with a rising complexity (including algal growth and death at the highest complexity level). The influences of the different methods alone and in combinations on water quality model outputs (NO_3-N, NH_4-N, PO_4-P) were analysed for the outlet of the large-scale Saale basin in Germany. Experiments revealed that nutrient forms coming primarily from diffuse sources are mostly influenced by retention processes in the soils of the catchment, and river processes are less important. Nutrients introduced to the river mainly by point sources are more subject to retention by in-stream processes, but both nutrient retention and transformation processes in soils and rivers have to be included. Although the best overall results could be achieved at the highest complexity level, the calibration efforts for this case are extremely high, and only minor improvements of overall model performance with the highest complexity were detected. Therefore, it could be reasoned that for some research questions also less complex model approaches would be sufficient, which could help to reduce unnecessary complexity and diminish high uncertainty in water quality modelling at the catchment scale.

6.1 Introduction

Within a watershed, retention of nutrients by physical, chemical and/or biological processes can take place during transport from agricultural areas to rivers in soils or riparian wetlands, as well as during routing and turnover in the surface water bodies themselves (such as streams, rivers, or lakes). These processes cause either a removal or a short- or long-term storage of nutrients, inducing a temporary or permanent reduction in the amount of nutrient concentration in river water or a delay in nutrient transport through the basin. Many authors (e.g. Kronvang et al., 1999; Hejzlar et al., 2009) refer to denitrification, sediment adsorption, and plant and microbial uptake as the main retention processes affecting nitrogen in watersheds. Phosphorus adsorbs to sediments, organic matter and clay particles or can be taken up by microbial biomass, followed by physical settling of these compounds. Therefore, deposition in water bodies and on flooded areas is usually mentioned as main reasons for phosphorus losses from river waters. Water residence time (lag time) in the river basin significantly affects retention of both nitrogen and phosphorus.

When modelling water quality of a river basin nutrient retention processes in the catchment cannot be neglected. Comparing the sum inputs (including diffuse and point source contributions) within a watershed to measured loads at the river outlet, many river basins demonstrate discrepancies in the amount and composition of nutrients (for an example see Table 6.1). Ignoring chemical fate and transport processes in rivers often leads to large errors in model output compared to observed values, which can partially be diminished by accounting for any kind of a retention process during the modelling procedure (Behrendt & Opitz, 2000).

Model research approaches using the ecohydrological model SWIM (Soil and Water Integrated Model; Krysanova et al., 2000) for several subcatchments of different sizes within the Elbe basin in Germany revealed as well that assuming only diffuse and point source emissions of nutrients to the river network and their simple routing cannot deliver efficient modelling results. Capturing retention, transformation and decomposition processes in the river was necessary to achieve sufficient and realistic outcomes. To accomplish this task, a simple decomposition equation for nutrients introduced to the river network by point source emissions was used during modelling (Hesse et al., 2008), or complex algae and nutrient cycles in the river channels were implemented (Hesse et al., 2012). The last approach required a lot of new, and often unknown, parameters and extensive additional calibration. Due to the limited new data, the uncertainty in the model results increased. A decision had to be made regarding which processes were pertinent to simulate and to achieve realistic results, because higher model complexity with a large number of calibration parameters considerably increases uncertainty of the model outcome (Snowling & Kramer, 2001; Adams, 2007). Using a simpler approach for simulating retention and transformation processes in the river might reduce uncertainty and support a more user-friendly handling.

With the analysis in hand, the significance of retention and transformation processes in the landscape and river network was tested by modelling the large-scale Saale basin in Germany using SWIM. One would expect that including complex in-stream processes in the model seems to be closer to nature than using a simple equation to represent river retention. However, the question arises, whether only such detailed description of in-stream processes allows to reproduce the measured concentrations and loads, or whether sufficiently good results can also be achieved using a simpler approach with less parameters. To answer this question, several methods representing nutrient retention processes in rivers were inter-compared, also in combination with the approach to simulate nutrient diminishment in the soils of the catchment.

Publications can be found regarding a comparison of methods and results achieved by different individual models dealing with water quality and nutrient retention in river basins (e.g. Horn et al., 2004; Migliaccio et al., 2007; Hejzlar et al., 2009). However, a comparison of modelling results, achieved by using several model approaches of different complexity implemented into one model, could not be found, but will be presented in this research study.

The objective of the study was to identify the level of model complexity necessary to realistically represent nitrogen and phosphorus in-stream behaviour during water quality modelling aiming in a decrease of complexity and high uncertainty within water quality modelling at the catchment scale.

6.2 Material and methods

6.2.1 The model SWIM and implemented retention approaches

General model description The ecohydrological model SWIM (Krysanova et al., 1998; Krysanova et al., 2000) was developed on base of the two models SWAT (Arnold et al., 1993) and MATSALU (Krysanova et al., 1989) to simulate hydrology, nutrients (nitrogen and phosphorus), vegetation and water quality at the regional scale using climate, soil and land use conditions as driving forces and considering feedbacks (Figure 6.1). Hence, the model is a suitable tool for analysis of climate and land use change impacts on hydrological processes, agricultural production and water quality. According to Pechlivanidis et al. (2011) the SWAT model (and therefore also the similar SWIM model) can be characterised as a “hybrid physically-based-conceptual model” aiming “to simplify model structure by representing some of the mathematical-physics based processes in a conceptual manner, particularly in cases where physical parameters are difficult to measure.”

SWIM is a spatially semi-distributed dynamic model working with a daily time-step. It is connected to an interface of a Geographic Information System (GIS), which is used for model set-up and extraction of spatially distributed information and routing structure. The spatial aggregation units are subbasins derived from elevation data, which are additionally subdivided into hydrotopes by overlaying subbasin, soil, and land use maps of the modelled basin. Vertically up to 10 soil layers can be considered. It is assumed that hydrotopes behave in a similar way regarding water, vegetation, and nutrient cycles. Water fluxes, plant and nutrient dynamics are calculated on the hydrotope level, aggregated at the subbasin scale, and finally routed from subbasin to subbasin to the basin outlet taking into account transmission losses.

Simulation of hydrological processes is based on the water balance equation taking precipitation, snow melt, evapotranspiration, percolation, surface and subsurface runoff, capillary rise and groundwater recharge into account. Driven by climate conditions, vegetation needs, soil layering and soil characteristics of the corresponding hydrotope, water flows through the soil surface, the root zone, and contributes to the streamflow as surface, subsurface, or groundwater flow.

For calculation of the potential evapotranspiration the Priestley-Taylor-method is used, which is based only on solar radiation and air temperature as input data. Actual evaporation from soil and transpiration by plants are calculated separately. The snow melt component of the standard

SWIM version is a simple degree-day equation. Estimation of surface runoff is done by a non-linear function of precipitation and a retention coefficient (depending on soil water content, land use and soil type) as modification of the Soil Conservation Service (SCS) curve number method (Arnold et al., 1990) adapted to German conditions. Percolation and lateral subsurface flow are calculated together. In case the soil layer storage exceeds field capacity after percolation calculations, the water flows laterally and is accumulated at subbasin scale. Water flow from subbasin to subbasin is calculated using the Muskingum flow routing method. Furthermore, the hydrological cycle is influenced by vegetation via cover-specific retention coefficients and transpiration processes.

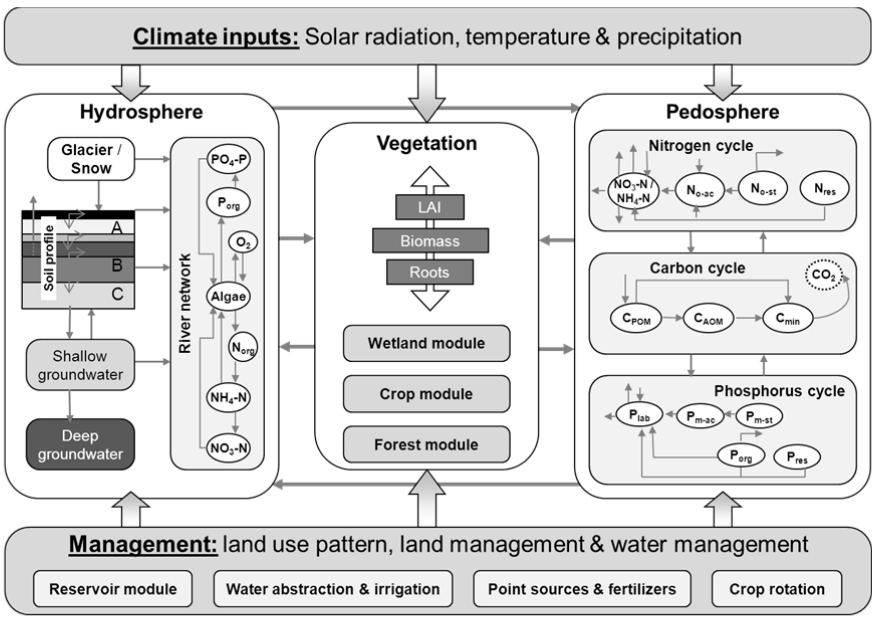


Figure 6.1 Conceptual diagram of the SWIM model showing compartments, processes and feed-backs included as well as driving forces and border conditions needed for model calculations.

The crop and vegetation module represents an important interface between hydrology and nutrients. Crop (e.g. summer barley, potatoes, maize, or winter wheat) and natural vegetation (e.g. grass, pasture, or broadleaf forest) are specifically parameterised (e.g. maximum leaf area index, maximum plant rooting depth, optimal nutrient content parameters, and harvest index dependent of accumulated heat units) and their dynamics are calculated using a simplified EPIC approach (Williams et al., 1984), where plant development and growth is based on such phenological descriptions aimed in enabling the parametrisation of the model at the regional scale. Crop type specific parameters for 74 crop/vegetation types were obtained in different field studies and collected in the database connected to SWIM (Krysanova et al., 2000; Neitsch et al., 2002b).

The nitrogen module for the soil layers includes several pools: nitrate nitrogen, active and stable organic nitrogen, and organic nitrogen in plant residues, as well as the flows: fertilisation, mineralisation, denitrification, plant uptake, input with precipitation, wash-off, leaching, and erosion. Two different pools are assumed to be sources for nitrogen mineralisation: crop residue and soil humus. The stable organic nitrogen pool is not subjected to mineralisation. Organic nitrogen flow between the stable and active pools assumes that the active pool fraction at equilibrium is 0.15. Nitrogen decomposition rate of residue is a function of the C:N and C:P ratios, soil temperature and water content. The latter two also influences mineralisation of active organic nitrogen. Denitrification occurs in times of oxygen deficit, which usually is associated with high water content in soil, and is a function of soil temperature and carbon content. Nitrogen uptake by plants uses a supply and demand approach and takes place from all soil layers that have roots. It starts at the upper horizon to proceeds downwards until the daily demand is met or until all nitrogen is depleted. The daily demand is calculated as a function of the optimal to the already accumulated nitrogen in the crop biomass at a specific growth stage. The amount of nitrogen lost from soil with surface, subsurface and groundwater flow is adjusted daily and defined to be the product of actual nitrogen concentration and total water loss of the day. To describe nitrogen soil processes in more detail, the ammonium nitrogen pool was added to the nitrogen cycle (Hesse et al, 2012) taking into account decomposition, mineralisation, nitrification, volatilisation, leaching, erosion, and plant uptake processes. In contrast to nitrate nitrogen the ammonium nitrogen leaching is influenced by its high adsorption potential to soil particles.

The soil phosphorus module is simulated in a similar way and includes the pools: labile phosphorus, the active and stable mineral phosphorus, the organic phosphorus and phosphorus in the plant residue, and the flows: fertilisation, sorption and desorption, mineralisation, plant uptake, erosion, and wash-off. The flows between the different phosphorous pools are governed by equilibrium equations. In contrast to the standard SWIM version the soluble phosphorous in this study is allowed to leach also vertically through the soil profile as a function of phosphorous concentration, the amount of leaving water and of the ratio between the phosphate phosphorous concentration in the soil to that in soil water (Hesse et al., 2008). While passing the soil layers the surplus phosphorous is added to the corresponding lateral water flows (interflow and base flow) to reach the river network.

The nitrogen and phosphorus substances transported with surface, subsurface and groundwater flows to the river network influence the resulting water quality at the basins outlet. During their passage through the catchment the nutrients are subject to varying retention and transformation processes in soils, wetlands and in the river system. As it is important for this study, these processes will be described in more detail in the following sections, although not all of them are included in SWIM by default.

Since the time of its development, SWIM has been applied and tested in river catchments of many sizes in several regions (e.g. Krysanova & Haberlandt, 2002; Habeck et al., 2005; Hattermann et al., 2005; Hesse et al., 2008; Huang et al., 2009; Yu et al., 2009; Martinkova et al., 2011). The model has been extended by different modellers in accordance with the particular research questions to improve its usability as a tool for impact assessment of climate and land use change (e.g. Hattermann et al. (2004) regarding groundwater dynamics, Wattenbach et al. (2005) regarding forest growth, Hattermann et al. (2006) regarding riparian zones and wetlands, Post et al. (2007) regarding carbon in soils, Huang et al. (2010) regarding snow melting in mountainous areas, and Hesse et al. (2012) regarding nutrient and algal in-stream processes).

Nutrient retention and decomposition in soils Nitrate nitrogen decomposition in soils of a watershed is strongly influenced by denitrification processes occuring in times when the soilwater content exceeds a certain threshold also depending on other environmental conditions such as carbon content or soil temperature; whereas ammonium nitrogen and phosphate phosphorus retention and leaching are mostly influenced by adsorption to the soil particles (whose intensity is defined in the model by the ratio of nutrient concentration in the soil to that in soil water). These processes are represented in the standard SWIM version.

In addition, retention of nutrients during their soil passage to the river network is included in the model (Figure 6.2a) using some first order kinetics as a parameter curve fitting procedure. The transport of nutrients from the agricultural land, grassland and forested land to the water bodies is coupled to the water flows from surface, subsurface and groundwater. The nutrients are subject to retention and transformation processes in the soil profile according to the geo-chemical conditions of the hydrotope. Therefore, the general retention of a nutrient in the landscape is a function of the mean residence time in the subsurface and the decomposition potential of the soil components.

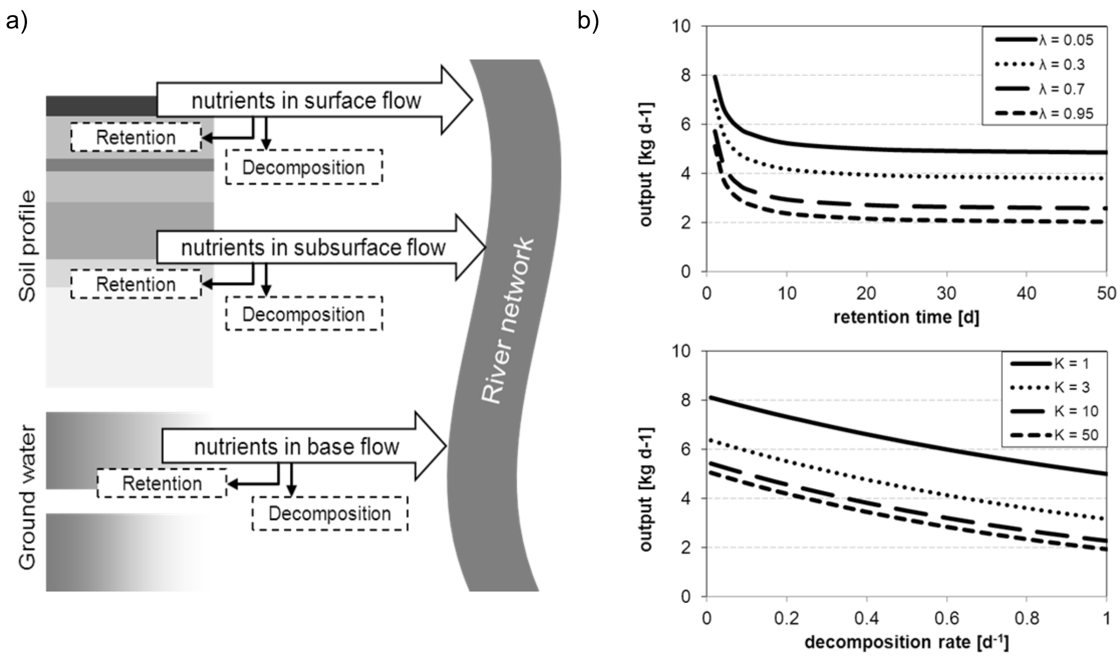


Figure 6.2 Landscape nutrient retention and transformation: (a) scheme illustrating processes consi-dered in SWIM (each simulated nutrient type follows these retention scheme separately), (b) nutrient output with water flow from a subbasin to the river as a function of retention time K with constant decomposition rate λ (above), and as a function of decomposition rate with constant retention time (below) assuming the input ($N_{t,in}$) of 10 kg d^{-1} and the previous output at the day before ($N_{t-1,out}$) of 5 kg d^{-1}.

Hattermann et al. (2006) introduced a retention function for nitrogen to the SWIM model to describe this behaviour mathematically, assuming a perfect mixture of the water volumes by diffusion and dispersion and a normal distribution of retention time and decomposition rate in the basin:

$$N_{t,out} = N_{t,in} \times \frac{1}{1 + K\lambda} \times \left(1 - e^{-\left(\frac{1}{K}+\lambda\right)}\right) + N_{t-1,out} \times e^{-\left(\frac{1}{K}+\lambda\right)}$$

where K is the mean residence time (d), and λ the decomposition rate (d^{-1}) of the specific nutrient (N) inflowing to (N_{in}) and outflowing from (N_{out}) a specific subbasin at the actual day (t) or the day before (t-1). Since SWIM distinguishes between nutrient fluxes in surface flow, interflow, and base flow, equation 1 is used basin-wide three times per nutrient with flux-specific parameters. In this study, the same equation was also used to simulate the ammonium nitrogen and phosphate phosphorus retention and transformation in the soils, each with specific coefficients. The effect of this retention equation on the modelled nutrient output with constant inputs is shown in Figure 6.2b.

Nutrient retention in rivers as a function of hydromorphology The chemical, physical, or biological transformation and/or decomposition processes in aquatic ecosystems are significant, because they influence nutrient transport in the river network, resulting in a delay, storage, or diminishment of the nutrient loads. The retention rate of a nutrient varies between 0 and 1 (meaning the percentage of the nutrient's load disappearing during river passage), and the remaining nutrient load can be described as the difference between the incoming and retained nutrient amounts. Consequentially, the effect of these retention processes on nutrients can be calculated according to the equation:

$$N_{out} = [1 - R] \times N_{in}$$

where R means the retention rate, N_{in} describes the incoming nutrients, and N_{out} the outflowing nutrients after retention impact.

Nutrient retention processes in water bodies can be linked to the morphologic and hydrologic characteristics of the river segments or embedded lakes. In general, wider water bodies with lower stream velocity increase the retention potential of a watercourse (as the sedimentation of particles with adsorbed nutrients is facilitated) with tendencies toward higher variations for phosphorous than for nitrogen due to the specific adsorption propensity and potential of each nutrient to suspended solids in the river water (Hejzlar et al., 2009).

In order to implement nutrient retention as a function of hydromorphology two different equations were tested. According to Grimvall & Stålnacke (1996), retention R_G is a function of stored water volume V and passing discharge Q (i.e. the hydraulic residence time) of a specific river reach segment and can be expressed as:

$$R_G = 1 - \frac{1}{1 + \tau \frac{V}{Q}}$$

where $\tau \geq 0$ represents an unknown calibration parameter. Equation (3) assumes a well and completely mixed water column. The resulting nutrient output as a function of water discharge and the calibration parameter τ is shown in Figure 6.3a. The most intense nutrient retention can be seen in cases with lower discharge and high parameter τ.

According to Doyle (2005), the portion of nutrients retained in a reach R_D is a function of discharge Q, length of stream reach L, mass transfer coefficient V_f, and channel morphology (dimensionless parameters a and b relating width to discharge):

$$R_D = 1 - \exp\left(-\frac{LV_f a}{Q^{(1-b)}}\right)$$

with similar effects (compared to the equation of Grimvall & Stålnacke (1996)) of a changing discharge or mass transfer coefficient on nutrient transport and output from a river reach (Figure 6.3b).

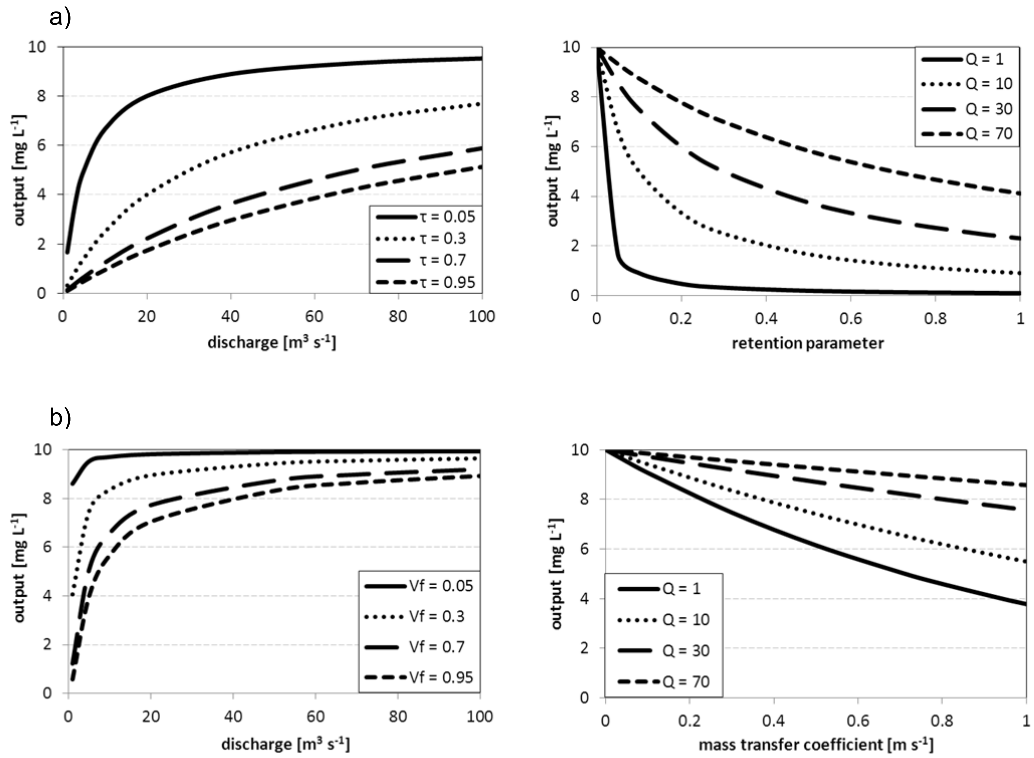


Figure 6.3 Effects of the hydro-morphological in-stream retention equations on nutrient concentrations assuming an input of 10 mg L^{-1}: (a) nutrient output from a river segment as a function of water discharge Q (left) and as a function of the retention calibration parameter τ (right) assuming the volume V of 100 m^3 using the equation of Grimvall & Stålnacke (1996); and (b) nutrient output from a river reach as a function of water discharge (left) and as a function of the mass transfer coefficient (right) assuming a length of 10 m, and constant parameters a and b of 0.3 using the equation of Doyle (2005).

Nutrient decomposition in rivers as a function of water temperature Besides the mainly physical retention processes linked to river hydro-morphology, the retention could also be linked to the water temperature, especially in regard to chemical and biological transformation processes. To model this behaviour in a simple way, a decomposition approach can be used, assuming nitrification from ammonium to nitrate and then loss of nitrate nitrogen and also loss of phosphate phosphorus (compare Figure 6.5a) as a function of water temperature. In this approach the nutrient retention time is coupled to the residence time of the river water and is not calibrated.

The mathematical description of the decomposition processes is the same for all substances, but with a nutrient specific decomposition rate δ (d^{-1}), which can be used for calibration. The coefficient D_T to describe temperature effects on nutrient degradation is introduced to the model related to river water temperature T_{wat} (°C) according to Whitehead et al. (1998):

$$D_T = \delta \times 1.047^{(T_{wat}-20)}$$

This coefficient is used to calculate the resulting nutrient amount N_{out} in the river segment using nutrient input N_{in} according to the equation:

$$N_{out} = N_{in} \times e^{(-D_T)}$$

Figure 6.4 illustrates the general effect of this equation on the model results. Nutrient losses are the most detectable and greater with higher water temperatures and decomposition rates.

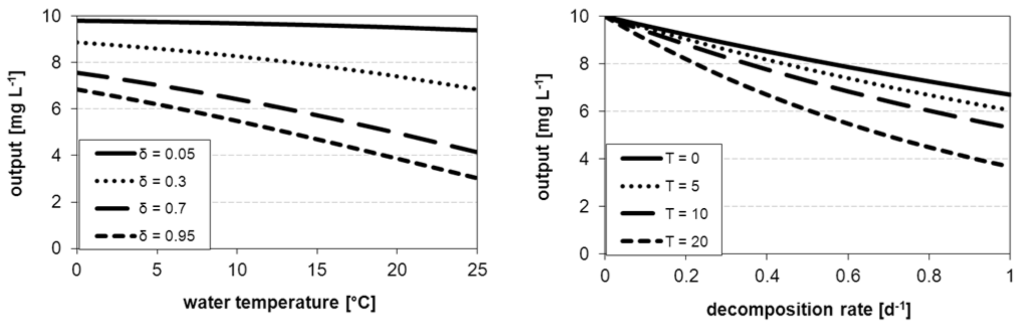


Figure 6.4 Nutrient output from a river segment according to the simple temperature related in-stream decomposition approach as a function of water temperature with constant decomposition rate δ (left), and as a function of decomposition rate with constant water temperature (T) (right) assuming N_{in} of 10 mg L^{-1}.

Detailed in-stream nutrient processes To describe the behaviour of nutrients in rivers, a model extension was introduced to the SWIM model using mainly in-stream equations of the SWAT model (Neitsch et al., 2002a) but extended by additional equations regarding losses of algal biomass caused by photoinhibition, temperature stress, and grazing (Hesse et al., 2012). As a result, the SWIM model now takes several in-stream processes into account, driven by water temperature and light and controlled by the amount of existing algae in the stream water body.

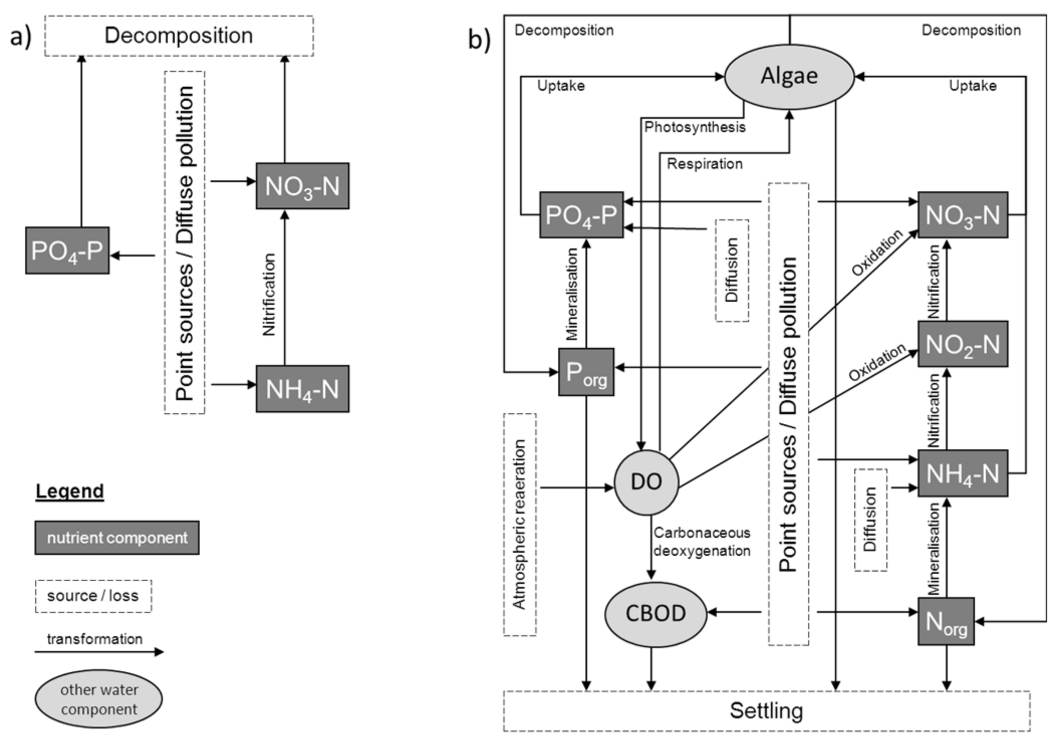


Figure 6.5 Comparison of nutrient processes considered for water temperature induced simple (a) and detailed (b) method to simulate nutrient cycles in the river network.

Besides the algal population, the in-stream components used for water quality calculations are: organic nitrogen (N_{org}), ammonium nitrogen (NH_4-N), nitrite nitrogen (NO_2-N), nitrate nitrogen (NO_3-N), phosphate phosphorus (PO_4-P), organic phosphorus (P_{org}), as well as dissolved oxygen (DO) and carbonaceous biological oxygen demand (CBOD). All these components are subject to different transformation processes and can influence each other (see Figure 6.5b and Hesse et al., 2012).

The rate constants (r) for the different processes (e.g. mineralisation, decomposition, or settling) are mostly adjusted to the local water temperature (T_{wat}) with different bases (B) and user defined local conversion rates at 20°C (κ, used for calibration):

$$r = \kappa \cdot B^{(T_{wat}-20)} \quad [1.024 \leq B \leq 1.074]$$

In relation to nitrification, the rate additionally depends on the in-stream DO concentration:

$$r = \kappa \cdot (1 - e^{-0.6 \cdot DO}) \cdot 1.083^{(T_{wat}-20)}$$

Hesse et al. (2012) includes full description of all equations used to simulate the detailed in-stream processes in SWIM.

6.2.2 Evaluation of model results

For calculating the performance ratings of achieved model results different measures of accuracy were used, taking into account only those days with available observational data within the period under investigation.

The coefficient of determination (R^2) specifies the degree of collinearity between the simulated and measured data (Moriasi et al., 2007) and describes the total variance in the measured data that can be explained by the model. The R^2 ranges from 0 to 1, higher values indicate better agreement. Although R^2 has been widely used for model evaluation, this statistic measure is oversensitive to extreme values (outliers) and is insensitive to additive and proportional differences between modelled and measured data (Legates & McCabe, 1999; Moriasi et al., 2007). Therefore, the R^2 cannot be used alone to describe the model accuracy and fit.

The percent bias (PBIAS) is also used to evaluate model results. It is a measure of over- and under-estimation of bias for predicted and measured values, expressed as a percentage (Gupta et al., 1999). PBIAS measures the average tendency of the simulated data to be larger or smaller than their observed counterparts. The optimal value of PBIAS is 0. Positive values indicate model bias toward underestimation, while negative values indicate model bias towards overestimation. The PBIAS should have values with a low magnitude.

The RMSE (Root Mean Square Error)-observations standard deviation ratio (RSR) was also described by Moriasi et al. (2007). This index criterion is used to quantify error in units of the variable being evaluated. To develop a performance rating for RMSE, it is divided by the standard deviation of the observed values. RSR incorporates the benefits of error index statistics and includes a scaling/normalisation factor so that the resulting statistic can apply to various constituents. The value of RSR ranges from 0 (perfect fit) to a large positive value (poor fit). The lower RSR, the better is the model simulation performance.

Predetermined levels of acceptable model performances for R^2, PBIAS, and RSR can be found in Moriasi et al. (2007) and Parajuli et al. (2009). In general, the rating should be done with a decreasing strictness looking at simulation results with an ascending complexity from river discharge, via nutrient loads to nutrient concentrations.

6.2.3 Calibration with PEST

The different model experiments were first calibrated manually to get optimal results before starting a final calibration run by dint of the PEST model (Model Independent Parameter Estimation; Doherty, 2005).

The PEST model is a standard software package for automatic parameter estimation and uncertainty analysis of complex environmental and other computer models. This package has been used in other watershed modelling studies (e.g. Doherty & Johnston, 2003; Liu et al., 2005; Doherty & Skahill, 2006). The PEST model writes model input files for the SWIM model by continuously changing the calibration parameters according to previously defined constraints within maximum and minimum values. Next, it compares the SWIM output files to the observed data, and then calculates statistics on the model performance and sensitivity, including correlation and covariances, for example, on the calibration parameters. The model continues until the optimal parameter combination is found, that provides the best model fit in terms of the weighted sum of squared differences between the simulated and measured values.

The PEST method for automatic calibration is based on the Gauss-Marquardt-Levenberg method of nonlinear parameter estimation and optimisation. This combines the advantages of the Hessian method and the steep descent method; as a result, a faster and more efficient convergence toward the objective function minimum is obtained (Baginska et al., 2003). In past studies, the results of automated calibration depended on the set of initial parameter values due to nonlinearity and high correlations between parameters within the model in use (Liu et al., 2005). In this study PEST was used to find the local optimum around an initial parameter set found by manual calibration.

6.3 Study area, data preparation and model setup

6.3.1 The Saale basin

The Saale river is a left tributary of the Elbe river with a catchment area of 24.167 km^2, a total river length of about 427 km, and an average discharge at its last gauge Calbe-Grizehne of 115 $m^3\ s^{-1}$ (FGG-Elbe, 2004b). The Saale catchment has lowland to low mountain range character with an altitude between 20 and 1140 m above sea level. Location and digital elevation model (DEM) of the basin are shown in Figure 6.6.

The climate is characterised by oceanic and continental influences. According to altitude and location, precipitation is heterogeneous and ranges from <500 (leeward areas and the central basin) until 1300-1600 mm y^{-1} (windward areas in the mountains). The central basin of the Saale catchment is one of the driest regions in Germany considering precipitation amount (Müller et al., 2001). For the time period 1996-2003 analysed in this study the average annual sum of precipitation for the entire Saale catchment is 628 mm y^{-1}; the average temperature covering temporal and spatial range is 9.1 °C.

Geographic, orographic and soil conditions are reflected in the land use patterns of the basin (Figure 6.6). Forests can be found especially in the mountain ranges (about 20% of the area).

The middle and lower courses of the Saale basin are characterised by wide and very fertile brown and loess soils (chernozems) used for agriculture (two thirds of the whole catchment). According to the land use map, only five percent of the basin is grassland. The Saale basin has a human population of about 4.2 million people (FGG-Elbe, 2004b). The settlements cover nearly 8.5% of the study area.

The Saale river has been drastically influenced by different hydraulic engineering measures during the last century (water reservoirs in the upper course, weirs and locks in the lower course) to enhance water availability and navigability and to use them as a “salt-load control system” by adding additional water during low flow conditions in order to dilute high salt concentrations in the downstream river reaches caused by mining and industrial activities in the catchment. Construction measures continue to have influences on water quality, discharge regime, structural diversity, particulate matter, and groundwater, affecting the vulnerability of the ecosystem (Rode et al., 2002).

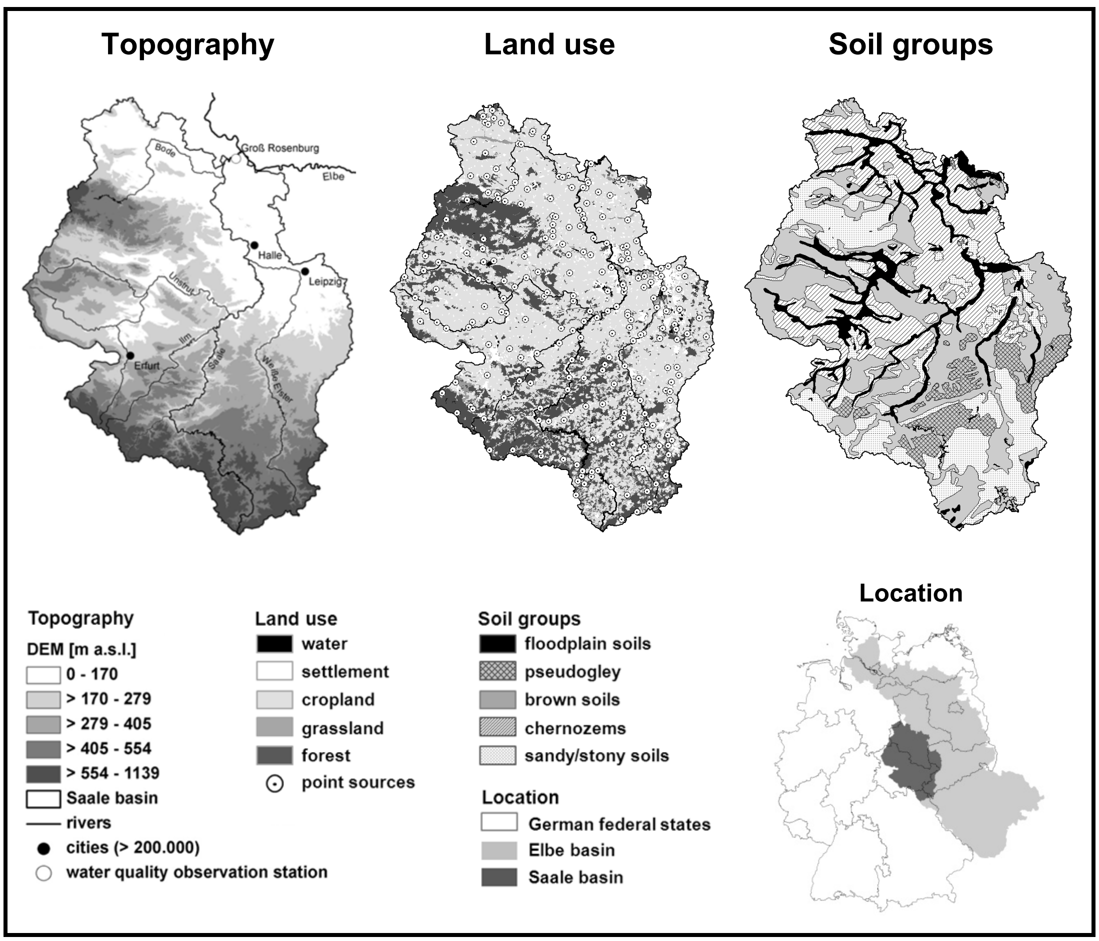


Figure 6.6 Location and natural conditions with anthropogenic influences of the Saale basin.

The water quality of the Saale river was considerably improved during the last two decades mainly due to better techniques in sewage treatment plants, and industrial enterprises as well as the closure of numerous industrial units (Lindenschmidt, 2005). However, there are still several industries in the Saale basin and, in conjunction with the intensive agricultural land use and the relatively high population density, the river and its flood plains are still suffering from nutrient, heavy metal, and salt pollution. The land use map in Figure 6.6 illustrates the high number of point sources in the Saale basin listed by the FGG-Elbe. According to these data, there is a total input of nitrogen to the river network of nearly 10.000 kg per day, and a total input of phosphorous of above 700 kg per day (FGG-Elbe, 2004b). However, nearly 70% of the nitrogen and phosphorus input to the Saale river system originates from diffuse sources (Behrend et al., 2001), which can be only hardly influenced by reducing fertiliser applications in agriculture with a considerable time-delay.

The resulting water quality can be evaluated by ranking the 90-percentiles of nutrient concentrations in water quality classes (LAWA, 1998). In accordance with this method, the water quality observation station Groß Rosenburg achieved the classes III (heavily polluted) regarding nitrate and ammonium nitrogen and the class II-III (critically polluted) regarding phosphate phosphorus (period 1996-2003).

Discrepancies between estimated point and diffuse nutrient emission amounts found in the literature and observed measurements at the river outlet identify gaps that point to retention processes occurring in the catchment and/or river network (Table 6.1).

Table 6.1
Comparison of total nitrogen (N) and total phosphorus (P) inputs to and outputs from the river network in the Saale basin for the time period 1998-2000, as well as the nutrient's natural background level.

	N [t a^{-1}]	P [t a^{-1}]
Background level (Behrend *et al.* 2003)	**4380**	**106**
Estimated input (Behrend *et al.* 2003)	**35150**	**2308**
point sources		
municipal	*4720*	*364*
industrial	*1390*	*21*
diffuse sources		
erosion	*1940*	*1194*
drainage	*7180*	*31*
atmospheric deposition	*520*	*10*
surface washoff	*190*	*59*
groundwater	*14770*	*105*
urban areas	*4430*	*518*
Measured output (LHW[a]) Groß Rosenburg	**25034**	**874**

[a] State Office of Flood Protection and Water Management Saxony-Anhalt

The ecological potential of the Saale river according EU-WFD (EC, 2000) is unsatisfactory and the environmental quality standards are not reached yet. This has negative impacts on the Elbe river, as its ecological status declines after the Saale river flows into it. Particularly, the nitrate nitrogen concentrations of the Elbe river are influenced by the confluence of the Saale river (Arge-Elbe, 2008). Additional measures to improve the ecological status of the Saale river are necessary to prevent further degradation. Water quality modelling of the catchment and improving the present models to minimise uncertainties is an important step towards water quality protection.

6.3.2 Data preparation

To generate the hydrotope classes, basin and routing structure and the attributes of subbasins and rivers, four different raster maps of the studied area are needed: elevation, subbasins, soil types and land use. For the Saale basin the DEM provided by the NASA Shuttle Radar Topographic Mission (SRTM), the Elbe subbasin map provided by the German Federal Environment Agency (UBA), the general soil map of the Federal Republic of Germany (BÜK 1000) originating from the Federal Institute for Geosciences and Natural Resources (BGR), and the land use map CORINE Land Cover 2000 prepared by order of the UBA by the German Aerospace Center (DLR), all maps with a resolution of 100 x 100 m, were used.

The model input requires daily data of minimum, maximum and mean temperature, precipitation, solar radiation, and air humidity. These data were provided by the German Weather Service (DWD). The values of 246 real climate observation stations located within and around the Saale basin (20 km buffer) were interpolated to the centroids of 263 subbasins by an inverse distance method.

Daily output and locations of municipal and industrial point sources were derived from one average annual data delivered by the River basin Community Elbe (FGG-Elbe, 2004b). So, the emissions were added to the daily water and nutrient amounts of the corresponding subbasins with constant values throughout the total modelling period. Due to the fact that only values of the total nitrogen and total phosphorus inputs per source (without differentiating into the single nutrient phases and without seasonal variations) were available, which were simply split into the different nutrient forms by equal amounts, these data have a high degree of uncertainty within the model simulations.

Fertilisation data and crop management represent the diffuse sources in the Saale basin. Fertilisation dates and amounts were derived according to regional conditions and regulations assuming a “good agricultural practice” (TLL, 2007).

The model was calibrated for water discharge and water quality using daily discharge and fortnightly to monthly water quality data of the gauge Groß Rosenburg at the watershed outlet. These data were provided by the State Office of Flood Protection and Water Management Saxony-Anhalt (LHW). Delivered concentration data named as “below the threshold of measurement” were assumed to be 50% of this quantification limit. The model was set up and evaluated for the time period 1996-2003 due to an obvious decreasing trend in ammonium emissions in the first half of the 1990s, which was not represented by available point source data.

After collecting the data, preparing the required model input files, and running the GIS interface, the model simulations were completed using a three-step modelling procedure of SWIM. First, water, nutrient and vegetation dynamics are calculated for each of the 5030 hydrotopes derived within the Saale catchment. Next, the outputs from these hydrotopes are used to calculate the area-weighted average to estimate the subbasin outputs. Finally, these outputs are calculated according to the routing structure of the basin, taking transmission losses into account.

In this study, for the comparison of different retention and decomposition approaches, the SWIM code was altered to simulate the different retention and decomposition methods, which can be turned on or off.

6.3.3 Design of model experiments and calibration parameters

The retention and decomposition methods described in section 6.2.1 were tested alone and in combinations to evaluate and compare the effects of these model approaches on model outputs regarding nutrient loads and concentrations at the outlet gauge of the Saale river (Groß Rosenburg) for an eight year time period, 1996-2003, with a daily time step. The numbering and composition of 12 different investigated model runs are presented in Table 6.2.

Table 6.2
Overview of the model experiments performed to test and to compare the effects of the retention and decomposition approaches on the model out-put. The Plus symbol (⊕) means process equation was turned on; the Minus symbol (–) means the process equation was turned off.

		Landscape Retention and Decomposition	**River** Retention R_G	**River** Retention R_D	**River** Decomposition D_T	**River** Detailed in-stream processes
Base	**B0**	–	–	–	–	–
Single model approaches	**S1**	⊕	–	–	–	–
	S2	–	⊕	–	–	–
	S3	–	–	⊕	–	–
	S4	–	–	–	⊕	–
	S5	–	–	–	–	⊕
Combined model approaches	**C1**	⊕	⊕	–	–	–
	C2	⊕	–	⊕	–	–
	C3	⊕	–	–	⊕	–
	C4	⊕	⊕	–	⊕	–
	C5	⊕	–	⊕	⊕	–
	C6	⊕	–	–	–	⊕

The base version (B0) with all possible retention processes turned off was run to visualise the overall influence of retention and decomposition processes in the soils and rivers as represented in SWIM nutrient outputs. Resulting nutrient loads and concentrations simulated with the B0 experiment show the probable nutrient output without any diminishing processes in the basin.

During the experiments with one retention approach either in the landscape or river network (S1 to S5) one of the five methods was on. Experiment S1 calculates nutrient retention in the soils of the catchment, but the resulting nutrient loads introduced to the river network are simply added and routed through the channels to the outlet of the basin. The experiments S2 and S3 neglect terrestrial nutrient retention, rather deal with nutrient retention in the river water as a function of hydromorphology according to Grimvall & Stålnacke (1996) (S2) and Doyle (2005) respectively (S3). The two last single model approaches S4 and S5 refer to nutrient decomposition processes in the river waters as a function of water temperature while ignoring soil retention potential: S4 deals with the simple approach, whereas S5 tests the influence of the stand-alone detailed in-stream processes on modelled nutrient loads.

After that, the combined simulation experiments were conducted (C1 to C6), in which terrestrial nutrient retention and decomposition was always included and supplemented by one or two nutrient transformation processes in the river. The C1 experiment combines soil retention potential and river retention according to Grimvall & Stålnacke (1996), whereas C2 assumes an additional nutrient retention in the river using the equation of Doyle (2005). C3 tests the influence of simple nutrient decomposition based on water temperature together with terrestrial retention on model output. Combinations of one simple river morphology dependent retention approach (R_G or R_D) with the river temperature dependent decomposition (D_T) were realistically the only reasonable river retention experiments to consider together in addition to the basic nutrient retention in soils (C4 and C5 respectively). The last combined model approach C6 assumes terrestrial nutrient retention together with a detailed nutrient cycle in the flowing water induced by temperature- and light-dependent algal and nutrient decomposition processes.

Table 6.3 SWIM calibration parameters regarding nutrient retention and decomposition together with their ranges defined for PEST calibration.

parameter	description	unit	min	max
Landscape retention and decomposition: *12 parameters (each per NO_3-N, NH_4-N, and PO_4-P)*				
K_{int}	retention time in interflow	d	1	500
K_{grw}	retention time in groundwater flow	d	30	5000
λ_{int}	decomposition rate in interflow	d^{-1}	0.001	0.5
λ_{grw}	decomposition rate in groundwater flow	d^{-1}	0.001	0.5
River retention R_G: *3 parameters (each per NO_3-N, NH_4-N, and PO_4-P)*				
τ	unknown calibration parameter	-	0.001	5.0
River retention R_D: *9 parameters (each per NO_3-N, NH_4-N, and PO_4-P)*				
V_f	mass transfer coefficient (benthic nutrient uptake rate)	d^{-1}	0.001	5.0
a	dimensionless parameter relating width to discharge	-	0.1	0.5
b	dimensionless exponent relating width to discharge	-	0.1	0.5
River decomposition: *3 parameters (each per NO_3-N, NH_4-N, and PO_4-P)*				
δ	nutrient decomposition rate in the river	d^{-1}	0.001	0.5
Detailed in-stream processes: *12 parameters*				
μ_{max}	maximum specific algal growth rate	d^{-1}	1.0	5.0
$\rho_{a,20}$	algal respiration or death rate at 20°C	d^{-1}	0.05	0.5
T_{opt}	optimal temperature for algal growth	°C	5.0	35.0
PR_{20}	predation rate in the reach at 20°C	d^{-1}	0.01	0.5
Rad_{opt}	optimal radiation for algal growth	ly	100	500
$\sigma_{1,20}$	local algal settling rate at 20°C	$m \cdot d^{-1}$	0.15	1.82
$\sigma_{3,20}$	benthic source rate for ammonium at 20°C	$mg \cdot (m^2 \cdot d)^{-1}$	0.05	0.5
$\beta_{N,1,20}$	rate constant for oxidation of NH_4 to NO_2 at 20°C	d^{-1}	0.001	1.0
$\beta_{N,2,20}$	rate constant for oxidation of NO_2 to NO_3 at 20°C	d^{-1}	0.002	2.0
$\beta_{N,3,20}$	rate constant for hydrolysis of N_{org} to NH_4 at 20°C	d^{-1}	0.04	0.4
$\sigma_{2,20}$	benthic source rate for dissolved phosphorus at 20°C	$mg \cdot (m^2 \cdot d)^{-1}$	0.05	0.5
$\beta_{P,4,20}$	rate constant for mineralisation of P_{org} to PO_4 at 20°C	d^{-1}	0.05	5.0

Table 6.3 gives an overview of the parameters used for calibration of nutrient transformation processes in landscape and rivers together with their minimum and maximum values defined from literature and used during the PEST calibration. Due to the aim of this study, only those parameters related to calibration of retention and transformation processes in soils and rivers are mentioned. Detailed explanations about hydrological modelling with SWIM (which had to be done in advance of this assessment) and most appropriate hydrological calibration parameters can be found in Krysanova et al. (2000) or Hattermann et al. (2005).

6.4 Results and discussion

As introduced in Table 6.2, 12 model runs were performed in order to test the influence and effects of five different nutrient retention and decomposition approaches and their combinations on the modelling results. The results are presented in Figures 6.7 to 6.12.

6.4.1 Simulation results: visual representation

The seasonal dynamics (mean monthly averages) for eight analysis years 1996 to 2003 are presented in Figure 6.7. Depicted are the nitrate and ammonium nitrogen as well as phosphate phosphorous concentrations for the simulation experiments based on the single approaches (S1-S5) or on combinations of the terrestrial and in-stream retention approaches (C1-C6) in comparison to the observed values with their standard deviations, as well as to the results of the base scenario without any retention in landscape or river waters (B0) for the Saale river, gauge Groß Rosenburg. Mean monthly observed and simulated water discharges at the outlet of the basin as well as monthly observed climate parameters (precipitation and temperature) are additionally depicted in Figure 6.7 to facilitate interpretation of achieved model results. The climatic parameters are distinguished into observations averaged for the entire Saale basin and for the subbasin containing the most downstream Saale gauge Groß Rosenburg. Groß Rosenburg shows a slightly warmer and obviously drier climate than the basin on average.

The base scenario B0 with all retention and decomposition approaches of landscape and river turned off in the model mainly delivers overestimated nutrient concentrations. This is especially observed in winter time and is characterised by high inputs from diffuse sources due to leaching and wash-off with the lateral water flows. As a result of decreased diffuse nutrient inputs in the drier summer months, the simulated concentrations are generally lower, especially for nitrate nitrogen and phosphate phosphorus. In this time, an overestimation of ammonium nitrogen and a significant underestimation of nitrate nitrogen concentrations can be noticed. It is concluded that for the realistic modelling of nitrate nitrogen concentration at the outlet of the basin, a smoothing of the curve (e.g. via retention process) is necessary. The seasonal dynamics of ammonium nitrogen and phosphate phosphorus seem to be represented better, but with some overestimation. An overestimation of phosphate phosphorus can be seen in winter/spring months. The relative better fit can be explained by the nutrient specific characteristics in the model, which act as a “natural retention” function due to a specific high adsorption potential to soil particles defined in the soil leaching equation for phosphate phosphorus as well as for ammonium nitrogen.

Looking at the other model experiments performed, it can be readily observed that realistic modelling of nitrate nitrogen requires implementation of the retention and decomposition processes in the landscape. Only terrestrial retention (S1) is able to reproduce measured concentrations at the basin outlet, whereas all other separately used retention and decomposition processes in the river network (S2-S5) are not able to smooth the monthly-mean-curve sufficiently. The attempts to reduce nitrate nitrogen in winter time lead to lower concentrations in summer months as well. The version S5 with the highest achieved summer nitrogen concentrations among the single approaches delivers the worst winter concentrations. The combined model approaches (C1-C6) generally show good results with small variations. It can be concluded that modelling of nitrate nitrogen requires retention and decomposition functions in the soils of the catchment, whereas the riverine processes alone are not sufficient.

Still looking at Figure 6.7, it can be seen, that using the single terrestrial retention approach S1 independently does not allow for sufficient modelling results of the ammonium nitrogen concentrations. In general, correct modelling of ammonium nitrogen behaviour is complicated because of its low stability in ecosystem and its fast change to nitrate nitrogen in short time. This nitrification process can cause low ammonium nitrogen concentrations in soil solution and in stream water although the deposition load on the soils is much higher (Yu et al., 2012). Retention during the lateral flow of ammonium nitrogen passing through terrestrial soils accounts for lessening the total diffuse inputs to the river in winter time, but does not decrease the inputs in summer when point sources dominate. Simulation with riverine processes alone (variants S2-S5), in contrast, lessens the summer concentrations of ammonium nitrogen in the river to the measured values, but simultaneously declines the winter concentrations to an unrealistically low level. Most of the combined approaches (C1-C5) indicate the same problem: a general smoothing of the seasonal dynamic and decrease in summer concentration accompanied by a decreased winter concentration. The best result was achieved with experiment C6 (retention in landscape together with the detailed in-stream processes). This approach allows for simulating ammonium nitrogen concentration more realistically, probably due to capturing behaviour in two directions: decrease of ammonium in spring and summer months due to excessive consumption by algal biomass, combined with a moderate increase in autumn and winter time due to terrestrial retention (acting as a reducing effect) and algal decomposition and diffusion of ammonium from the sediments (acting as an increasing effect).

Regarding phosphate phosphorus, the main problem can be detected in the winter and spring months, when concentrations are mostly overestimated (Figure 6.7). Using the single approach taking into account retention in soils only (S1) leads to smoothing of seasonal dynamics, which is too strong (underestimation in October-December). Single riverine approaches (S2-S5) generally indicate higher variability, but they either overestimate the winter/spring concentrations or underestimate the autumn/winter phosphate phosphorus concentrations. The problem of a rather strong smoothing is visible in the combined approaches due to the main influence of the terrestrial retention in periods with higher diffuse inputs. Approach C6 reproduces seasonal dynamics better, probably due to taking into account such processes as desorption from sediments and algal consumption.

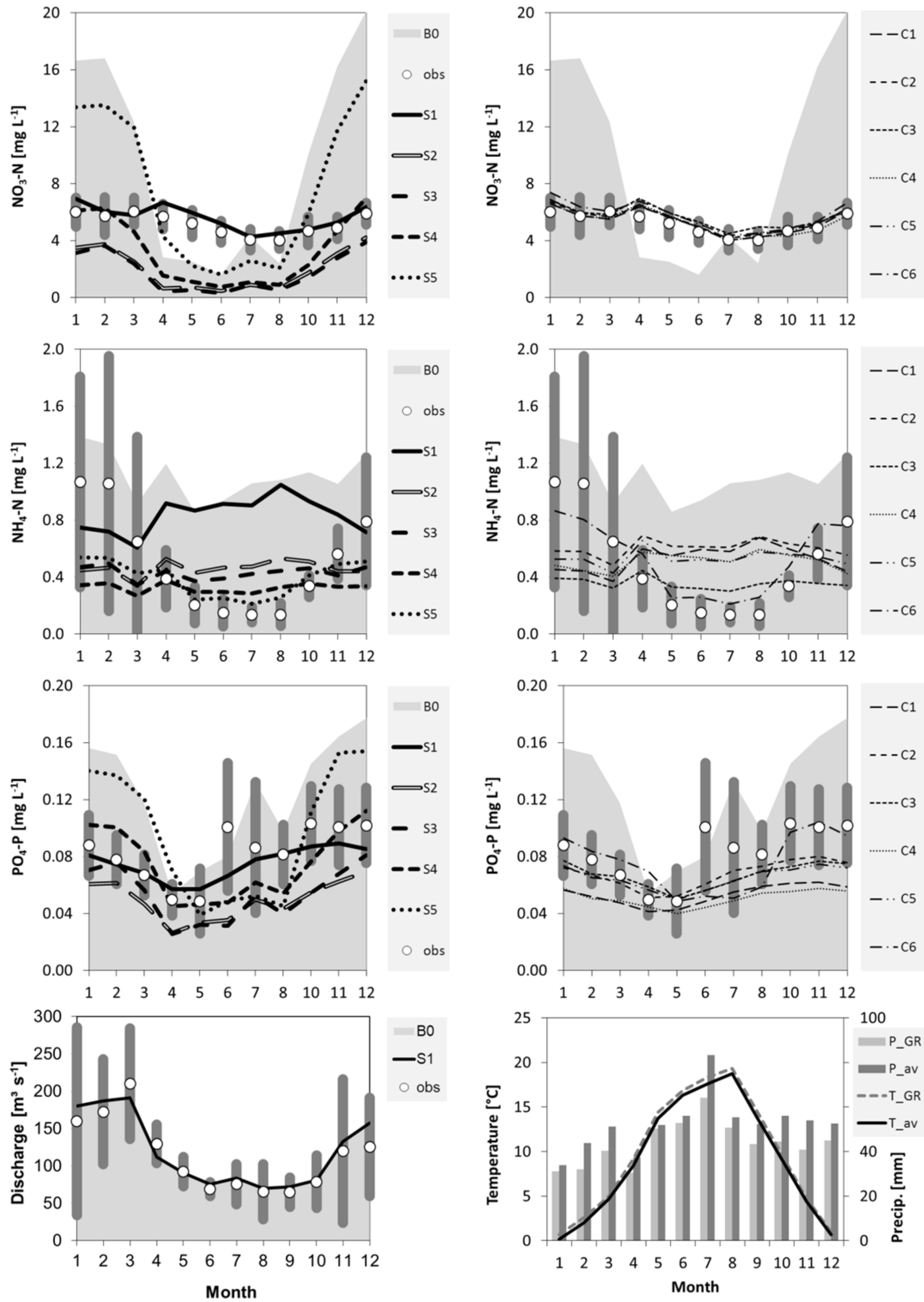


Figure 6.7 Observed (with standard deviation) and simulated monthly averages of nitrate nitrogen concentration (above), ammonium nitrogen concentration (middle), and phosphate phosphorus concentration (below) at the Saale gauge Groß Rosenburg for all model approaches in the time period 1996-2003, supplemented by measured and simulated mean monthly discharges at the outlet of the basin as well as with monthly temperature (T) and precipitation (P) averages for the total basin (av) and for the last gauging station Groß Rosenburg (GR) covering the same time period (bottom).

Figure 6.8 illustrates daily model results for the three nutrients in two selected years 1999 and 2000 to facilitate presentation and interpretation of model outcomes. The graphs include concentrations simulated by the single approach with retention in soils (S1) and by the combined simple and detailed methods additionally dealing with transformation and decomposition processes in the river itself as a function of water temperature (C3 and C6) in comparison to fortnightly measurements and the results of the B0 model run.

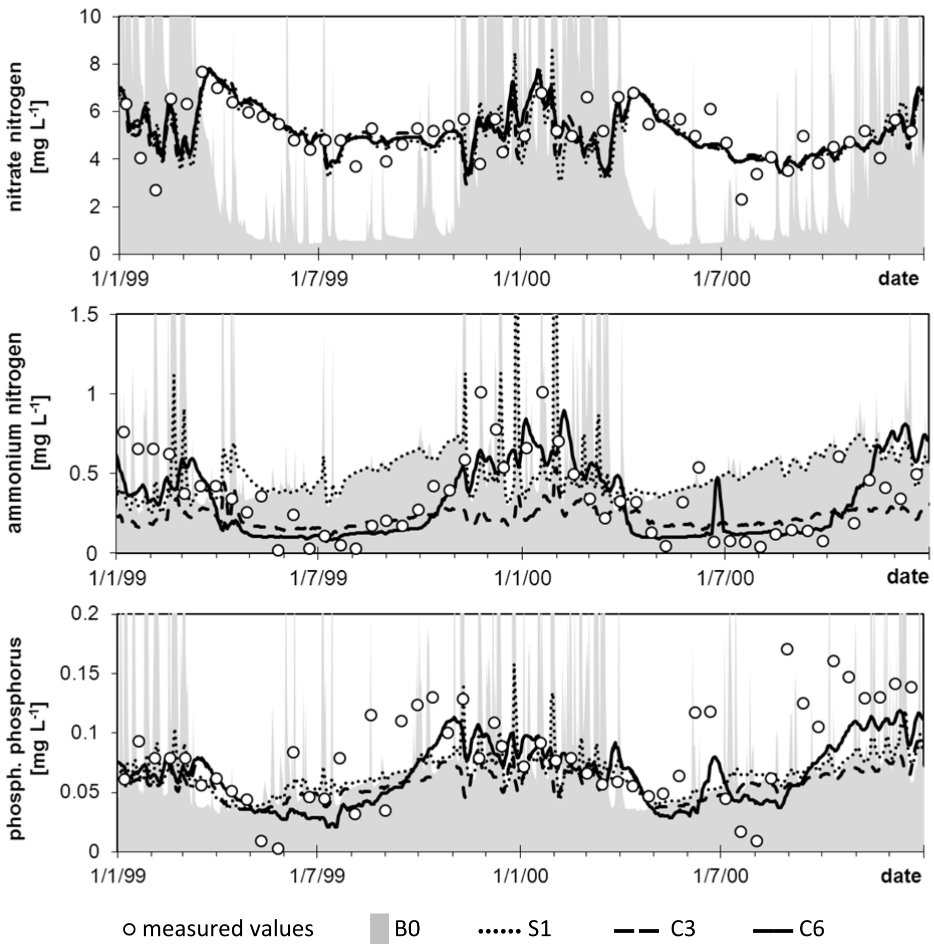


Figure 6.8 Daily model results of selected experiments compared to measured data at the outlet of the Saale basin (observation station Groß Rosenburg) in 1999 and 2000.

Looking at the simulated daily concentrations of B0, many narrow peaks are noticeable that correlate with intense rain events in the basin. These events are smoothed by natural (and also by modelled) retention processes. For ammonium nitrogen and phosphate phosphorus the base experiment does not reach the measured high winter concentration values, possibly because of reduced leaching through soils due to their high adsorption potential.

It can be readily determined that neither simple nor detailed in-stream processes are necessary to simulate nitrate nitrogen concentrations (Figure 6.8, upper graph) realistically. The nitrate nitrogen dynamics depend very much on the retention processes in the landscape. When the model accounts for terrestrial retention and decomposition, simulation results are sufficient.

Due to a lack of more detailed data, point-borne nutrient inputs to the Saale river could only be considered as yearly constants with an unknown composition and a high uncertainty. As a result, the ammonium nitrogen concentrations (Figure 6.8, middle graph) are notably influenced by point source emissions. In model applications without an appropriate retention potential of the river water, the ammonium nitrogen concentration increases with a decrease in water discharge in late summer and autumn due to less dilution. Therefore, riverine decomposition and transformation processes are important to simulate measured data of ammonium nitrogen. Whereas the simple approach C3 diminishes summer as well as winter concentrations, the detailed approach C6 considering algal growth is most useful, as it allows to simulate both summer minimum and winter maximum of ammonium nitrogen well.

Regarding the phosphate phosphorus concentrations (Figure 6.8, lower graph) the same conclusions can be drawn. Only C6 approach delivers the most reasonable seasonal dynamics, including summerly nutrient peaks according to the dynamics of algal biomass.

An additional experiment was conducted to test the influence of hydromorphology and water temperature on model output when using the simple in-stream retention and decomposition equations of the approaches C1, C2 and C3 (Figure 6.9). The daily results of these three methods were compared regarding ammonium nitrogen with a possible retention or decomposition without considering hydromorphology or water temperature respectively (nutrient load reduction was treated as a constant). Both comparisons obviously show the influence of temperature and discharge especially in winter time and an improvement of results when using inconstant retention rates. High discharge or low water temperature cause lower nutrient retention/decomposition potential in the river than by assuming a constant retention value all over the year, but the amplitude between the simulated summer and winter concentrations is still too small to match the observed values. It can also be seen that the second approach dealing with hydromorphology (C2) is much more sensitive to water discharge than the first method (C1).

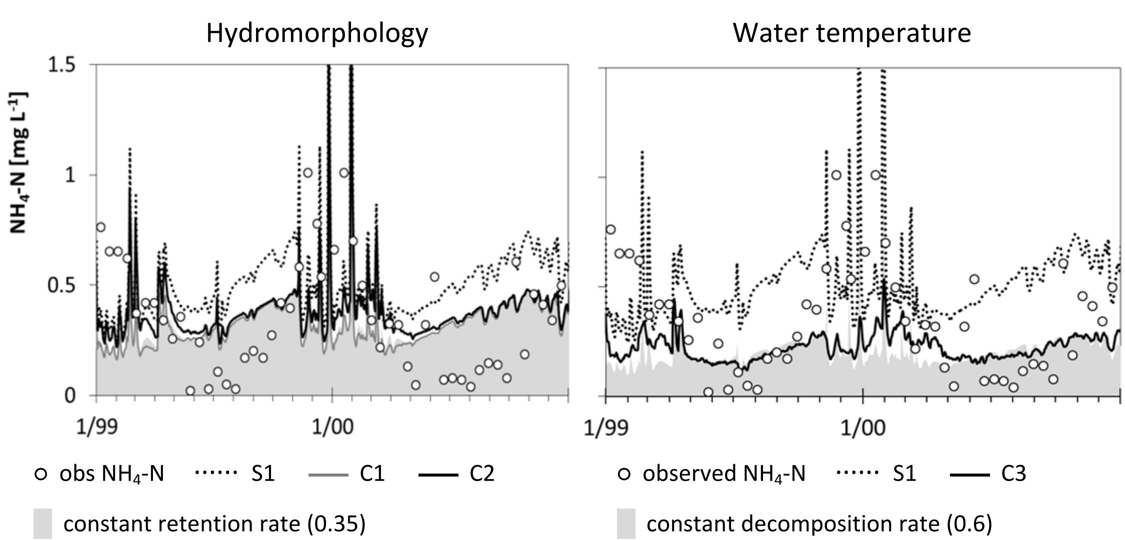


Figure 6.9 Additional experiment illustrating the influence of hydromorphology (left) and water temperature (right) on resulting ammonium nitrogen concentrations: Daily model outputs achieved using the simple in-stream retention and decomposition approaches as simulated in experiments C1, C2 and C3 are compared with results obtained when assuming a constant retention or decomposition rate impacting nutrient loads.

Figure 6.10 shows mean model results regarding accumulated nutrient loads for the selected experiments S1, C3, and C6 in comparison to observed loads and to model results without any retention (B0) for the time period 1996-2003. Whereas the nitrate nitrogen loads can be reproduced by any of the retention and decomposition methods, the ammonium nitrogen loads are definitely best depicted by using the combined approach with detailed in-stream processes (C6). The mean amounts of accumulated phosphate phosphorus loads are modelled sufficiently by all selected methods; the approach S1 exclusively simulating retention and decomposition in the soils of the catchment surprisingly delivered already good results.

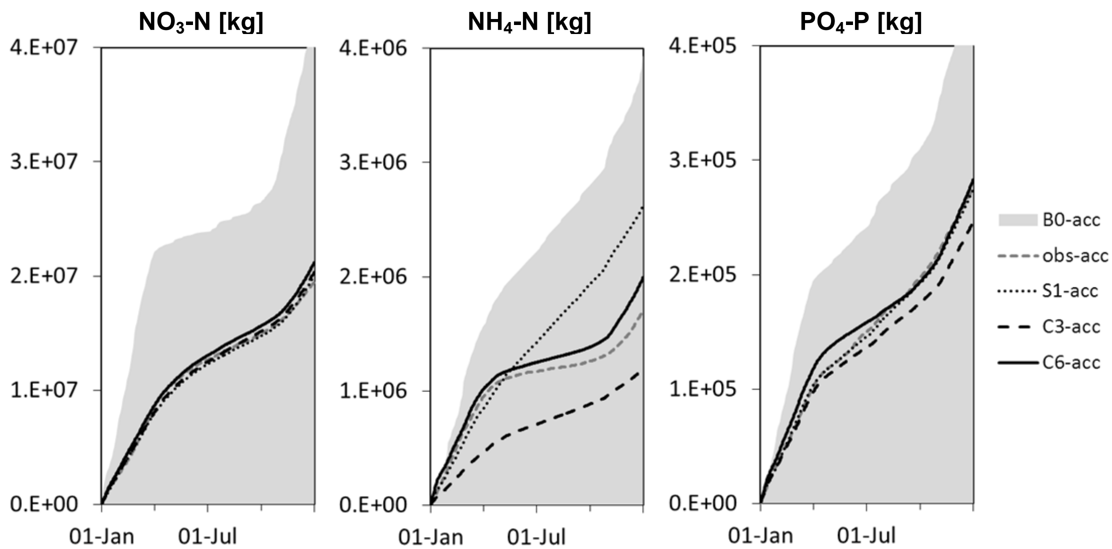


Figure 6.10 Comparison of observed and simulated yearly accumulated nutrient loads in the mouth of the Saale river for selected model experiments (average of the years 1996-2003).

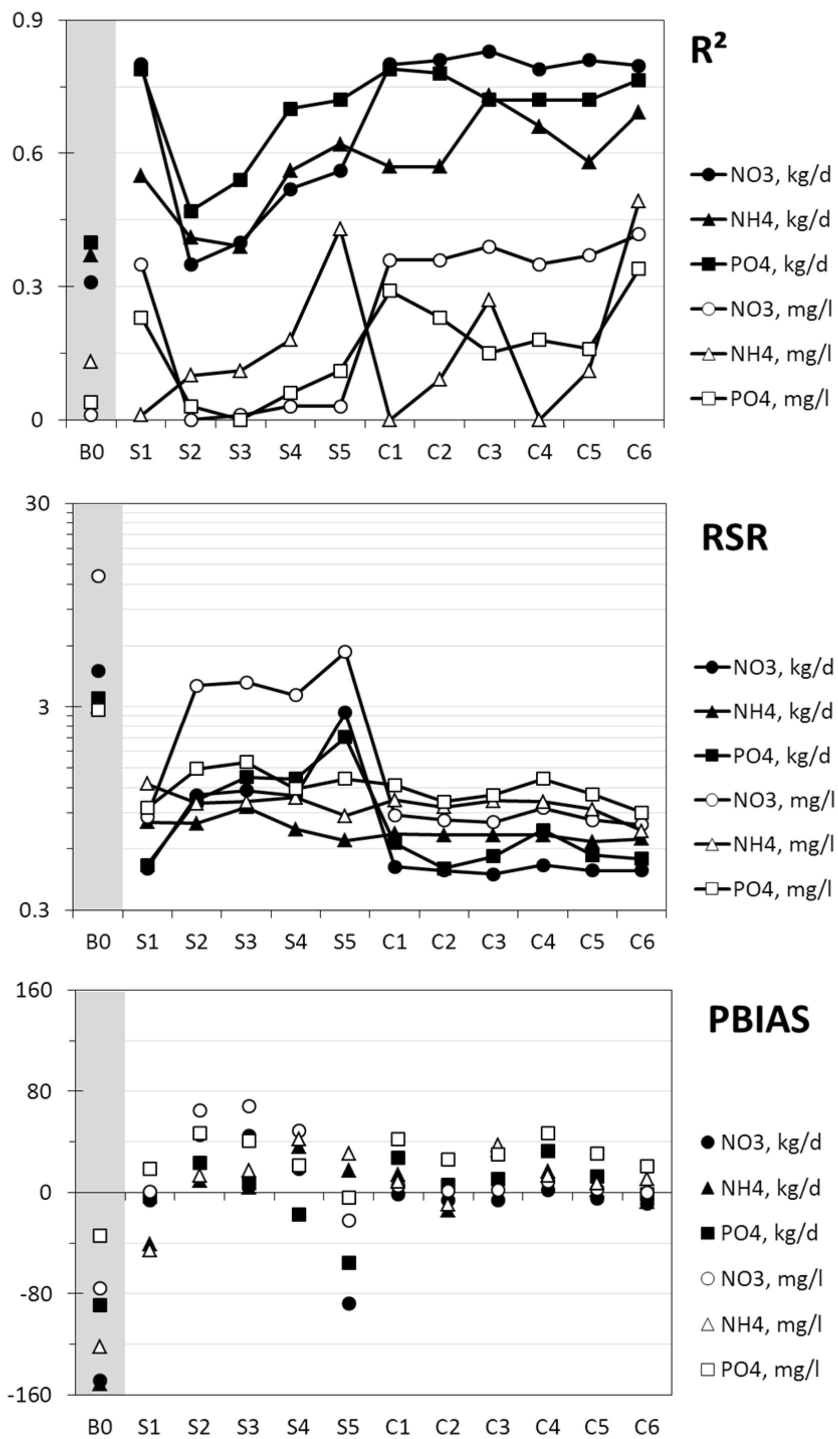
6.4.2 Evaluation of model approaches: criteria of fit

The quality of the different model approaches was statistically evaluated by different measures for the goodness of fit (R^2, RSR and PBIAS). The performance parameters were estimated separately for loads and concentrations of the three nutrients per each model approach for the two years 1999 and 2000, which were already used for analysing and visualising daily nutrient dynamics above.

In water quality modelling and management distinction between nutrient loads and concentrations is important to estimate the absolute weight of the impacting component. As the nutrient concentration is a function of water discharge and nutrient load, a river can feature the same nutrient concentration in winter times with several times higher discharges than in summer times, meaning that it is simultaneously carrying several times higher nutrient loads. That is why pollutant loads provide much more information for assessing the impact potential of a river, whereas water quality standards and pollution indices are by necessity based on pollutant concentrations (Michaud 1991). So, a watershed model should be able to sufficiently provide both resulting nutrient loads and concentrations.

Figure 6.11 illustrates the differences in model performance between the experiments B0-C6 and between nutrient loads and concentrations. In general and as expected, nutrient loads indicate a better performance: R^2 is higher and RSR and PBIAS values are lower than those for nutrient concentrations due to high correlation of loads with water discharge (especially for nutrients coming mainly from diffuse sources) and strong dependence of nutrient concentration model output on realistic results of the previous water discharge simulation. Similar experiences were also reported by other authors, who achieved better watershed model performances for nutrient loads than for concentrations (e.g. Bärlund & Kirkkala, 2008).

Figure 6.11 Model performance for the two years 1999 and 2000: Comparison of the nutrient form specific R^2, RSR, and PBIAS of all model approaches and all three nutrients under observation.



Simulations for nitrate nitrogen loads and concentrations deliver the highest goodness of fit in all cases when the retention and decomposition equations for catchment soils are used (S1 and C1 – C6). In contrast, using the single methods with transformation and retention processes only in the river (S2 – S5) results in worse outcomes, especially regarding nitrate nitrogen.

The performance ratings are highly variable between the approaches as well as for loads and concentrations within one approach. So, to rank the different model experiments done, a mean performance rating was evaluated for each model approach by calculating the average of all six R^2 values within a method and the average of the absolute values of PBIAS for the time period 1996-2003. The results of this evaluation are presented in Figure 6.12.

The base version B0 shows the worst evaluation criteria regarding R^2 and PBIAS (Figure 6.12), whereas the standard SWIM version with implemented retention in landscapes, but without riverine processes (S1), already delivers acceptable results. The sequence of experiments from S2 to C6 demonstrates a more or less steady improvement of the mean performance ratings. In general, the single approaches using only riverine retention and transformation processes (S2-S5) cannot reach similar goodness of fit values as the ones with terrestrial processes included. The approach S5 with detailed in-stream processes implemented delivered improved results for R^2, but worse absolute values of PBIAS compared to the S1 approach. Within the combined approaches, the version C3 with a simple decomposition method according to the water temperature, accomplishes a better mean performance than the standard SWIM version. The performance of the simulation experiment using the combined approach with implemented detailed in-stream processes (C6) is the highest in terms of R^2 (0.40), and exceeds the performance of results, which could be achieved using the standard SWIM version (0.33) by 21%. The model improvement can also be seen looking at PBIAS: version C6 (10.1) shows a decrease in bias by -62% compared to S1 (26.3). The relative low values for R^2 shown in Figure 12 are the result of averaging all performances achieved for three different behaving nutrients for both loads and concentrations, the latter one usually more difficult to realistically model.

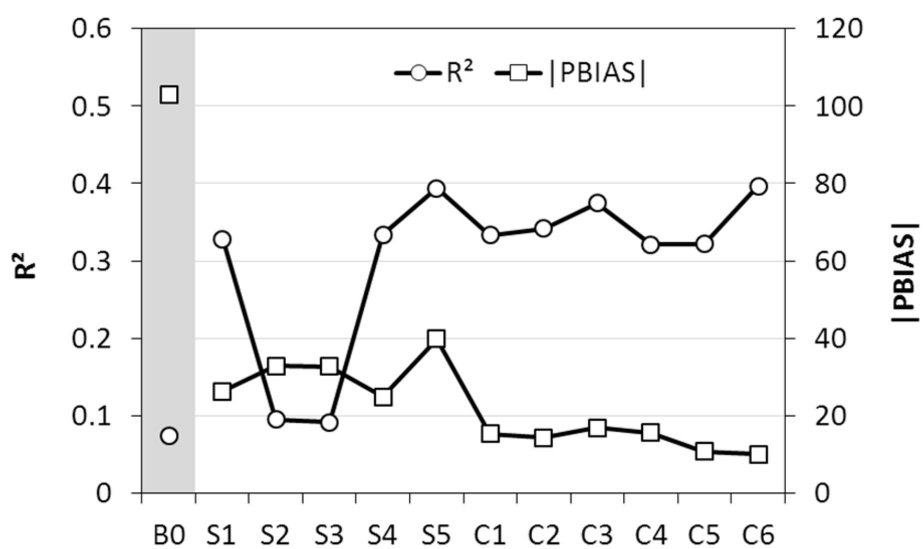


Figure 6.12 Total ranking of the variants of retention modelling: R^2 and absolute values of PBIAS per model approach as an average for six model variables (considering loads and concentrations per nutrient form) for the time period 1996-2003.

But it should be kept in mind that usually even a little increase in goodness of fit requires more calibration efforts. The number of calibration parameters rises with the increasing model complexity, and the model uncertainty increases as well. Physically or process based models are usually overparameterised and include a lot of parameters, which could be only calibrated. A corresponding danger of overparametrisation exists with conceptual models which are configured in a distributed manner (Adams, 2007). Hejzlar et al. (2009) stated that the more complex and process oriented models were likely to give a higher variation in nutrient retention values for different catchments. This is because these models are calibrated against observed riverine nutrient loads or concentrations and the deviations in model outputs during the calibration process can be compensated at the expense of either riverine retention or processes exporting nutrients from soil to surface waters. "The implication of this is that while highly parameterised models generally contain enough flexibility to fit observations well, the selected parameter set may not be physically meaningful" (Blakers et al., 2011). Therefore, realistic modelling of nutrient outputs for large-scale river basins remains a difficult task, due to some specific obstacles in water quality modelling (Krysanova et al., 1998).

6.5 Conclusions and outlook

For an adequate representation of nutrient concentrations and loads measured at the outlet of a mesoscale or large river basin, it is often necessary to consider terrestrial and in-stream nutrient retention and decomposition processes during water quality modelling. Decomposition and transformation processes lead to retardation of nutrient transport, and as a consequence, to an increase in retention potential of the observed river reach. But it is important to distinguish between the different nutrient components and their main sources. In this study, nutrients coming mainly from diffuse sources (such as nitrate nitrogen in the Saale catchment) are mostly influenced by retention in the landscape, and additional retention or transformation processes in the river network could be ignored in the model simulations. On the other hand, nutrients introduced to the rivers mainly by point sources (e.g. ammonium nitrogen) clearly need implementation of transformation processes in the flowing water itself. It could be concluded that neither sole terrestrial nutrient retention nor a single in-stream retention process was able to reproduce ammonium nitrogen and, less obvious, phosphate phosphorus concentrations sufficiently well, but a combination of both approaches succeeded.

Not all versions of riverine processes introduced to the standard SWIM model with implemented nutrient retention in the soils of the catchment resulted in better model performance for nutrients coming mainly from point sources. The two approaches simply coupled to the hydromorphology of the river (C1 and C2), or the method simulating a simple decomposition as a function of water temperature (C3), were not able to considerably improve seasonal dynamics of nutrients, not even in combinations (C4 and C5). This is mainly due to the fact that those methods generally decrease the concentrations in the river throughout the year and produce a counterproductive smoothed nutrient concentration curve. In contrast, the detailed river approach simulating in-stream nutrient processes (C6) allows ammonium nitrogen and phosphate phosphorus concentrations to rise in river reaches in winter by increasing the diffusion rate from the sediments. Furthermore, this method is capable to reproduce summer minimums of nutrient concentrations by algal consumption. Hence, application of this modelling approach enabled an increase in the accuracy of model fit to observed data.

Model evaluation should consider that with increasing complexity of a model approach and with rising number of calibration parameters, the time requirements and uncertainties may increase dramatically. The problem could be exacerbated in the case of correlation between some parameters. Completing sensitivity analysis aimed at finding the most responsive parameters to model output in advance of calibration, and analysis of correlation between parameters is recommended. This implies a careful choice of the appropriate model approach with the lowest possible complexity according to research question, special basin characteristics and scale of the case study to avoid unnecessary calibration efforts and unreasonable uncertainties (Drewry et al., 2006; Adams, 2007). The chosen complexity should be as high as necessary whereas the resulting uncertainty should be as low as possible to get the most realistic and useful model results (Snowling & Kramer, 2001). Related to the scale of the modelled study area different processes are dominating and define the necessary complexity: soil and crop type, nutrient cycling and leaching are most important on the plot scale, hydrological processes dominate at the hillslope scale, and land use, rainfall and topography are important influences on the catchment scale (Drewry et al., 2006). Model experiences with SWIM revealed that at the large scale, model errors caused by the uncertainties related to the different processes within a river basin often compensate each other and facilitate realistic simulation of measured data. It seems to be easier to achieve reasonable results for larger basins than for smaller ones, also with a lower model complexity.

Unfortunately, PEST was not able to find the optimal parameter settings by itself starting at any point within the maximum and minimum borders. It searched for the local optimum around the starting values; therefore, the model results were highly dependent on the previous manual calibration per model experiment. The uncertainty of the model approaches within this study is not only model specific, but also model user specific.

Basin-wide constant nutrient retention and decomposition parameters in the soils may be unrealistic in large-scale water quality modelling. According to the geo-chemical conditions in the soils, the intensity of denitrification (which is probably the main process responsible for loss of nitrogen from soil) or sorption (the same regarding phosphorus) processes, and also the residence time for nutrients in the lower and deeper soil profiles can vary and may change from hydrotope to hydrotope. Spatially distributed terrestrial retention parameters could be beneficial for the improvement of the model performance. But the usefulness of soil specific distributed retention and decomposition parameters was not confirmed for the same Saale basin in a previous study (Huang et al., 2009). This approach may be helpful in larger and more heterogeneous river basins, such as the entire Elbe or Rhine river basins.

Apart from the precautions and uncertainties mentioned above, the model experiments presented in this study increased the understanding of the importance, usefulness, and necessity of implemented retention processes in landscape and rivers and their effects on the simulated river water quality. With regard to the main source of a certain nutrient introduced to a river, it could be demonstrated that applying either terrestrial (in regard to diffuse pollutants) or a combination of terrestrial and riverine retention and transformation processes (in regard to point pollutants) support improving the modelling performance.

CHAPTER 7

IMPACT ASSESSMENT FOR THE TOTAL ELBE RIVER BASIN

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Abstract

Ecohydrological water quality modelling for integrated water resources management of river basins should include all necessary landscape and in-stream nutrient processes as well as possible changes in boundary conditions and driving forces for nutrient behavior in watersheds. The study aims to assess possible impacts of the changing climate (ENSEMBLES climate scenarios) and/or land use conditions on resulting river water quantity and quality in the large-scale Elbe river basin by applying a semi-distributed watershed model of intermediate complexity (SWIM) with implemented in-stream nutrient (N+P) turnover and algal growth processes. The calibration and validation results revealed the ability of SWIM to satisfactorily simulate nutrient behavior at the watershed scale. Analysis of 19 climate scenarios for the whole Elbe river basin showed a projected increase in temperature (+3 °C) and precipitation (+57 mm) on average until the end of the century, causing diverse changes in river discharge (+20%), nutrient loads (NO_3-N: −5%; NH_4-N: −24%; PO_4-P: +5%), phytoplankton biomass (−4%) and dissolved oxygen concentration (−5%) in the watershed. In addition, some changes in land use and nutrient management were tested in order to reduce nutrient emissions to the river network.

7.1 Introduction

Changes of the world's and Europe's climate and increased anthropogenic pressure on natural resources have already been detected in the past, and this development is likely to continue in the future (IPCC, 2007; IPCC, 2013; EEA, 2010; Cassardo & Jones, 2011; RIKS, 2010; Alcamo et al., 2007b).

Looking at the climate aspect, a global rise in mean temperature, change in precipitation pattern as well as an increase in intensity and frequency of extreme events can be recognised (IPCC, 2007; IPCC, 2013; Christensen & Christensen, 2004), impacting the water cycle (Kløve et al., 2014; Kundzewicz, 2008; Wang et al., 2013b), vegetation and biodiversity (Linderholm, 2006; Vittoz et al., 2013; Kittel, 2013; Lindner et al., 2014) as well as human health (Gabriel & Endlicher, 2011; Haines et al., 2006) and economy (Koch et al., 2015; Liersch et al., 2013). The potential warming in Europe could reach values from +1 to +6 °C by the end of this century (Alcamo et al., 2007a), depending on the location. The annual mean precipitation is expected to increase in Northern Europe and decrease in most parts of Southern Europe and Mediterranean regions up to ±20% (EEA, 2012). The catchment of the Elbe river, mainly located in Germany and the Czech Republic in Central Europe, is already experiencing changes in climate conditions as well as changes in extreme temperature and precipitation values, and this trend is expected to continue. During the last century (1882–2013) the average temperature in Germany increased by 1.2 °C, whereas the precipitation amounts rose by 10.6% on average with a high spatial and temporal variability (UBA, 2015). Application of ensembles of climate scenarios shows increasing trends in floods for the Elbe basin in Germany (Huang et al., 2015) as well as in the Czech Republic (Kyselý & Beranová, 2009), especially in wintertime.

Climate change will have direct and indirect impacts on river water quantity and quality (Whitehead et al., 2009; Kundzewicz et al., 2007; Crossmann et al., 2013; Dunn et al., 2012; Mimikou et al., 2000). With the rising temperature, water availability will decrease due to increased evapotranspiration, and a reduced discharge will facilitate algal growth and reduce dilution of point source pollutants. Higher temperatures and lower flow velocities would additionally stimulate turnover processes and increase system respiration rates, causing oxygen deficits in river reaches. All these processes lead to the degradation of water quality and ecological status of a waterbody connected with a higher probability of algal blooms (Whitehead et al., 2009; Desortová & Punčochár, 2011; Hardenbicker et al., 2014) and increasing problems for water supply and treatment (Kundzewicz et al., 2007).

As phytoplankton growth is a key factor for water quality in lowland river ecosystems (Scharfe et al., 2009), the algal processes should be included in evaluating impacts of global change on water quality. Light and nutrients are generally deemed to be the most important external drivers of phytoplankton dynamics in rivers, along with temperature which also has a positive relationship with phytoplankton, and discharge which has a negative relationship (Scharfe et al., 2009; Desortová & Punčochár, 2011; Hardenbicker et al., 2014).

Additionally, climate change would influence nutrient turnover and transport processes (denitrification, nitrification, volatilisation and leaching) in the catchments, due to altered temperature and precipitation (Barclay & Walter, 2015; Whitehead et al., 2006; Macleod et al., 2012), and the terrestrial processes will also influence the final river water quality at the outlet of the basin. River systems are also affected by anthropogenic impacts (land use composition, population and industry) causing nutrient pollution from point (factories, sewage treatment plants) and diffuse sources (agricultural fields), which lead to eutrophication processes and a decrease in river water quality (Vollenweider, 1968; Anderson et al., 2002; Pieterse et al., 2003; Schindler, 2006).

Due to the high pressure of rising population, growing industry and increasing transport demand on landscapes and natural vegetation, many changes in land use could be recognised in Europe in the past. The current tendencies include a decreasing trend in crop and pasture acreages in Spain, Czech Republic and Northern Germany, slowly growing forested areas in Northern Europe and Portugal, and notably growing urban areas in France and Western Germany (EEA, 2007a; RIKS, 2010). It is expected that these trends will continue in the coming 10–20 years.

Population density and human activities are important underlying factors for point and diffuse nutrient pollution entering rivers (Seitzinger et al., 2010). During the last decades, many efforts to reduce nutrient inputs to the rivers by construction and improvement of sewage treatment plants and optimisation of fertiliser application on cropland were undertaken in Europe. They resulted in a remarkable reduction of phosphorus emissions (mainly from point sources), but only a small decrease of nitrogen inputs (mainly from diffuse sources) due to the lag time of diffuse nutrients in soils (Bouraoui & Grizzetti, 2011; de Wit et al., 2002; Grizzetti et al., 2012). It is widely recognised that the control of diffuse source emissions is much more difficult. So it is expected that the inputs of nutrients from households and industry will be further reduced in the future, and diffuse inputs from fertilisers and manure will become the main sources of nutrient pollution in Europe (de Wit et al., 2002).

Climate as well as land use change impacts on river water quality superimpose each other and create a very complex system of interactions and feedbacks (Dunn et al., 2012; Mehdi et al., 2015; Huttunen et al., 2015). The nitrate loads in the rivers, for example, are climate-dependent, and were likely influenced by former climate variations, so it is difficult to define and interpret the pure effects of management changes in the past (Bouraoui & Grizzetti, 2011). Furthermore, adaptation measures and policy responses to projected climate change, e.g., subvention for bio-fuels or control of greenhouse gas emissions, affect freshwater quality as well (Whitehead et al., 2009). A combined land use and climate change impact assessment would be an important step facilitating an integrated river basin management. The system characteristics and variable boundary conditions should be taken into account by default in modern management strategies (Scharfe et al., 2009) to support the implementation of adaptation measures in river basins.

The process-based ecohydrological watershed models driven by climate and land use parameters can be useful for assessing potential future developments in a changing world. Watershed models including both landscape and in-stream nutrient processes, which are able to simulate nutrient turnover processes in a catchment and river network, may represent effective tools for the evaluation of river water quality at the basin scale (Horn et al., 2004; Daniel et al., 2011). However, it should be kept in mind that current water quality modelling at the watershed scale still has more weaknesses and uncertainties compared to pure hydrological modelling due to the higher complexity of modelled processes and the requirement to include more input data and parameters.

In former applications of the semi-distributed ecohydrological Soil and Water Integrated Model (SWIM) (Krysanova et al., 2000) for water quality modelling in river basins in Germany, it was observed that nutrient retention and decomposition solely in the soils of the watershed is not sufficient for tackling nutrients coming from different sources, especially in larger basins (Hesse et al., 2008). Therefore, SWIM was extended by a new module representing nutrient and oxygen turnover processes and algal growth in rivers, which was already tested for the mesoscale Saale river, a subcatchment of the Elbe river with an area of about 25,000 km^2 (Hesse et al., 2012). The aim of this study is to apply the new SWIM version for a combined climate and land use change impact assessment on the entire Elbe basin including the upstream part in the Czech Republic and the lower part in Germany (total drainage area about 150,000 km^2). This can support the development of management strategies and adaptation measures to potential changes in the future in this large-scale river basin.

In particular, the following objectives were pursued in this study:

- Testing the in-stream SWIM module for the large scale by modelling water quality parameters (nitrate nitrogen (NO_3-N), ammonium nitrogen (NH_4-N), phosphate phosphorus (PO_4-P), dissolved oxygen (DOX), and chlorophyll *a* (Chla)) at the basin outlet and at confluences of the large Elbe tributaries in the historical period;
- Analysis of climate scenarios for the region provided by the European ENSEMBLES project (van der Linden & Mitchell, 2009), and climate change impact assessment on water quantity and quality for two future periods (2021–2050 and 2071–2100) with unchanged management;
- Simulation of selected land use change and management scenarios aiming at the reduction of point and diffuse nutrient loads in the basin; and
- Analysis of the combined climate and land use change impacts on water quantity and quality to derive ideas for suitable measures for adaptation to climate change.

The model-based assessments of climate and land use change impacts on water quality are rare in literature so far compared to impact assessments on the hydrological cycle, especially at the large scale. The recently implemented in-stream module enables a more realistic representation of all interrelated processes for the impact study. Therefore, this study is an important step forward to large-scale application of water quality models with distributed calibration for impact studies in general, as well as towards a fully integrated water resources assessment in the Elbe catchment in particular.

7.2 Study area: The Elbe catchment

The Elbe river (1094 km) originates at 1386 m a.s.l. in the Giant Mountains located between Poland and the Czech Republic, drains an area of 148,268 km^2 and flows into the North Sea (IKSE, 2005). The Elbe has the fourth largest catchment area among the European rivers (Scharfe et al., 2009). 65.5% of its catchment belongs to Germany, 33.7% to the Czech Republic, 0.6% to Austria and 0.2% to Poland (see Figure 7.1). The discharge regime (861 $m^3 \cdot s^{-1}$ on average) usually shows high water levels in winter and spring and low water levels in summer and autumn. In total, 24.5 million people live in the Elbe basin, which also includes the large cities Berlin, Hamburg and Prague (IKSE, 2005).

Table 7.1 gives an overview of the main characteristics of the Elbe basin until the gauge Neu Darchau, and its six main tributaries, covering catchment areas above 5000 km^2. In this table some topography-specific differences can be detected between the tributary subbasins, namely in regard to climate parameters, soil conditions and, as a consequence, land use distribution, which also affect nutrient concentrations in the rivers. So, in the subcatchments with dominating agricultural land use due to fertile loess soils (e.g., Saale and Mulde) the nitrate and nitrogen concentrations are higher (see Table 7.1), resulting from fertiliser application and leaching. In contrast, the catchment of the Havel river has the highest share of low fertile soils consisting of almost two-thirds of sandy grained particles (about 70% of the total area) and shows the lowest nitrogen pollution but the highest phosphorus level. The high phosphate concentrations of the Havel river can be mainly explained by desorption from historically polluted sediments (Bronstert & Itzerott, 2006).

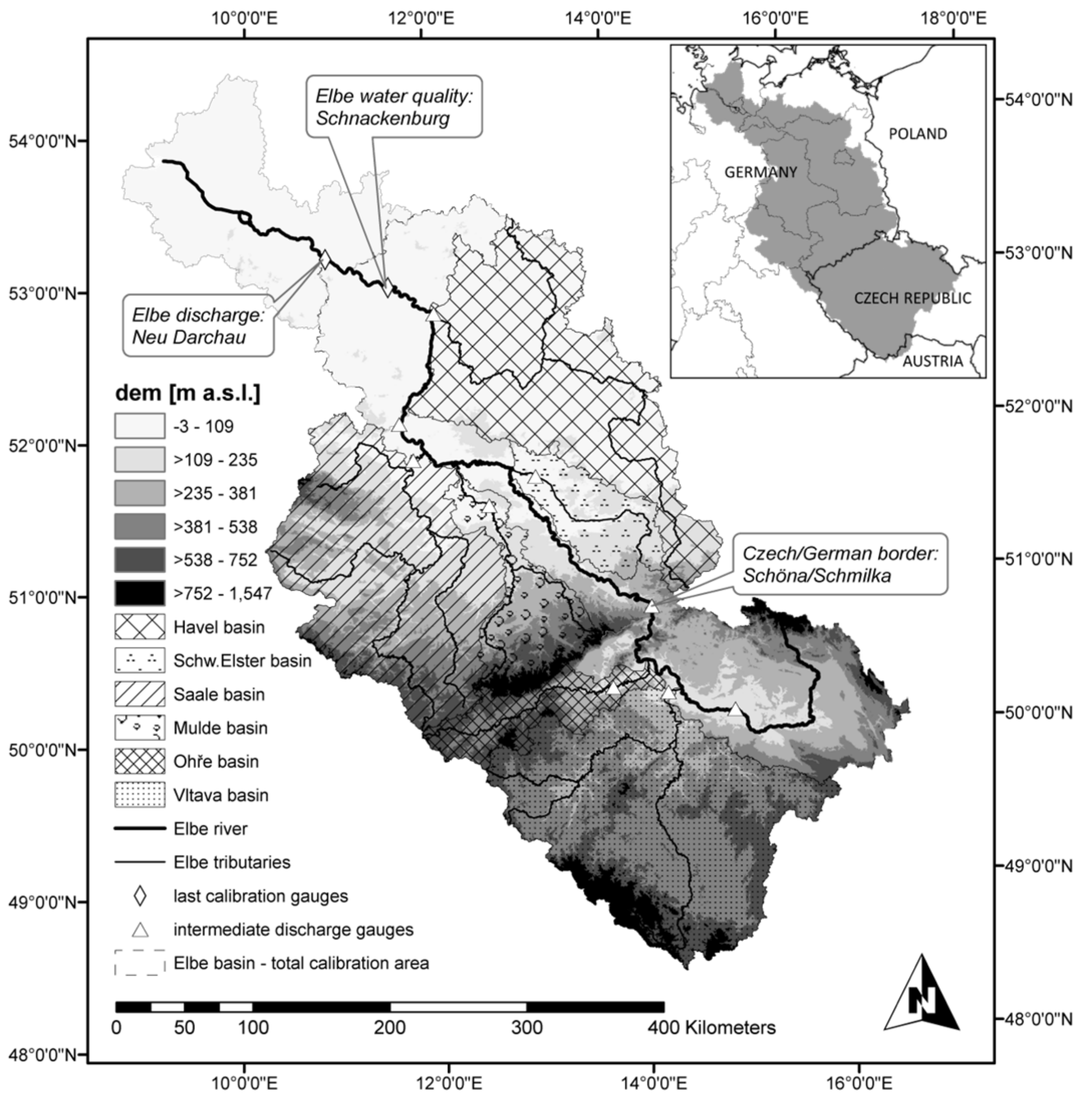

Figure 7.1 Location and digital elevation model of the Elbe river basin and six catchments of its main tributaries (drainage area > 5000 km^2), as well as location of the observation gauges used for calibration.

According to the German classification of water quality (LAWA, 1998), which uses the 90th percentile for nutrients and the 10th percentile for dissolved oxygen to compare with certain water quality thresholds, the highest nitrate level results in water quality class III (Mulde and Saale), the highest ammonium value belongs also to class III (Vltava), the maximum phosphate phosphorus level represents water quality class II–III (Vltava and Havel), and the lowest dissolved oxygen concentration results in water quality class II (Havel). There is quite high diversity between the rivers in this respect, and no river exists which has the worst or best status for all components.

Table 7.1 Characteristics of the Elbe river catchment and its main tributaries of second (classical) order for the time period 2001-2010.

River *gauges (discharge / water quality)*	**Elbe** *Neu Darchau / Schnackenburg*	**Vltava** *Vraňany / Zelčín*	**Ohře** *Louny / Terezín*	**Schwarze Elster** *Löben / Gorsdorf*	**Mulde** *Bad Düben / Dessau*	**Saale** *Calbe-Grizehne / Groß Rosenburg*	**Havel** *Havelberg / Toppel*	**Unit**
Length [1]	907	430	305	179*	314	434	334	km
Mean discharge [1]	711	145	38	21	67	117	114	$m^3 s^{-1}$
Catchment area [1]	131 950	28 090	5 614	5 705	7 400	24 079	23 858	km^2
Average altitude	281	523	507	131	394	287	74	m a.s.l.
Average temperature [2]	8.9	7.8	7.6	9.7	8.9	9.2	9.6	°C
Av. sum of precipitation[2]	698	713	771	652	822	680	616	$mm y^{-1}$
Land use [3]								%
Agriculture	51.3	49.7	42.2	48.1	53.3	63.0	38.6	
Forest	31.7	36.8	37.7	35.0	28.8	23.3	38.2	
Grassland	8.4	7.8	13.6	7.2	6.9	4.6	11.1	
Settlements	6.3	4.3	3.9	5.9	9.4	7.6	7.9	
Soil texture [4]								%
clay	16.2	20.3	22.1	8.5	17.1	20.0	9.0	
silt	38.2	37.4	39.6	29.8	47.9	54.9	26.3	
sand	45.6	42.3	38.3	61.7	35.0	25.1	64.7	
Point sources [5]								$t y^{-1}$
TN	22318	4704	570	183	1673	3557	2768	
TP	1870	564	73	29	155	357	167	
Nutrients [6]								$mg L^{-1}$
NO_3-N *av.*	3.17	3.73	2.38	2.31	4.35	4.68	0.82	
90-perc.	4.60	4.91	3.20	4.30	6.10	6.15	1.56	
NH_4-N *av.*	0.16	0.31	0.08	0.20	0.16	0.21	0.10	
90-perc.	0.33	0.94	0.11	0.53	0.36	0.46	0.23	
PO_4-P *av.*	0.07	0.12	0.03	0.02	0.06	0.09	0.13	
90-perc.	0.11	0.22	0.05	0.03	0.09	0.13	0.24	
DOX *av.*	11.7	11.7	10.6	9.7	10.6	10.3	10.6	
10-perc.	9.7	9.4	8.0	7.8	8.5	7.8	6.7	
Chlorophyll [6]								$\mu g L^{-1}$
CHLA *av.*	77.1	36.7	8.0	9.3	10.7	21.8	37.6	
90-perc.	184.0	96.1	14.2	18.0	28.5	61.7	73.0	

* Wikipedia; Data sources: [1] IKSE (2005), [2] DWD/PIK, [3] Corine2000, [4] Germany: BÜK1000, Czech Republic: Košková et al. (2007), [5] Germany: FGG-Elbe (2004a), Czech Republic: IKSE (1995), [6] German gauges: FIS, Czech gauges: IKSE

The Elbe river is the most important river draining the eastern part of Germany. The natural flow regime is influenced by reservoirs and regulation of small rivers, drainage of wetlands and brown coal mining (Klöcking & Haberlandt, 2002). Due to former political and socio-economic conditions, the Elbe was one of the most polluted rivers in Europe with a low ecological potential. The water quality improved after the German reunification in 1990 due to closure or upgrading of sewage treatment plants and industrial enterprises in the basin, as well as to a substantial decrease in fertilisation rates on agricultural land (Lehmann & Rode, 2001; Hussian et al., 2004). However, contamination problems still exist, especially looking at sediments, which are characterised by a high adsorption of heavy metals and other polluting substances (Schneider & Reincke, 2006). There are also no significant improvements regarding chlorophyll *a* concentrations in the Elbe river (Lehmann & Rode, 2001).

In general, the Elbe river is characterised by a strong phytoplankton growth in the free-flowing section due to inputs from the reservoirs of the upper Elbe and Vltava and high nutrient loads from tributaries (Quiel et al., 2011). The high primary productivity leads to substantial differences in nutrient concentrations along the river with remarkable intra- and interannual variations (Quiel et al., 2011), and the season of main biological activity is between March and October (Scharfe et al., 2009). Low flow velocities in the lowland tributaries with many natural lakes in the river course (e.g., Havel) and in rivers influenced by weirs and barrages (e.g., Vltava, Saale) facilitate good conditions for algal growth and cause high concentrations of chlorophyll *a*.

The middle course of the Elbe river in Germany contains several protected natural areas with a high diversity of flora, fauna and landscape types. Large parts of the river in Germany are free-flowing and not influenced by barrages. However, the original floodplain areas have often been cut off by flood protection measures for settlements, agriculture and industry during the last centuries. Approximately 84% of the floodplain along the Elbe river course in Germany is protected by dikes (Grossmann, 2012). The reduced flooding area not only causes problems in times of very high water levels (e.g., during the last decades when immense flood events and damage occurred), but also hinders the natural nutrient retention capacity of the river ecosystems. This induces an intensification of nutrient pollution problems in the river waters.

7.3 Material and methods

7.3.1 Soil and Water Integrated Model (SWIM)

The Soil and Water Integrated Model (SWIM) is an ecohydrological model of intermediate complexity simulating the hydrological cycle and vegetation growth integrated with nutrient turnover processes within a river basin driven by climate parameters and taking soil conditions and land use management into account. SWIM was developed on the base of the Soil and Water Assessment Tool (SWAT) (Arnold et al., 1993) and the MATSALU model (Krysanova et al., 1989) specifically as a tool for the analysis of climate and land use change impacts on hydrological processes, agricultural production and water quality at the regional scale. More details can be found in (Krysanova et al., 2000).

Being a spatially semi-distributed dynamic model working with a daily time step, SWIM calculates all hydrological, vegetation and nutrient processes on a hydrotope level (set of elementary units in a subbasin with the same land use class and soil type). Lateral fluxes (surface, subsurface and groundwater flow with associated nutrients) are summarised at the subbasin level and routed through the river network to the outlet of the catchment.

Hydrological processes on the hydrotope level are based on the water balance equation, taking precipitation, evapotranspiration, percolation, surface and subsurface runoff, capillary rise and groundwater recharge into account.

The available water content in soil is influenced by crop and vegetation types, which are parameterised in a database connected to SWIM (Krysanova et al., 2000). The crop database is the same as in SWAT (Neitsch et al., 2002b), and only some parameters were adapted during calibration. The vegetation affects nutrient turnover as well, as plants are important nutrient consumers as well as sources (from plant residue).

The nitrogen module of the applied SWIM version (compare Hesse et al., 2012) calculates nutrient processes in the soil profile and includes several pools: nitrate and ammonium nitrogen, active and stable organic nitrogen, and organic nitrogen in plant residues. They are influenced by fertilisation, mineralisation, volatilisation and (de-)nitrification processes, plant uptake, wet deposition, wash-off, leaching and erosion. Leaching is calculated differently for nitrate and ammonium nitrogen, as the latter has much higher bonding capacity to soil particles.

The soil phosphorus module includes labile phosphate phosphorus, active and stable mineral phosphorus, organic phosphorus and phosphorus in the plant residue. The phosphorus pools are influenced by fertilisation, (de-)sorption, mineralisation, plant uptake, erosion, and leaching. The equation applied to calculate leaching of phosphate phosphorus through the soil profile can be found in Hesse et al. (2008).

Processes related to diffuse source nitrogen and phosphorus flows to the river network are surface runoff, subsurface runoff, groundwater flow, wash-off, leaching, erosion and retention of nutrients in the landscape. After simulating all nutrient-specific processes in the soil profile, nitrogen and phosphorus are transported with surface, subsurface and groundwater flows to the rivers. During their passage through the basin, nutrients are subject to retention and transformation processes in soils, wetlands and in the river system. These processes and model equations, as well as the testing of different retention methods, were described in detail in previous publications (Hattermann et al., 2006; Hesse et al., 2012; Hesse et al., 2013).

Additional information about the general SWIM model concept, necessary input and output data, calibration parameters, process equations as well as the GIS interface for model setup can be found in the User Manual (Krysanova et al., 2000).

7.3.2 Data preparation and model setup for calibration

SWIM model setup requires spatial and temporal data sets as well as major water and land use management information. The spatial maps include a digital elevation model (DEM), a soil map with soil parametrisation, a land use map and a subbasin map. The temporal data sets include the daily historical observed or projected future climate parameters (temperature, precipitation, solar radiation and relative air humidity) as external drivers of the model. The observed river discharge and nutrient concentrations, at least close to the catchment's outlet, are necessary for the model calibration and validation. Additional monitoring data at intermediate gauges and tributaries allow a multi-site calibration, which is more reliable, especially for large-scale catchments. Necessary management data include water abstraction, storage or transfer, major crops with their planting and harvesting dates, as well as fertilisation rates and dates and effluents from industrial sites or waste water treatment plants.

The model setup for the Elbe river was based on spatial maps with a 250 m resolution. The DEM map was resampled from the data provided by the NASA Shuttle Radar Topographic Mission (SRTM). The general German soil map "BÜK1000" delivered by the Federal Institute for Geosciences and Natural Resources (BGR) was combined with the soil map and soil parametrisation of the Czech Republic (Košková et al., 2007) and the European Soil Database (ESDB) provided by the Joint Research Centre of the European Commission to cover the entire Elbe river catchment. The land use map was obtained from the CORINE land cover (CLC2000) data set of the European Environment Agency (EEA) and reclassified to the 15 SWIM land use classes required by the model. The subbasin map was combined from the standard maps of the Federal Environment Agency (UBA) for Germany and the T.G.M. Water Research Institute for the Czech Republic, and included 2268 subbasins.

The historical climate data of 348 climate observation stations located within and 20 km around the Elbe catchment were used to interpolate the climate parameters to the centroids of all subbasins by an inverse distance method for calibration and validation of the SWIM model, taking climate information of at least one to maximum four neighboring stations into account. The station density with available climate data was higher in the German than in the Czech part of Elbe river catchment.

The observed discharge and water quality data for selected gauges located at the Elbe river and its main tributaries in Germany originated from the Data Information System (FIS) of the River Basin Community Elbe (FGG-Elbe) and were downloaded in December 2012. The Czech monitoring data with a monthly time step were taken from the publications of the International Commission for the Protection of the Elbe river (IKSE). In case the observed nutrient concentrations were indicated to be below the detection limit, the minimum detectable concentration was halved and assumed for this day. Data on nutrient inputs from point sources at the German part of the basin were taken from FGG-Elbe (2004a). For the Czech part, assumed data on nutrient emissions from point sources were derived from a report of the IKSE for the year 2000 (1995). As there were only temporally aggregated data available, the point source emissions were implemented in the model as daily constant values.

The standard SWIM does not consider crop rotation management on agricultural fields so that only one main crop type could be assumed on the entire arable land. According to data in the statistical yearbooks of the German federal states in Germany considerably overlaying with the Elbe basin (Thuringia, Saxony-Anhalt, Brandenburg, Saxony and Mecklenburg-West Pomerania), winter wheat was selected to be the main crop. Assuming some nutrient storage in the soils, 100 kg N/ha and 12 kg P/ha were assumed as an average fertilisation level in accordance with recommendations of the federal agriculture agencies. However, fertilisation is recommended to be increased with increasing yield expectations (TLL, 2011a). To implement this option, arable land was classified according to the expected yield as simulated by SWIM (as a function of soil quality, water availability and climate conditions under constant fertilisation). Then the medium yield class received the average fertilisation, and fertilisation of the low/high yield classes was reduced/increased by 20%.

In order to better represent specific behavior of vegetation in lowland areas with its connection to groundwater and the increased evapotranspiration potential, the simpler of two approaches for wetland simulation as described in Hattermann et al. (2008a) was used in SWIM. In total, 22.6% of the entire Elbe river basin belongs to wetlands, with especially high shares in the Schwarze Elster catchment (41%), the lower Elbe reaches (40%), and the Havel river catchment

(33%). In the catchments of the other large tributaries (Saale, Mulde, Ohře and Vltava), wetlands make up 10%–16% of their total areas.

The model calibration and validation for the whole basin was performed for five years, each within the period 2001–2010, considering observed data at the last gauges at Neu Darchau (discharge, Elbe, km 536.4) and Schnackenburg (water quality, Elbe, km 474.5), which are undisturbed by tidal influences. The nutrient loads at the gauge at Schnackenburg were calculated as products of concentration and discharge using the discharge of the gauge at Wittenberge (km 453.9) with the correction factor 1.001 (IKSE, 2007).

The calibration of water discharge (Q) and nutrient loads was done by adjusting the main model calibration parameters described in the SWIM manual (Krysanova et al., 2000), and listed in former SWIM model applications (Hesse et al., 2008; Hesse et al., 2012; Hesse et al., 2013; Hattermann et al., 2005; Huang et al., 2009). During the model calibration it was realised that a global calibration parameter set was not sufficient to represent the basin- and river-specific water and nutrient processes for the several catchments of the Elbe tributaries, which can be highly variable due to different combinations of elevation, soil, land use and river characteristics. Therefore, it was decided to use the most important calibration parameters spatially distributed for the seven large river catchments, which were calibrated individually. Table 7.2 lists and describes those parameters for water quantity and quality calibration used in a distributed mode within the Elbe river basin.

Table 7.2. SWIM calibration parameters applied spatially distributed in the Elbe river basin.

Module	Parameter	Description	Unit
Hydrology	bff	baseflow factor used to calculate return flow travel time	-
	delay	time needed for water leaving root zone to reach shallow aquifer	day
	roc2/roc4	coefficients to correct the storage time constants for surface and subsurface flows	-
Soil nutrients	ret	retention times of nitrate nitrogen (NO_3-N), ammonium nitrogen (NH_4-N) and phosphate phosphorus (PO_4-P) in the lateral subsurface and groundwater flows (6 parameters)	day
	deg	degradation rates of NO_3-N, NH_4-N and PO_4-P in the lateral subsurface and groundwater flows (6 parameters)	day^{-1}
	deth	soil water content threshold for denitrification of NO_3-N	%
	dad/dkd	ratios of adsorbed NH_4-N and PO_4-P to that in soil water	-
In-stream processes	mumax	maximum specific algal growth rate	day^{-1}
	tempo	optimal temperature for algal growth	°C
	lio	optimal radiation for algal growth	ly
	pr20	predation rate in the reach at 20 °C	day^{-1}
	ai1/ai2	fractions of algal biomass that is nitrogen and phosphorus	$mg \cdot mg^{-1}$
	rs1	local algal settling rate in the reach at 20 °C	$m \cdot day^{-1}$
	rs2/rs3	benthic source rates for PO_4-P and NH_4-N in the reach at 20 °C	$mg\ (m^2 \cdot day)^{-1}$
	rs5	organic phosphorus settling rate in the reach at 20 °C	day^{-1}
	rk2	oxygen reaeration rate in the reach at 20 °C	day^{-1}
	bc3	rate constant for hydrolysis of organic nitrogen to NH_4-N at 20 °C	day^{-1}
	bc4	rate constant for mineralisation of organic phosphorus to PO_4-P at 20 °C	day^{-1}

7.3.3 Evaluation of model results

The ability of SWIM to simulate water and nutrient processes in the Elbe catchment and to reproduce the observed monitoring values was evaluated in different ways for water quantity and quality.

The simulated daily and/or monthly discharges were assessed using the Nash-and-Sutcliffe efficiency (NSE, Nash & Sutcliffe (1970)) as well as the deviation in water balance (DB) (compare Hesse et al., 2008). The non-dimensional NSE is a measure to analyse the squared differences between the observed and simulated values, and DB describes the long-term differences of the observed values against the simulated ones for the whole simulation period in percent.

The model's efficiency to represent the water quality parameters was evaluated at the long-term average monthly basis using three criteria, $\Delta\mu$, $\Delta\sigma$ and r, according to Gudmundsson et al. (2012). Here $\Delta\mu$ is a balance measure defined as the relative bias of the mean annual observed and simulated values. Criterion $\Delta\sigma$ evaluates the amplitude or the spread from the lowest to the highest monthly values of the mean annual cycle by comparing the relative difference in standard deviations of the observed and the simulated values. Also, the usual Pearson's correlation coefficient r, which is sensitive to differences in the shape as well as in the timing of the mean annual cycle, was applied.

Table 7.3 lists the possible ranges, optima and aspired results of the different performance criteria used in this study.

	Range	Optimum	Aim in this study
NSE	-∞ to 1	1	>0.65
DB	-∞ to +∞	0	>-20% - <20%
Δμ	-∞ to +∞	0	>-0.2% - <0.2%
Δσ	-∞ to +∞	0	>-0.2% - <0.2%
r	-1 to 1	1	>0.5

Table 7.3
Description of performance criteria used in this study to evaluate model results.

7.3.4 Description, evaluation and processing of climate scenario data

The ENSEMBLES project (van der Linden & Mitchell, 2009) delivered projections for a possible climatic future of Europe by running an ensemble of different Regional Climate Models (RCMs) using the boundary conditions produced by several General Circulation Models (GCMs). All models assumed the A1B emission scenario with a balanced use of fossil and non-fossil fuels in a world with a rapidly growing economy, population growth until 2050 and a decline afterwards, and fast development of new and effective technologies (IPCC SRES, 2000). According to this scenario an average global temperature rise of 2.8 °C (with a range between 1.8 and 4.4 °C) is estimated (IPCC, 2007) until the end of the 21st century.

The resulting ENSEMBLES climate scenarios differ in resolution (25 or 50 km grids) and simulation period (1951/1961–2050/2100). For our study, 19 scenarios covering the period until 2100 were chosen (Table 7.4). As climate data necessary for SWIM modelling were not available for all scenarios until 2100, only data until 2098 were considered in all cases. A scenario-specific number of grid cells with data were treated as virtual climate stations for climate interpolation to the centroids of the 2268 subbasins within the Elbe basin using an inverse distance method.

Table 7.4 Numbering of the chosen ENSEMBLES scenarios as combinations of General Circulation Models (GCMs) and Regional Climate Models (RCMs), the responsible institute, resolution [km], starting year, and number of grid cells used for interpolation of the projected climate in the Elbe catchment.

ID	Institute	GCM	RCM	Reso-lution	Start year	Number of grid cells
1	SMHI	HadCM3Q3	RCA	25	1951	316
2	HC	HadCM3Q0	HadRM3Q0	25	1951	316
3	HC	HadCM3Q3	HadRM3Q3	25	1951	316
4	HC	HadCM3Q16	HadRM3Q16	25	1951	316
5	C4I	HadCM3Q16	RCA3	25	1951	316
6	ETHZ	HadCM3Q0	CLM	25	1951	316
7	KNMI	ECHAM5-r3	RACMO	25	1951	316
8	SMHI	BCM	RCA	25	1961	316
9	SMHI	ECHAM5-r3	RCA	25	1951	316
10	MPI	ECHAM5-r3	REMO	25	1951	316
11	CNRM	ARPEGE_RM5.1	Aladin	25	1951	300
12	DMI	ARPEGE	HIRHAM	25	1951	316
13	DMI	ECHAM5-r3	DMI-HIRHAM5	25	1951	316
14	DMI	BCM	DMI-HIRHAM5	25	1961	316
15	ICTP	ECHAM5-r3	RegCM	25	1951	282
16	KNMI	ECHAM5-r1	RACMO	50	1951	79
17	KNMI	ECHAM5-r2	RACMO	50	1951	79
18	KNMI	ECHAM5-r3	RACMO	50	1951	79
19	KNMI	MIROC	RACMO	50	1951	79

To analyse the projected trends of single climate scenarios, climate change signals were calculated for two future periods for temperature, precipitation and solar radiation. Climate change signals describe the differences between the mean climate parameter values in a future period and in the reference period of the same scenario. The signals were derived taking all scenario grid cells into account and were evaluated for the annual mean climate parameter values as well as for their seasonal dynamics.

The 19 climate scenarios were used to drive the calibrated SWIM model, each for the reference period 1971–2000 (p0) and the two future periods 2021–2050 (p1) and 2071–2098 (p2).

It is very important which downscaling approach is used to generate climate scenarios, and whether it is statistical or dynamical. The choice of a hydrological model is less important in terms of its contribution to uncertainty, especially when only the long-term mean annual changes are compared (Gädeke et al., 2014). Often it was detected that results achieved with one hydrological model under two or more climate scenarios differ more than the results of different hydrological models achieved by using only one climate scenario (Arheimer et al., 2012; Piniewski et al., 2014). Hence, many authors suggest using an ensemble of climate change scenarios to get the full range of uncertainty between the different scenario projections (Huang et al., 2015; Tebaldi & Knutti, 2007; Kling et al., 2012). The last two authors also mentioned that there is no direct link between the climate model performance in the historical period and the robustness of trends in the future, and thus the application of a smaller number of best fitting scenarios could not be recommended. Therefore, in our study we did not try to find the most probable future climate scenarios by their comparison with the historical measurements.

The observed climate data are also often used for bias correction of climate scenarios before applying them for impact assessment in order to avoid unrealistic simulations of runoff or nutrient loads. However, there is no consistent opinion on the usefulness of bias correction for impact assessments. While Teutschbein & Seibert (2010) recommend an application of bias correction, other authors complain about the lack of physical justifications of corrections damaging the physical consistency between the variables (Gädeke et al., 2014; Ehret et al., 2012). The latter do not appreciate this method as a "valid procedure", and complain that an additional uncertainty is added to the model chain. In our study it was decided not to use bias correction and to simply compare the simulations driven by 19 RCMs between periods to detect trends and the relative changes caused by climate change.

7.3.5 Processing of socio-economic change experiments

In addition to climate change simulations, five land use change experiments were applied for testing the effects of specific socio-economic measures aimed at reducing point or diffuse nutrient emissions.

The applied land use change scenarios are listed in Table 7.5 together with the description of the changes implemented in model input data. Two scenarios are dealing with the direct reduction of nutrient emissions ("Point sources" and "Fertilisation") by 10% or 20%. The decrease of point source emissions was assumed with different percentages for the two nutrients, as it was supposed that phosphorus reduction potential in sewage treatment is higher. The third scenario ("Retention") indirectly tested the effects of a possible increase of the retention potential and decomposition rate in the soils of the Elbe catchment by 10%. This could be achieved by different measures, for example by extension of wetland areas around the watercourses or intensified cultivation of plant communities with a high nutrient intake rate (mycorrhiza, legumes). In addition, two such measures were tested directly in the model ("Buffer" and "Slope") by changing the land use composition in the catchment. Due to the spatial resolution of the SWIM project with 250 × 250 m raster maps, water courses in agricultural areas were converted to 250 m raster cells in the "Buffer" experiment, containing extensive meadows without fertilisation. In the "Slope" scenario, all agricultural areas with a slope >4% were converted to extensively used meadows to study the effects on water quantity and quality in the catchment (see e.g., BMVEL (2002) where hillsides with slopes >4% are considered as being a risk of facilitating erosion).

Table 7.5 Description of applied land use change experiments in the Elbe river catchment.

Scenario name	Description
Point sources	Reduction of emissions from point sources (nitrogen -10%, phosphorous -20%)
Fertilisation	Reduction of N and P fertilisers on agricultural land by 20%
Retention	Increase of nutrient retention time and decomposition rate in soils by 10% each
Buffer	Conversion of all agricultural lands around water courses to extensive meadow
Slope	Conversion of agricultural lands to extensive meadows on hillsides with slopes >4%

The socio-economic experiments were run under the 19 ENSEMBLES climate scenarios to allow evaluation of the combined climate and land use change impacts on water quantity and quality in addition to the land use change impacts only. As 19 climate scenarios were applied with specific climate conditions, the results were different, not only for the combined impacts, but also for the land use change impacts. To show the possible effects of scenarios, the 19 single percental changes of the model outcomes were analysed regarding their medians and 25th/75th percentile values, representing the most probable 50% range of all scenario results.

7.4 Results

7.4.1 SWIM model calibration and validation

A successful calibration of a model for water quality requires a well-calibrated hydrological model. During the hydrological and water quality calibration, the observed and simulated values at the most downstream Elbe gauges, at the gauges located close to the German-Czech border, as well as at the main tributaries were compared and statistically evaluated for the period of 2001–2010.

Figure 7.2 presents the observed and simulated daily discharges for the 10-year period (left), and the long-term daily averages (right) at the two main Elbe gauges Schöna and Neu Darchau. The discharge dynamic is well reproduced, reaching the good to very good performance ratings. The performance criteria for the daily model results are better at the downstream gauge Neu Darchau. The long-term seasonal dynamics are reproduced well at both gauges.

However, not all simulation results at the tributaries reach the same model performance (Table 7.6). The most difficult river to simulate was the Schwarze Elster, which is highly influenced by human activities and regulation (opencast lignite mining, discharge regulation and stream straightening), so that the hydrological processes are no longer natural. As these site-specific management measures were not implemented in the model, the model does not perform well enough at the Löben gauge. Similar problems apply to the lowland catchment of the Havel river, which is characterised by a high number of wetland areas and stream lakes, and is also highly affected by lignite mining in its upper course, all this leading to lower NSE values at gauge Havelberg.

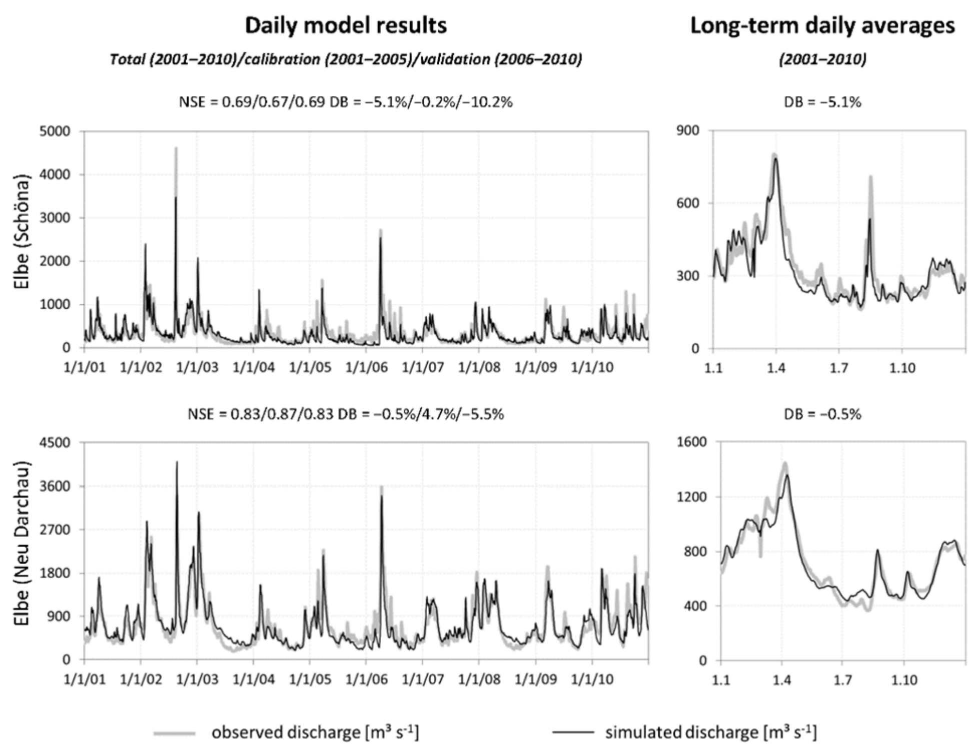

Figure 7.2 Calibration results for the Elbe river discharge at the most downstream gauge Neu Darchau and the intermediate Elbe gauge Schöna (Czech/German border) for the time period 2001–2010, separated into calibration and validation subperiods.

Table 7.6 Model performances for four discharge gauges of the Elbe river and six gauges of its main tributaries from the upstream to downstream location of tributaries.

River	Gauge	Time period	NSE [-]		DB [%]
			daily	*monthly*	
Elbe	Nymburk	11/2002-10/2010		0.75	-13.5
Vltava	Vranany	11/2002-10/2010		0.64	-10.5
Ohře	Louny	11/2002-10/2010		0.86	-0.3
Elbe	Schöna	2001-2010	0.69	0.77	-5.1
Schwarze Elster	Löben	2001-2008	0.25	0.60	13.4
Mulde	Bad Düben	2001-2010	0.74	0.88	1.7
Saale	Calbe-Grizehne	2001-2010	0.61	0.84	1.5
Elbe	Magdeburg	2001-2010	0.82	0.86	1.1
Havel	Havelberg	2001-2010	0.54	0.68	-1.5
Elbe	Neu Darchau	2001-2010	0.83	0.86	-0.5

Only monthly measurements for a shorter time period were available for the three gauges located in the Czech part of the Elbe basin. The best results here could be achieved for the smaller and mountainous river Ohře. The upper part of the Elbe river (gauge Nymburk), as well as the largest Elbe tributary, Vltava, show a slight underestimation of discharge. This could be explained by water regulation measures in the water course of these rivers, with a high number of barrages and dams to ensure water availability for shipping and for flood protection, which were not implemented in the model. However, the hydrological model performance in terms of NSE and DB for the Elbe and its tributaries mostly meet the aim (compare Table 7.3), so that it was used for the subsequent water quality calibration.

Figure 7.3 presents the results of water quality calibration for two main gauges in the Elbe river: Schmilka at the Czech-German border and the most downstream Elbe gauge Schnackenburg. The long-term average daily observed loads were calculated based on interpolated values between biweekly measurements and have some degree of uncertainty. The calibration was aimed at visually and statistically matching the inner-annual dynamics and minimising the deviation in balance of the mean annual nutrient loads for the 10-year period of 2001–2010.

In Figure 7.3, a specific annual cycle of the three nutrients can be observed, which is reproduced quite well by the SWIM model. The nitrate nitrogen loads (mainly coming from diffuse sources) generally follow the discharge curve with a spring peak and low values in summer. Ammonium nitrogen and phosphate phosphorus are more algae-influenced. The periods with high concentrations of chlorophyll *a* especially result in ammonium depletion in the river due to the high ammonium preference factor of the algae defined in the model. Algal influences on the phosphate loads are less significant, but also obvious, especially during the spring algal bloom. The dissolved oxygen loads are highly connected to the water amounts and are simulated very well. The balance measure $\Delta\mu$ is low in all cases and is located within the aimed range, also reflecting sufficiently good calibration results.

Figure 7.4 and Table 7.7 show results on water quality for the main tributaries of the Elbe river and for selected Elbe gauges. Figure 7.4 plots the simulated versus observed long-term average monthly values and illustrates the variation of the long-term seasonal cycle ratios around a diagonal of perfect fit, and Table 7.7 analyses the model's performance statistically.

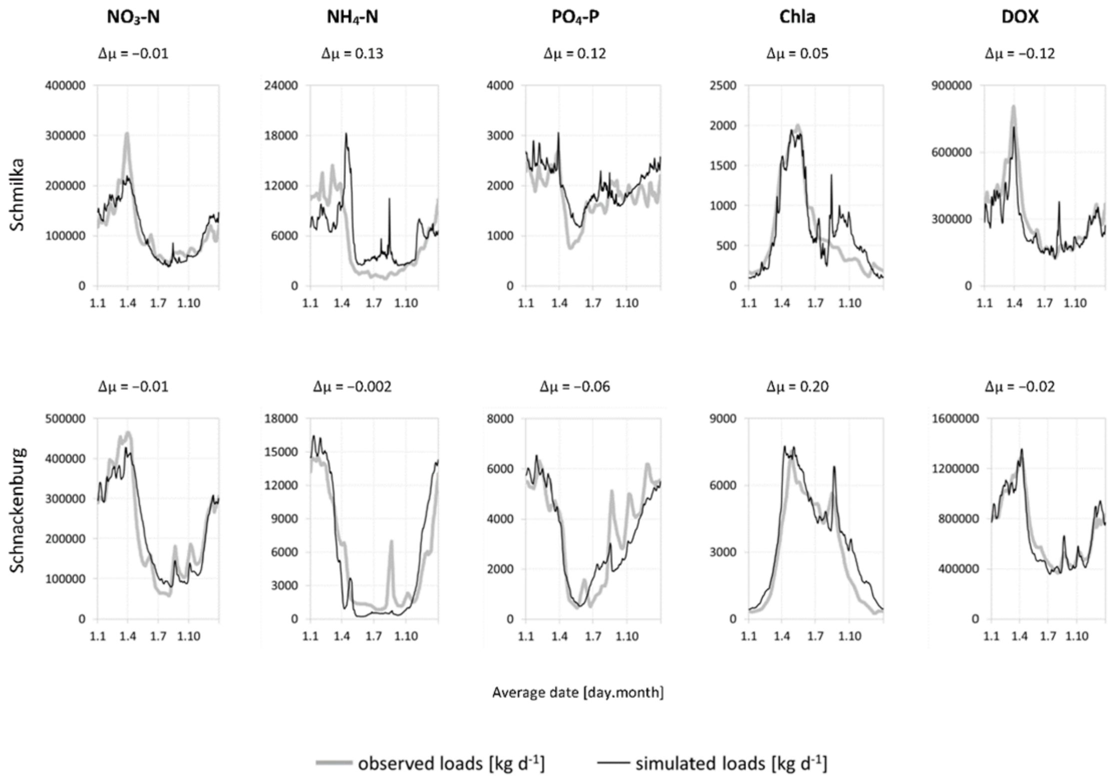

Figure 7.3 Long-term average daily observed and simulated loads of nitrate nitrogen (NO_3-N), ammonium nitrogen (NH_4-N), phosphate phosphorus (PO_4-P), chlorophyll *a* (Chla) and dissolved oxygen (DOX) at the two Elbe gauges Schmilka (corresponds to the total Czech loads) and Schnackenburg (most downstream gauge) for the time period 2001–2010.

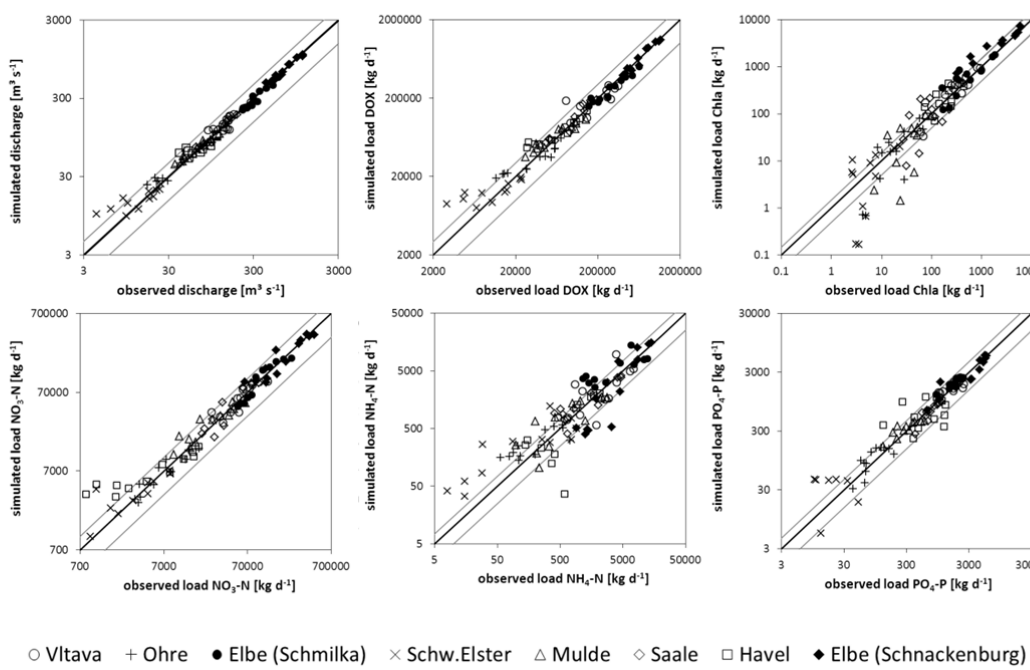

Figure 7.4 The long-term average monthly observed and simulated discharge and loads per tributary and at two selected Elbe gauges in the period 2001-2010 (diagonals: black – perfect fit, grey – ± 50% intervals).

Table 7.7 Model ability to simulate the long-term monthly average loads of water quality variables for six main tributaries as well as three selected Elbe water quality observation gauges in the time period 2001-2010 after spatially distributed model calibration. The model performance variables were calculated according to Gudmundsson et al. (2012) and are described in section 7.3.3.

	Vltava *Zelčín*	Ohře *Terezín*	Elbe *Schmilka*	Schwarze Elster *Gorsdorf*	Mulde *Dessau*	Saale *Groß Rosenburg*	Elbe *Magdeburg*	Havel *Toppel*	Elbe *Schnackenburg*
Time period	2001-2004	2007-2010	2001-2010	2004-2010	2001-2010	2001-2010	2001-2010	2001-2010	2001-2010
					NO_3-N				
Δμ	-0.01	-0.09	-0.01	-0.13	0.04	0.10	0.09	-0.01	-0.01
Δσ	-0.11	-0.23	-0.04	-0.27	-0.20	0.18	0.03	-0.42	-0.07
r	0.91	0.93	0.93	0.96	0.93	0.94	0.93	0.97	0.95
					NH_4-N				
Δμ	0.02	0.12	0.13	0.17	-0.08	-0.01	0.17	0.05	0.01
Δσ	0.17	-0.25	-0.23	0.02	-0.31	-0.19	0.08	0.13	0.26
r	0.64	0.74	0.68	0.53	0.85	0.97	0.92	0.94	0.95
					PO_4-P				
Δμ	-0.01	0.11	0.12	0.12*	0.03	-0.11	0.10	-0.10	-0.06
Δσ	-0.40	0.01	-0.02	0.39*	-0.37	-0.03	0.00	-0.19	-0.03
r	0.73	0.70	0.87	0.13*	0.87	0.93	0.92	0.24	0.94
					Chl. a				
Δμ	0.08	-0.02	0.05	0.03	-0.08	0.04	0.06	0.12	0.20
Δσ	0.06	0.12	-0.07	0.05	0.17	0.04	-0.07	0.18	0.00
r	0.95	0.82	0.94	0.82	0.80	0.82	0.91	0.78	0.97
					DOX				
Δμ	-0.06	-0.12	-0.12	0.02	-0.01	0.06	0.04	0.03	-0.02
Δσ	-0.28	-0.39	-0.30	-0.50	-0.37	0.08	-0.02	-0.25	0.02
r	0.85	0.95	0.98	0.91	0.95	0.97	0.96	0.98	0.98

*2008-2010

As already detected in the hydrological calibration, the largest discrepancies between the observed and simulated values can be seen for the Schwarze Elster river. The intensive human activities within this catchment (e.g., surface water management due to lignite mining) influence nutrient processes, but are not fully implemented in the model, resulting in model outputs different from observations. Some problems can also be seen for the Havel and (partly) the Mulde tributaries. The largest dispersion around the diagonal of perfect fit is obvious for ammonium nitrogen, which is difficult to model as it is highly influenced by point source emissions involving input data uncertainty as well as by algal consumption processes (parameter uncertainty). The latter, due to their complex behavior influenced by many physical, chemical and biological interactions, are difficult to model, especially in large basins. The results in terms of statistical criteria (Table 7.7) with mostly high r and low Δμ and Δσ confirm the visual impression.

Generally, the calibrated SWIM model for the large-scale Elbe river basin matches observations well, and can be used for climate and land use change impact assessment.

7.4.2 Climate change signals of the ENSEMBLES scenarios

Before applying the 19 ENSEMBLES climate scenarios to the Elbe basin, they were analysed for their trends in temperature, precipitation and solar radiation averaged over the whole basin by comparing two future scenario periods, p1 and p2, with the reference period p0. The comparison was done for the long-term average annual values as well as for the long-term average monthly values of all scenarios and periods.

The climate change signals per scenario can be found in Table 7.8. The results show an increase in temperature by 1.3 °C for the first period and by 3 °C for the second period on average, as well as an increase in precipitation by +41/+57 mm on average for all 19 climate scenarios. The increase in precipitation is accompanied by a decrease in solar radiation of −15/−27 J cm^{-2} on average, probably due to increased cloudiness with higher precipitation amounts. There is a wide spread in signals between the scenarios, which is increasing in the second period. Regarding temperature, all scenarios agree on increasing trend, but the increase in period p2 ranges between 2 and 5 °C depending on the scenario. The agreement of the single scenarios with the overall trends is lower for precipitation (15 of 19 scenarios agree with the trend) and solar radiation (14 scenarios agree). However, a majority of scenarios correspond to the average trends.

Table 7.8 Climate change signals for temperature, precipitation and radiation of 19 analysed ENSEMBLES climate scenarios and on average for the two future periods 2021-2050 (p1) and 2071-2098 (p2) compared to the reference period 1971-2000 (p0) for the Elbe basin.

Scenario	Temperature [°C]		Precipitation [mm]		Radiation [J cm^{-2}]	
	p1-p0	p2-p0	p1-p0	p2-p0	p1-p0	p2-p0
S1	1.5	2.9	67	95	-26	-76
S2	2.1	4.0	-2	16	27	28
S3	1.7	3.4	34	17	8	7
S4	2.2	5.0	48	-49	1	43
S5	1.8	4.1	104	94	-57	-67
S6	1.7	3.5	24	13	-22	-12
S7	0.9	2.6	35	110	-12	-20
S8	0.7	1.9	63	86	-30	-48
S9	0.8	2.4	47	112	-29	-65
S10	0.9	2.6	14	47	-18	-42
S11	1.1	2.8	-4	-68	5	36
S12	0.9	2.0	14	-31	-16	-111
S13	0.6	2.0	57	157	-21	-73
S14	0.9	2.5	37	99	-29	-47
S15	0.9	2.6	29	87	1	7
S16	1.0	3.1	52	63	-12	-5
S17	1.4	3.3	65	54	-22	-11
S18	0.9	2.6	36	99	-16	-20
S19	1.8	3.9	50	76	-26	-40
$mean_{all}$	1.3	3.0	41	57	-15	-27
$stdev_{all}$	0.5	0.8	26	60	18	42

The seasonal climate change signals are visualised in Figure 7.5. Looking at the changes per month, it is obvious that the value as well as the spread of the climate change signals is higher in the second period. The increase in temperature is confirmed for the entire course of the year, and it is lowest in May and highest in winter months (December–February) and in August. The changes in precipitation and solar radiation vary around the zero-line and show an opposite behavior (probably due to connection of precipitation and cloudiness). In the first period precipitation is slightly decreasing in July and August, and in the second period negative changes in precipitation are projected from June to September. The changes in solar radiation show almost the opposite trends. In general, the 19 ENSEMBLES climate scenarios project a warmer and wetter climate with less sunshine hours from autumn to spring, but a warmer, dryer and sunnier climate in the summer months for the region.

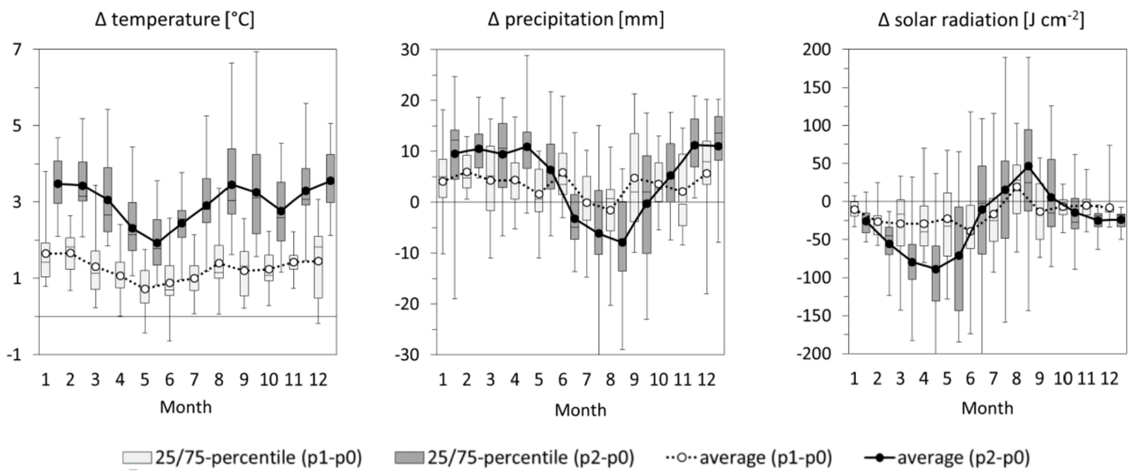

Figure 7.5 Ranges of seasonal climate change signals for temperature, precipitation and solar radiation of 19 ENSEMBLES climate scenarios for the two future periods compared to the reference period of the same scenario for the Elbe basin. The plots represent median (line), $25^{th}/75^{th}$ percentiles (box), min/max values (whiskers) and the average (dots) change of all 19 scenarios.

7.4.3 Climate change impacts

The projected changes in climate lead to changes in simulated water quantity and quality variables in the Elbe basin in future periods. The results are shown Figure 7.6 for the two Elbe river gauges Schöna and Neu Darchau. They present changes in the long-term average seasonal dynamics comparing the average and the $25^{th}/75^{th}$ percentile ranges of six variables from simulations driven by 19 climate scenarios in the future and the average of the reference period 1971–2000.

Following the increasing trend for precipitation in the Elbe basin, the discharge is projected to increase as well, both at the last Elbe gauge and at the gauge of the Czech-German border. The increase can be observed during almost the whole year, with the highest values in winter months (due to higher rainfall) and the lowest values, or even negative changes in the p1 period, in April (due to lower or missing snow melt peaks). Though a decrease in precipitation is projected in the summertime (compare Figure 7.5), the projected discharge in summer months is higher than in the reference period, probably due to the capability of soils to retain additional winter and spring water causing delayed subsurface and groundwater flows. However, the uncertainty ranges for the projected discharge are quite high, especially at the most downstream gauge.

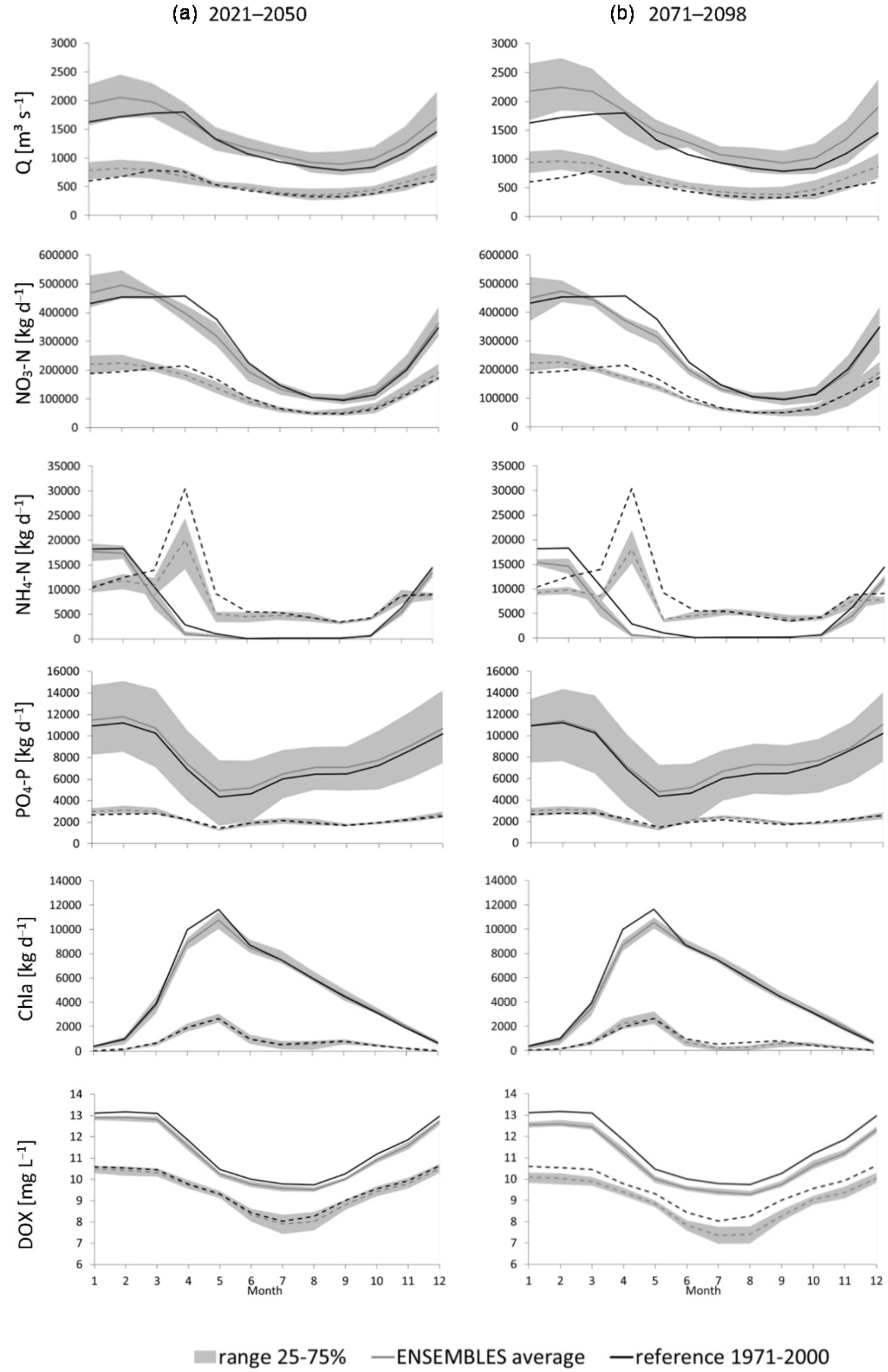

Figure 7.6 The long-term average monthly values of simulated discharge (Q), nutrient and chlorophyll *a* loads (NO_3-N, NH_4-N, PO_4-P, Chla) and dissolved oxygen concentrations (DOX) with uncertainty ranges (25^{th}/75^{th} percentiles corresponding to 19 simulations) at the two Elbe gauges Neu Darchau (full lines) and Schöna (dashed lines) for the future periods 2021–2050 (p1, a) and 2071–2078 (p2, b) in comparison to the corresponding average values of the reference period 1971–2000 (p0).

The nitrate nitrogen load performs similarly to the discharge, as nitrate nitrogen comes to the river mainly dissolved in water from diffuse sources. A moderate increase can be observed in the first winter months, followed by some decrease in spring, whereas the second half of the season shows only minor changes on average compared to the reference period (due to higher retention time of nitrate nitrogen compared to water as well as impacts of vegetation).

The ammonium nitrogen loads are higher on average in the upstream part of the Elbe (gauge Schöna) than downstream (gauge Neu Darchau) due to higher loads in the Czech part of the catchment as well as to progressively increasing phytoplankton concentration downstream of the Elbe. The decrease in ammonium load caused by changes in climate conditions is obvious in the first half of the season (especially during spring flood). The decrease in NH_4-N loads is probably connected to the rising temperatures, as mineralisation processes and the emergence of leachable ammonium in soils are temperature-related and occur mainly within a certain temperature range. The uncertainty ranges around the ENSEMBLES average, representing the most probable 50% of the 19 scenario results, are quite narrow.

The average phosphate phosphorus load shows a slight and almost constant increasing trend throughout the season, but the uncertainty ranges are the largest for this nutrient, caused by the high uncertainty and climate-dependence of phosphorus-related processes in the Havel catchment (compare with Figure 7.7). The increase in loads is probably connected to increasing erosion and leaching processes with higher precipitation in the future, washing more phosphorus from sandy and highly permeable soils. It could also be a result of less ingestion by a decreasing algae population in the future.

The chlorophyll *a* load is projected to decrease in the spring blossom time, when warmer temperatures (temperature stress) and lower solar radiation (below the optimum value) may hamper phytoplankton growth and less ammonium is available for algae consumption.

The dissolved oxygen concentration in the Elbe river is projected to decrease, and the changes remain almost constant throughout the season. This is probably connected to the increasing water temperature, resulting in lower values of oxygen saturation in the water. The uncertainty ranges for future dissolved oxygen concentrations are higher upstream, probably due to the generally higher ammonium loads modelled in the upper river reaches, where oxygen is used for nitrification in the water column.

In addition to the temporal analysis of climate impacts, Figure 7.7 illustrates some spatially distributed results for the Elbe and its tributaries. For that, average percental changes were calculated for six main tributaries of the Elbe and two Elbe gauges (the same as in Figure 7.6).

The overall trend for the entire basin can be generally detected regarding different variables in Figure 7.7, though there are some outlying subcatchments. For all gauges an increasing discharge is projected, which becomes higher in the second period. Also, the uncertainty ranges increase in p2. The differences between gauges are small.

The nitrate nitrogen load decreases on average for the entire Elbe river basin (Neu Darchau). The decrease is largest for the Saale catchment, which is characterised by the highest share of agricultural areas due to very fertile soils with a high nutrient retention capability. There are also some subcatchments where a small increase (or no change) in nitrate load on average is simulated. This is probably connected to an increased diffuse pollution with increased precipitation in these subareas.

The impacts on ammonium nitrogen loads are almost all negative, and show a high diversity between the subcatchments. The uncertainty ranges are highest in the Vltava and Schwarze Elster subcatchments, where ammonium pollution is generally at its highest level, and have more space for variability due to climate change impacts.

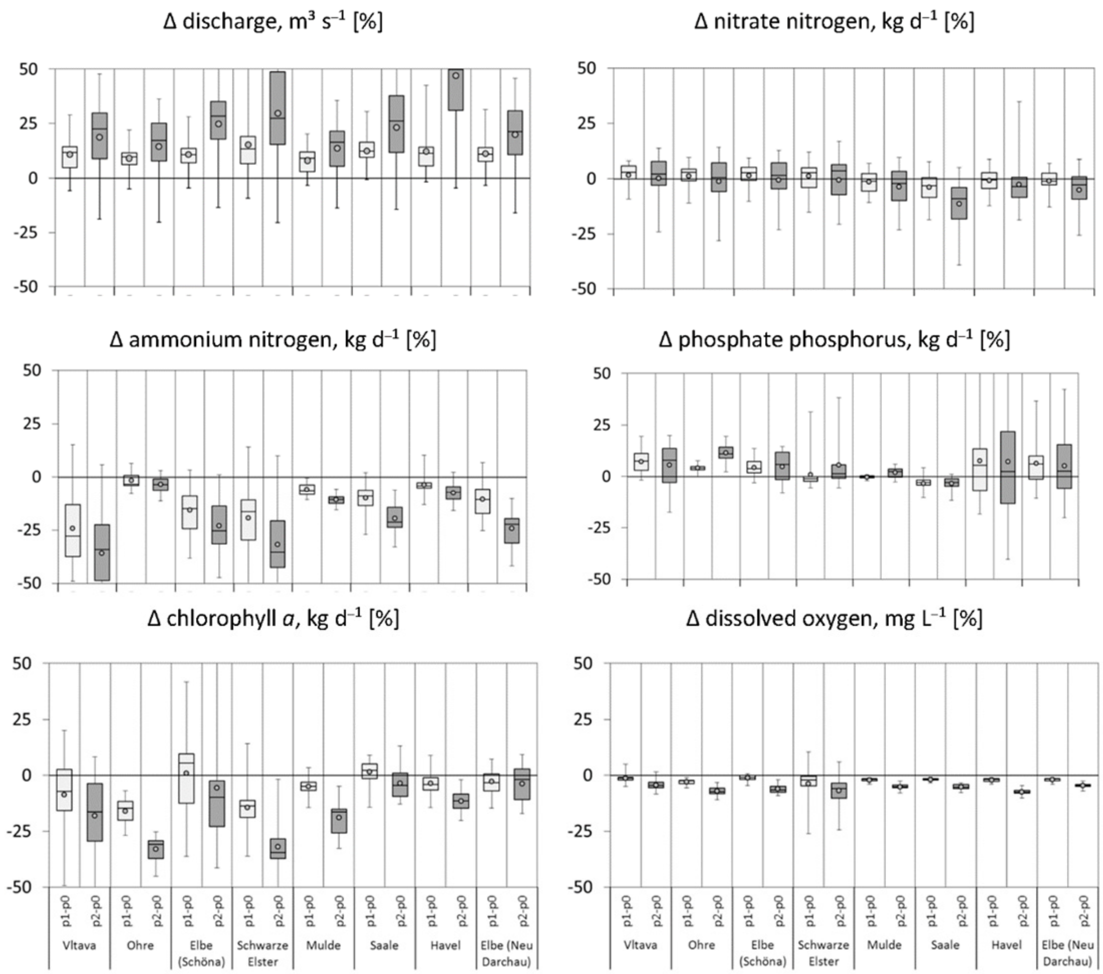

Figure 7.7 Ranges of the percental changes of 30-year-average river discharges, nutrients and chlorophyll *a* loads, as well as dissolved oxygen concentrations in the Elbe river and its main tributaries simulated with SWIM driven by 19 ENSEMBLES climate scenarios (in future periods p1 (light) and p2 (dark) compared to the reference period p0 of the same scenario). The plots visualise the following ranges: min/max (whiskers), 25th/75th percentiles (boxes), median (line) and average (dots) changes of all 19 scenarios.

Except for the Saale subcatchment with its fertile soils and high nutrient retention potential, the climate change impact on phosphate phosphorus shows increasing loads due to increased leaching and erosion processes. The uncertainty ranges are extremely high in the Havel subcatchment, where phosphorus contamination is the highest in the Elbe drainage area, and a high share of permeable and sandy soils causes a high phosphorus leaching potential with higher precipitation amounts.

Chlorophyll *a* demonstrates a decreasing trend on average almost everywhere. The uncertainty ranges, especially in the upper tributaries, are quite high, due to the high complexity of algae processes simulated in the model, which are influenced by many system-internal and external drivers.

Changes in the dissolved oxygen concentrations have a very small uncertainty range and show a decreasing trend on average for all gauges due to increased temperatures and lower oxygen saturation capacity. The highest range in average changes can be observed for the Schwarze Elster subcatchment, which is quite heavily polluted with ammonium nitrogen. The latter is highly sensitive to climate change impacts and is connected to the oxygen processes in the river water.

7.4.4 Socio-economic change impacts under climate change

In addition to the climate change impact assessment, five land use change experiments were run to test the model's reaction on certain management measures aimed at reducing nutrient inputs to the river network. The aim was to check whether such measures are able to be reversed, intensify or revoke climate change impacts. The land use change experiments were run 19 times, driven by the 19 ENSEMBLES climate scenarios for the near future period 2021–2050 (p1), and the results were compared with the results achieved under the reference management conditions for the period 1971–2000 (p0) of the same scenarios (combined impacts) as well as with the climate scenario-driven results with the reference management for period p1 (land use change impacts only).

The single and combined impacts were analysed for the two Elbe gauges Schöna (Czech/German border) and Neu Darchau (Elbe outlet) as well as for the outlets of the two selected tributaries Saale and Havel (Figure 7.8). The results are shown as median values with a 25th/75th percentile range. In some cases, even the single land use change impact shows some range of relative changes caused by different behavior of temperature- and water-dependent nutrient processes under different climate conditions used as an external driver.

The socio-economic changes related to nutrient inputs to the river network (experiments "Point sources" and "Fertilisation") and an increased nutrient retention potential in soils (experiment "Retention") have no influence on water discharge. Only the combined impacts show an increase in discharge of about 10% due to climate change. The solely socio-economic impacts of a changed land use composition ("Buffer" and "Slope") on river discharge show a decrease (due to increased evapotranspiration of the enlarged grassland areas), but it is quite low, and cannot compensate the increase in Q caused by the projected climate change, so that all combined impacts for these experiments have a positive direction.

The reduction of point source emissions has the highest influence on phosphate and ammonium loads, as these nutrients mainly originate from anthropogenic inputs of water treatment plants or industrial units. The projected climate change even intensifies the reduction of ammonium nitrogen loads in the rivers, whereas the decrease of phosphate phosphorus is reduced by climate change impacts (except for the Saale basin). The sole reduction of point source emissions predominantly results in a decrease of chlorophyll *a* loads in the rivers due to less available ammonium and phosphate as algal food.

The decrease in fertiliser application causes lower nitrate loads in all analysed river parts, as this nutrient originates mainly from diffuse sources (predominantly from agricultural fields).

The reduction is only marginally influenced by climate change. A decrease in fertilisation affects NH_4-N only partly, and causes decreased ammonium loads, particularly in the upper part of the Elbe basin. As the changes in NH_4-N and PO_4-P loads are less distinct under the "Fertilisation" experiment, chlorophyll *a* loads are only marginally influenced. The on-average-increasing chlorophyll *a* trend caused by climate change impacts in the upper Elbe and Saale catchments cannot be reversed by a simple reduction of fertilisation in the combined experiments.

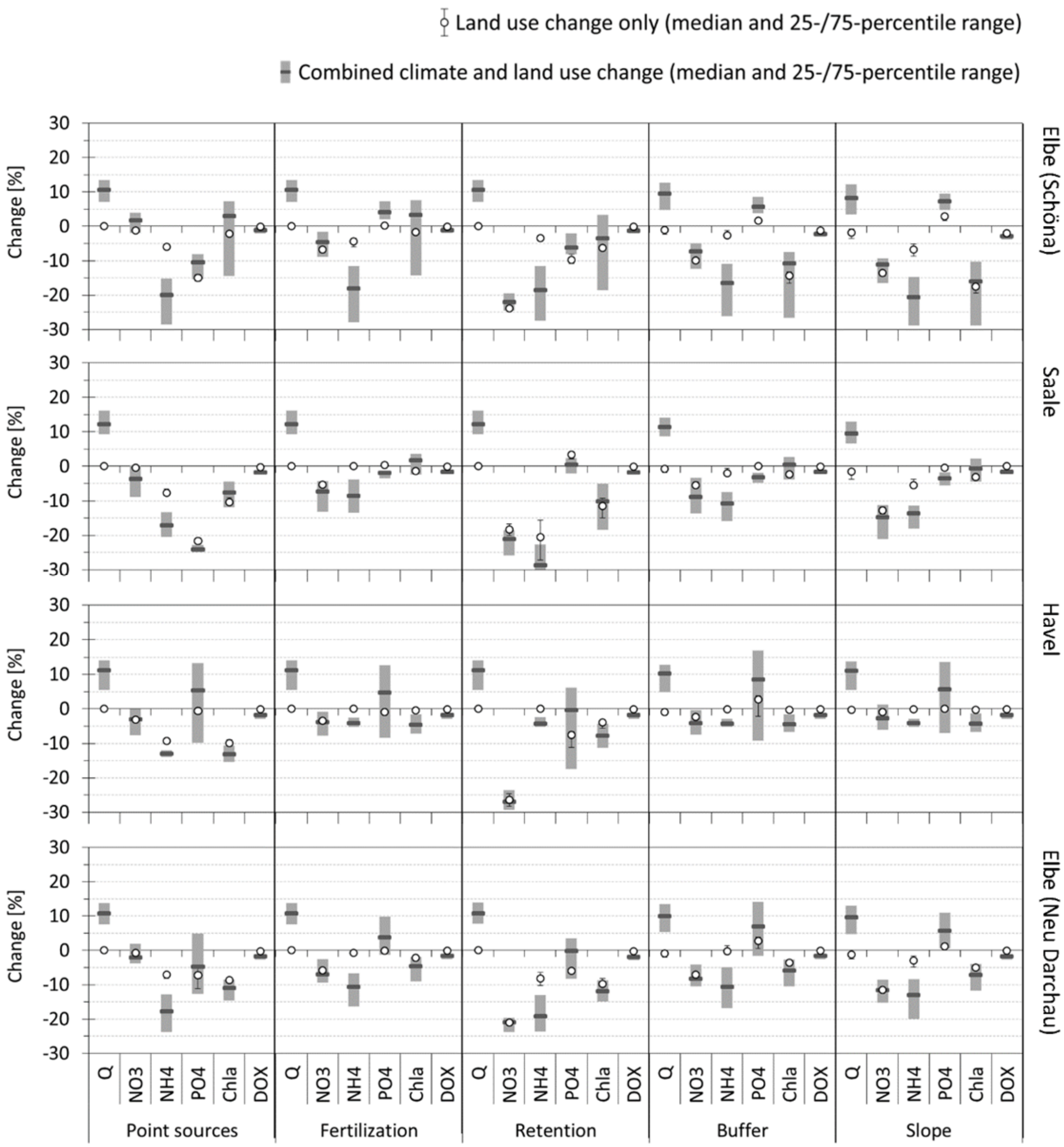

Figure 7.8 Impacts of socio-economic changes and combined climate and socio-economic changes on the average water discharge (Q), nutrient (NO_3-N, NH_4-N, PO_4-P) and chlorophyll *a* (Chla) loads and dissolved oxygen concentrations (DOX) of the Elbe river at two stations and at two main German tributaries. The dark grey bars and white dots show the median of 19 percental changes together with their 25th/75th percentile ranges (light grey ranges and black whiskers).

An increased nutrient retention and decomposition potential in the soils of the landscape ("Retention") has the highest impact on nutrient loads. Especially the diffuse nitrate nitrogen loads are affected, but also ammonium and phosphate show some reactions, though with different magnitudes for the four analysed gauges. The diversity in the magnitude of changes for the river parts can be explained by the heterogeneity and distribution of land use patterns and point sources as well as by the diversity in projected climate change within the catchment. As NH_4-N and/or PO_4-P are remarkably reduced under the retention experiment, chlorophyll *a* shows a decreasing trend due to a lack of nutrients. This reduction is even able to reverse the increasing trend in chlorophyll *a* caused by climate changes in the upper Elbe and Saale subcatchments.

Two experiments dealing with a changed land use composition ("Buffer" and "Slope") result in more meadows and less agricultural areas in the subcatchments and show similar results in the different river parts. Nitrate nitrogen is reduced most in the majority of cases due to less agricultural area with fertiliser application and hence lower total fertiliser loading under the experiments. The highest diversity of changes can be seen under the "Slope" experiment in the upper Elbe and Saale subcatchments, which are characterised by a high share of mountainous areas, where the share of transformed land use areas is higher than in the lowland subcatchment of the Havel river. For the latter, the "Slope" experiment has nearly no impact on the model outputs, and the combined changes result only from the climate scenario impacts.

The concentrations of dissolved oxygen are not visibly influenced by the changes in land use or management. The decreasing trend due to increased water temperature is more obvious in the upper part of the Elbe basin (gauge Schöna), probably due to less oxygen production with decreasing chlorophyll *a* loads in the river.

In general, the shares of cropland and distribution of point sources, as well as the distribution of soils with their specific nutrient retention potentials, are very important factors influencing the nutrient loads coming with the rivers. However, in the model application presented here, it is often difficult to distinguish between the single impacts on nutrient loads caused by certain land use or management changes and the secondary impacts due to altered chlorophyll *a* concentrations and a resulting change in nutrient uptake in the water body. The in-stream processes include a complex behavior of nutrients with a high number of interactions and feedbacks with the algae population. Chlorophyll *a*, for example, increases with decreasing NH_4-N availability and vice versa, causing increase (or decrease) of PO_4-P due to less (or more) algal uptake. Therefore, the resulting impacts are not only directly caused by land use changes, but are also indirectly caused by the subsequently changed conditions in the river water.

7.5 Discussion

A comparison of obtained results with the results of previous studies dealing with global change impacts in the Elbe river catchment is sometimes difficult, as different scenarios and downscaling methods were used by different authors. The whole range of model outputs illustrates a high uncertainty in climate change impact assessment.

The majority of published studies for the Elbe basin deal with climate change impacts on the hydrological cycle. The simulated effects of climate change on water cycle and river discharge presented in literature are diverse and differ in intensity and even in direction of change, resulting mainly from the diversity of precipitation change signals projected by different climate scenarios. Studies using 100 realisations of the Statistical Analogue Resampling Scheme (STARS), with a distinct decrease in summer precipitation and a moderate increase of precipitation in winter, project lower river discharge in the Elbe basin (Roers et al., 2015; Huang et al., 2010; Hattermann et al., 2008b; Conradt et al., 2012). However, we have to note that recently the STARS model was critically discussed (Wechsung & Wechsung, 2014 & 2015) regarding its suitability for producing climate scenarios. Model runs using the Inter-Sectoral Impact Model Intercomparison Project (ISI-MIP) climate scenarios (Warszawski et al., 2013) for the Elbe basin also project a decreased discharge on average, but the magnitude of changes is less pronounced (Roers et al., 2015). Huang et al. (2013) report diverse results depending on the driving climate model: the projections driven by the empirical-statistical model WETTREG (WETTerlagen-basierte REGionalisierungsmethode) produce negative trends in flood occurrence, whereas the projections forced by the two dynamical regional climate models REMO (REgional MOdelling) and CCLM (COSMO-Climate Limited-area Modelling) show various results with the prevalence of increasing trends in flood occurrence for this region. Applications of the ENSEMBLES scenarios for assessing future risks of floods and droughts in Germany showed an increasing trend of floods but no significant increase in droughts for the Elbe basin (Huang et al., 2015). This is also reflected in our study, where under the same ENSEMBLES climate scenarios' higher discharges are projected on average (compare Figure 7.7).

There are some studies on the management change impacts on river water quality for often only small parts of the Elbe region (e.g. Kersebaum et al., 2003; Meissner et al., 2002; Ullrich & Volk, 2009), but only a few publications exist covering water quality issues under climate change. So, Quiel et al. (2011) used the outputs of a model chain driven by selected realisations of the statistical model STARS as boundary conditions to run the river model QSim for a 700 km reach of the Elbe river. Soluble phosphorus concentrations decrease in all tributaries under all scenarios compared with the reference period for the same scenario. This results in an increased phytoplankton growth along the studied river reach and a shift of the chlorophyll *a* maximum under the dry and medium scenarios, but in a decrease in chlorophyll *a* concentration under the wet scenario conditions (Quiel et al., 2011). The latter is in accordance with the results for chlorophyll *a* presented in our study (compare Figure 7.7), as the ENSEMBLES climate projections produce a wetter climate in the future as well.

It seems that the projected nutrient loads presented in literature often correspond to the precipitation change signals, especially when ecohydrological models using a simple routing of nutrients through the river network are applied. The increased precipitation causes higher nitrogen leaching through soils as well as higher phosphorus erosion rates with surface flow to the river network. Both processes increase nutrient loading to the river waters. Therefore, statistically downscaled climate scenarios with a negative trend in precipitation (e.g., STARS) mostly project decreasing nutrient loads in the Elbe catchment, whereas dynamic climate scenarios (e.g., REMO or the wet years of ISI-MIP scenarios) mostly result in increasing nutrient loads in the river due to positive precipitation change signals (e.g. Martinkova et al., 2011; Roers et al., 2016). This simple relationship between precipitation change signals and final nutrient load projections can be disturbed by including in-stream and algal processes in the eco-hydrological models, due to included transformation and ingestion of nutrients in the river network.

Nevertheless, the same conclusion as for river discharge is valid for the water quality impact assessment: a wide range in projections can be found in literature (as well as in our study). However, the diversity in discharge and water quality projections may not necessarily be the result of the application of different model approaches or climate scenario sets. Even with one scenario and one model, a high spatial variability can be observed, and some subregional trends can actually be opposite to the overall average trend of a large-scale basin, or local effects can be masked by large-scale aggregation (Arheimer et al., 2012; Piniewski et al., 2014). This could also be seen in our study, where changes of model outputs due to climate impact differ in magnitude and intensity or even in the direction of change when comparing several tributaries of the Elbe (Figure 7.7).

In climate and socio-economic impact assessments in addition to the general (and often large) uncertainty associated with climate scenarios as drivers, there is also uncertainty connected to applied watershed models. The so-called structural and parametrisation uncertainty is related to the ability of ecohydrological models to represent the interrelated processes in landscape, vegetation and river network. The parametrisation uncertainty can be especially large in a model with a high number of calibration parameters influencing each other, as in the SWIM model with implemented in-stream processes. Often several calibration parameter combinations exist, delivering the same or very similar model performance, so that it could happen to be "right for the wrong reasons" (Dayton, 1973; van der Laan et al., 2014). In general, such uncertainty rises with the rising model complexity, and goes along with a rising need in calibration efforts (Hesse et al., 2013), and this should be taken into account when the model is extended by adding new processes. To overcome the limitations and weaknesses of a single ecohydrological or climate model approach, it is useful to apply several models with the same input parameter sets (model intercomparison) and ensembles of climate scenarios for a more comprehensive assessment of uncertainties and elicitation of robust outputs (Warszawski et al., 2013; Schewe et al., 2013).

The land use change experiments applied in this study do not represent the "full" set of potential future land use scenarios in the Elbe region, which could be elaborated considering options of future socio-economic development. For example, changes in urbanisation or forest patterns could also have effects on the environment and the water resources (O'Driscoll et al., 2010; Wei et al., 2013). In our study only the effects of single measures connected to nutrient sources and agricultural practices (which are currently considered in the planning of land/water management) on water quantity and quality were tested, also in combination with climate change. This could be regarded as a first step to finding suitable methods for adaptation to climate change impacts. However, for further studies it is recommended to apply a combination of different measures under consideration of the future socio-economic development for a more realistic land use change impact assessment. As climate change can strengthen, revoke or even inverse the land use change impacts, this aspect should always be included in such studies.

7.6 Summary and conclusions

The SWIM model supplemented by an in-stream module was successfully calibrated and validated for the entire Elbe river basin, and applied for climate and land use change impact assessment in the region. For that, the commonly used technique was applied, using 19 climate scenario data sets provided by the ENSEMBLES project to drive an ecohydrological model for 30-year periods in order to evaluate changes in water quantity and quality for the two future periods of 2021–2050 and 2071–2098 in comparison to the reference period of 1971–2000.

The calibration and validation of the extended SWIM for the Elbe region was complicated due to the high number of calibration parameters and the spatial variability within the catchment. Satisfactory model results could be still achieved by applying spatially distributed calibration parameter sets to capture variability in soil type distribution, land use pattern and economic development in the subcatchments.

The analysis of a potential future climate, as projected by 19 scenarios for the Elbe catchment, indicates increasing trends in temperature and precipitation, but a decreasing trend in solar radiation on average. However, looking at the climate change signals of the 19 scenarios separately, differences can be seen in the intensity and – for precipitation and solar radiation – also in the direction of change signals. The standard deviation of the whole set of climate change signals increases in the second future period.

The results of the climate change impact assessment on water quantity and quality show a high spatial variability within the catchment according to the individual characteristics of the tributaries within the basin. For the entire Elbe catchment, river discharge is projected to increase by 11% and 20% on average for the two future periods. Dissolved oxygen concentration is projected to decrease by 2% and 5%, mainly due to the increased water temperature. The projected changes in nutrient loads do not show the same change direction. While NO_3-N loads slightly decrease on average (−1% and −5%), and NH_4-N shows a distinct decreasing trend (−11% and −24%), PO_4-P loads are expected to increase by 6% and 5% on average. The simulated reaction of nutrient loads to climate change is always influenced by the phytoplankton population, and vice versa. The chlorophyll *a* concentrations decrease slightly under the future conditions, by 3% and 4% on average, at the last downstream Elbe gauge.

Five simulation experiments dealing with possible changes in nutrient emissions were applied in the study, also in combination with climate change scenarios. Water discharge was mainly influenced by climate change impacts, and land use change measures had little or no influence on runoff. A reduction of agricultural area or fertiliser application mainly influenced the resulting nitrate nitrogen loads in the Elbe, whereas the reduction of point source emissions had the highest impacts on ammonium nitrogen and phosphate phosphorus loads. The chlorophyll *a* concentrations reacted to a changed food supply in the river, and would be reduced with a reduced nitrogen and phosphorus availability. An increase in nutrient retention and decomposition potential within the catchments would certainly be beneficial to reduce all types of nutrient loads in the river waters.

Nevertheless, the model application in the Elbe basin comes along with a certain degree of structural, parametrisation and scenario uncertainty. Due to the lack of more detailed information on the case-specific observations and processes, not all possible methods to reduce uncertainties could be applied in this study, and the climate scenario–related uncertainty is unavoidable. The climate change impact assessment and land use change simulation experiments presented here deliver the first results and rough estimation on probable future developments in the Elbe river basin under climate change. For future research, in order to diminish and better assess (but not to eliminate) uncertainty, it could be recommended to apply two to three ecohydrological models, as well as a "full" set of socio-economic scenarios, for a more reliable combined climate and land use change impact assessment. It could be also advantageous to additionally include management measures neglected in this model application so far (e.g., reservoirs or different crop types and rotations). These methods would help to identify future risks and threats more realistically, and to virtually test possible adaptation measures, as efforts to cope with the future climate conditions and their impacts are generally needed. Watershed models offer a suitable tool to guide decision-making on water quantity and quality for a sustainable management of water resources to match the requirements of the European Water Framework Directive (WFD).

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CHAPTER 8

DISCUSSION, CONCLUSIONS AND OUTLOOK

In addition to the already included discussions and conclusions of the individual research articles presented in Chapters 3 to 7, this chapter aims in summarising and integrating the results on model development and applications related to the two main objectives of this study stated in Section 1.3, and in deriving general conclusions on water quality modelling with SWIM in the Elbe river basin. Furthermore, uncertainties of model results and limitations of the model approaches are discussed, and further research needs and possible developments in water quality modelling and management in the Elbe river basin are outlined.

8.1 Discussion of the main new approaches implemented in SWIM

Ecohydrological watershed models usually have incomplete representation of biogeochemical processes in river basins mainly due to an extreme complexity of natural systems, but also due to missing knowledge, incomplete data and/or lacking computational capacity. Modelling is generally aimed in simplifying the process description as much as possible in order to get satisfactory calibration results for the main output variables. Hence, many natural processes are simply neglected in water quality modelling, and such models are still appropriate for solving important research questions.

However, with the rising interest in river water quality assessments mainly based on biological indicators (such as phytoplankton, macrozoobenthos and fish), hydromorphological structure, and only supplemented by chemical criteria (such as oxygen or nutrients), the ecohydrological models should be able to include the biotic indicators, in order to perform reasonable and useful model-based impact assessments on water quality. These are also essential factors for implementation of the European Water Framework Directive (WFD) in a changing world.

The standard SWIM version (Krysanova et al., 2000) describes nutrient processes in soils in detail at the hydrotope level, but nutrient transport through the catchment and river network is simulated by quite simple equations. The retention of nutrients in lateral flows in the landscape has already been included by Hattermann et al. (2006) using a retention and decomposition equation, but an adequate representation of nutrient retention in wetlands and rivers was still missing in the model. Therefore, this was one of the main objectives of this study to improve the nutrient retention and transformation in the routing process through the river network to the outlet of the catchment.

During the calibration of SWIM in different model applications in the Elbe river basin, several changes of the model code were implemented, in order to improve water quality modelling and to better integrate nutrient processes in the ecohydrological watershed model. All changes were already listed and shortly described in section 2.2.2. Three main new modelling approaches for further development of SWIM will be finally discussed here. They are related to an enhanced but simple modelling of the water and nutrient processes in lowlands (Chapter 3), to the implementation of in-stream processes including algal growth (Chapter 5), and to the testing of several approaches to describe retention processes in watersheds for better simulation of seasonal variations in nutrient loads and concentrations in river waters (Chapter 6).

For comparing the usability of new approaches to improve model performance, it is important that they are well calibrated and not simply switched on or off without refinement of the calibration parameter sets. This, of course, has been done for the results presented in Chapters 3, 5, and 6 of this study.

8.1.1 The simple wetland approach

The calibration of the standard SWIM model in the lowland catchment of the Rhin river revealed a continuous overestimation of discharge and connected nutrient loads during the summer months. A solution to improve the model results was found in integrating typical wetland processes in the SWIM model. A simple wetland approach was applied for the Rhin catchment, and the model performance increased.

Wetlands and riparian zones act in several ways to deliver hydrological, ecological and other services, e.g. by storing water in wet periods and maintaining flow in dry periods, by retaining nutrients on the way to the river network, and by providing recreational areas for the society. They are characterised by higher groundwater tables, so that the water and nutrient supply for vegetation is more stable during the year allowing higher water and nutrient consumption by plants.

In ecohydrological modelling the exact definition and detailed simulation of such wetland areas with their high groundwater tables and the complex interactions and feedbacks between hydrological process, vegetation and nutrients is difficult. However, the simple wetland approach applied in this study (see Chapter 3) revealed that it is possible to improve model results by such uncomplicated means, if they properly describe reality. There was also a dynamic and much more detailed and data demanding approach developed for wetlands and riparian zones in SWIM, which is additionally described in Hattermann et al. (2008a) (Chapter 3), however, this work was not done by the author and will therefore not be discussed here.

The simplicity consists mainly in the stable definition of the wetland regions correlated to the soil map and its parametrisation. Such stable definition does not consider the typical variations in groundwater tables or changes in groundwater availability during the year. Vegetation located in hydrotopes with the predefined wetland soils was allowed to increase its water and nutrient uptake in times when the demand is higher than the supply, and the potential value of plant transpiration is not reached. A limiting constraint is the root depth of vegetation, which should reach at least two thirds of the maximum root depth. As a consequence of the higher uptake rates, the percolation of water and leaching of nutrients to the aquifer was reduced by the same amount to keep the balance. The increased water and nitrogen uptake by plants resulted in a decrease of discharge and nitrogen loads at the outlet of the river basin.

Being a function of rooting depth and potential evapotranspiration (mainly correlated to air temperatures) the reduction in discharge can be primarily observed in the summer months (compare Section 3.3.1). But regarding nitrate nitrogen, a remarkable decrease of nitrogen loads could be also observed in the winter months. This is presumably connected with delay in nitrogen leaching to groundwater and during the lateral flows through the catchment. The largest amounts of leaching from arable land to the rivers can be expected in winter months with higher precipitation and low evapotranspiration (as a function of temperature and vegetation). However, the total amount of available nutrients in soils and subject to leaching in winter months is lower after increased consumption by plants in summer, so that the reduced nitrogen loads occur also in winter time in the catchment.

Using the simple wetland approach increased the model efficiency in the period of investigation, for river discharge as well as for nitrogen loads. It can be recommended to use this approach by default in regional ecohydrological modelling with SWIM, as it improves representation of special behaviour of wet areas in a catchment without needing additional data and high calibration efforts. This approach helps to come closer to description of natural conditions, although in a simplified and spatially static way. Nevertheless, it was used in all following SWIM applications presented in this dissertation (Chapters 4 to 7) in order to improve representation of typical lowland vegetation processes and influences on water and nutrients.

8.1.2 The in-stream module

The standard SWIM model simulates nutrient cycling in the soils of a watershed followed by retention and decomposition during nutrient transport with the lateral water flows to the river network (Hattermann et al., 2006). However, the standard model uses only a simple routing approach along the river courses without any further nutrient transformation or retention in the flowing waters. Such simplification does not correspond to the natural nutrient behaviour in river waters, where retention, transformation and algal processes are important, especially in large and slow flowing downstream water courses (Horn et al., 2004; Mischke et al., 2005).

The consideration of in-stream processes and nutrient retention could be helpful for increasing the model's performance in simulating nutrient loads and concentrations in large watersheds. The experience with the SWIM model applications for water quality simulation presented in Chapter 4 showed that inclusion of such processes could be beneficial especially for nutrients coming presumably from point sources to the rivers (such as phosphate phosphorus). The analysis of available data on nutrient input and output in the Saale river basin revealed as well that the retention processes must be considered, because the total input to the river was larger than the output at the outlet of the basin (see Table 6.1).

Besides, the in-stream approaches are also increasingly demanded in river water modelling due to the rising interest in a holistic ecohydrological approach for surface and groundwater protection as requested by the WFD. It was also stated in FGG-Elbe (2010) that it is of particular importance to consider nutrient pools within algae in the longitudinal nutrient observations of the Elbe river basin, as large amounts of the nutrient loads are ingested in the biomass between Valy and Hamburg, so that the observed concentrations are quite low in this river district with "hidden" nutrient pools in the phytoplankton biomass.

Therefore, an important aim of this dissertation was the further development of the SWIM model by implementation of the in-stream processes and the connected algal growth in meso- to large scale river basins. This work required substantial changes in the model code, and inclusion of several new equations and parameters (see Chapter 5 and Appendixes).

The implementation of in-stream processes was performed based on the corresponding module in the SWAT model, supplemented by three additional assumptions influencing the development of phytoplankton biomass: photoinhibition, temperature stress and grazing. Based on that, a substantial improvement of the model results for the Saale river basin could be achieved (see Chapter 5 and Figure 5.6). The main advantage of these additional assumptions was that they allowed to overcome the dominating temperature dependence of the processes describing in-stream nutrient transformation and algal growth, which contradicted the observed dynamics before (see Figure 8.1).

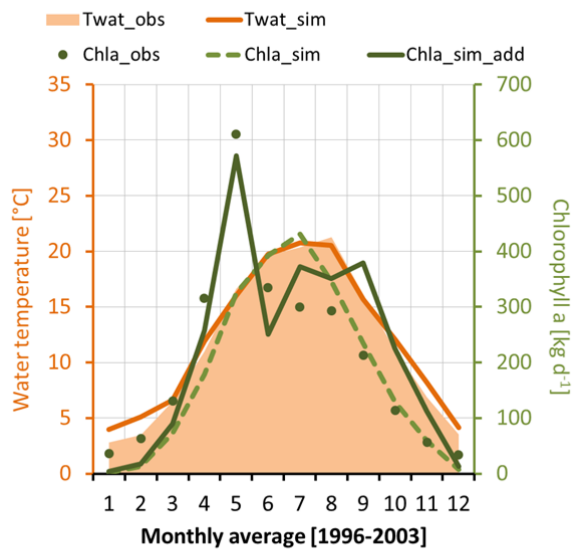


Figure 8.1 The observed (obs) and simulated (sim) water temperature (Twat) compared to the observed and simulated chlorophyll *a* (Chla) in the Saale river basin (gauge Groß Rosenburg) using SWIM with in-stream module, without and with (add) additional assumptions regarding phytoplankton growth constraints.

The implementation of in-stream processes was aimed to improve the SWIM model's applicability for future ecohydrological scenario simulations in meso- to large-scale basins. The improved SWIM model allows simulating impacts on riverine processes better than before, and the water quality modelling at the large scale is more realistic due to the improved process description and spatial distribution of included processes. In general, the modelling results could be notably improved using the extended SWIM model, especially for nutrients coming mainly from point sources directly to the river. Some discrepancies in the former model outputs could be eliminated by the new approach considering transformation processes in the river. The comparison of the observed and simulated nutrient and chlorophyll *a* concentrations at gauges within the catchment delivered sufficiently good results as well. Thus, the extended SWIM with an in-stream module can be rated as being closer to new requirements for water quality modelling, and is therefore an important and beneficial step for the SWIM modellers community and their further model applications.

Of course, even with the new developed in-stream approach of the SWIM model it was not possible to consider all naturally occurring nutrient processes in the model. The still assumed constant emissions from point sources, which are probably not realistic, could not be corrected due to the poor temporal resolution of available data. The new approach also includes some simplifications and neglects some processes, which could additionally influence the nutrient amounts in the river. For example, the sediment layer and the corresponding sorption and release processes of PO_4-P due to specific physico-chemical conditions (e.g. pH or oxygen concentration) are not included in the in-stream module. The sediments as a source and sink for nutrients are only marginally considered by using a benthic source rate for PO_4-P and NH_4-N and a settling rate for organic P and N, all based on water temperature. Another example is the effect of grazing on the phytoplankton biomass. The grazing intensity is considered as constant, without modelling the zooplankton community and its seasonal variations.

Furthermore, the new in-stream module introduced 36 additional parameters to the model outputs (compare Figure 5.4), and many of them are defined as ranges and could be subject to calibration if they show a high sensitivity. Besides, some of them can be assigned in a spatially distributed way. Thus, with this new module the calibration effort increased considerably, and the uncertainty of output regarding possible parameter ranges is very high. In addition, several parameter combinations could likely be used to achieve similar results at the end (equifinality problem). The parameters used in this model approach were not based on real measurements or observations in the Saale or Elbe case studies, but they were applied considering specific ranges found in literature. It is not known, whether these assumptions represent the real conditions in the simulated river reaches, and it would be desirable to set more realistic limits for these parameters based on real measured data in the river basin under study.

Therefore, due to the increased number of considered processes described by these parameters of the in-stream module, the calibration efforts are higher. Including additional in-stream processes in the model definitely brings some advantages but also an increasing uncertainty of the whole modelling system. This module should be used for water quality modelling mainly in the large-scale watersheds and phytoplankton dominated rivers, where the in-stream processes are more important, and when evaluation of the ecological status of a stream is planned. The in-stream processes can be neglected for pure assessments of diffuse emissions from agricultural fields to the river network, or for solely nitrate nitrogen modelling. It is possible to simply switch the in-stream module on or off in SWIM when simulating a river catchment.

8.1.3 The nutrient retention methods

Nutrients are subject to several retention and decomposition processes within river basins influencing the resulting loads and concentrations observed at the outlet of a catchment. The retention is based on processes in soils of the landscape (e.g. nitrification, sorption or volatilisation) supplemented by nutrient transformation and storage in the river waters (e.g. ingestion by algae, mineralisation or nitrification) and the underlying sediments (e.g. settling or sorption), causing a general decrease in nutrient loads along the route of transport.

Many watershed models (including the standard SWIM version) assume a simple routing of nutrients through the river network as soon as it is reached. This causes some problems in achieving good calibration results, especially for nutrients coming mainly from point sources. Therefore, the detailed in-stream processes were implemented in the SWIM model to overcome this problem, and to better simulate the observed nutrient concentrations (see Chapter 5 and the previous Section 8.1.2). However, this approach comes along with a high parameter-related uncertainty and calibration effort, and a question arose, whether more simple approaches representing retention in river reaches could also be helpful for this purpose. Using simpler methods for simulating retention and transformation processes in the river might reduce parameter uncertainty, and support a more user-friendly handling of the SWIM model.

This question was investigated in the application of SWIM for the large-scale Saale river basin in Germany. Three simple methods representing nutrient retention processes in rivers based on physical or hydromorphological boundary conditions of river reaches were compared with the detailed in-stream retention approach, also in combination with nutrient retention and decomposition during lateral flow in soils of the catchment (Chapter 6). Finally, eleven different model approaches were chosen and manually calibrated, and it was supplemented by a PESTassisted fine-tuning of several calibration parameters. The objective of this specific part of the dissertation was to identify the necessary model complexity in this respect to get sufficiently good results.

Looking at the results of these model experiments (Figure 6.7), it can be firstly concluded that a high importance of riverine retention could be confirmed for nutrients coming mainly from point sources (PO_4-P and NH_4-N in our application). In contrast, nutrients leached to the river predominantly from diffuse sources (such as NO_3-N) were mostly influenced by retention in the landscape, and an additional retention in the river practically did not improve the model results. It could be further concluded that neither sole terrestrial nutrient retention nor exclusive in-stream retention was able to simulate ammonium nitrogen sufficiently good, but the combination of both approaches helped to increase the model's performance in this respect.

The calculated performance ratings of the model runs showed that they are highly variable between the approaches as well as between the different nutrient forms. The concluding total ranking of the eleven approaches (Figure 6.12) indicated a more or less steady improvement of the mean performance along the sequence of riverine nutrient transformation experiments (representing the sequence of complexity). However, it could also be seen that in the total ranking the standard SWIM version with implemented retention in the landscape already delivered acceptable results on average. They could be only marginally improved by applying the additional in-stream retention methods. The best model performance in the total ranking can be found for the most complex approach. Although the approach with the highest complexity delivers the best total model efficiency, it could be seen that also simpler in-stream retention approaches in combination with landscape retention and decomposition are able to reach quite acceptable total performance rates.

However, the three simple approaches based on correlation of retention to hydromorphology or to water temperature were not able to match the seasonal dynamics of the observed nutrient concentrations at the river outlet, though they were also combined with the landscape retention processes. This was only possible by applying the detailed in-stream approach in combination with the landscape retention due to additional important processes (e.g. algal consumption, diffusion) considered. Therefore, the use of one of the simple retention and decomposition approaches for in-stream retention can not be recommended due to their limited ability to simulate the observed seasonal nutrient dynamics.

The seasonal effect of the in-stream processes mainly on ammonium and phosphate is coupled to the algae population, as NH_4-N and PO_4-P are supposed to be the favoured or most limiting nutrients for the algae in the river (Correll, 1998; Glibert et al., 2016). Comparing with the SWAT results of Migliaccio et al. (2007) it can be assumed that this distinct seasonal effect achieved with the in-stream approach in the SWIM model is probably the result of the temperature stress, photoinhibition and grazing assumptions hampering algal growth, which were implemented additionally to the originally used equations in SWAT (see Chapter 5, and Section 8.1.2).

The retention experiments presented in Chapter 6 helped to increase the understanding of the usefulness and importance of implemented retention processes in landscape and river network, and their effects on water quality modelling at the regional scale. With regard to the prevailing source of a certain nutrient, it could be demonstrated that applying either terrestrial (for diffuse source pollutants) or a combination of terrestrial and in-stream retention and transformation processes (for point source pollutants) leads to an improvement of the modelling performance. The effect of the landscape retention and decomposition (as taken from Hattermann et al., 2006) on the monthly averages of nutrient loads is shown in Figure 8.2, left. Figure 8.2 (right) illustrates the changing seasonal dynamics of PO_4-P loads with implemented in-stream processes (which fit better to the observed ones with their typical minimum in spring).

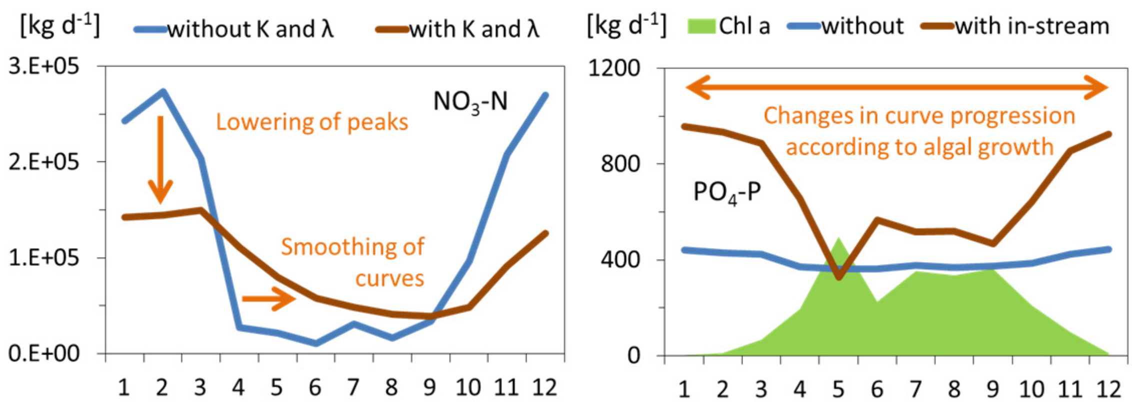


Figure 8.2 Schematic illustration of the influence of the calibration parameters K and λ representing landscape retention according to Hattermann et al. (2006) on the seasonal dynamics of nitrate nitrogen loads (left) as well as the influence of the in-stream processes and phytoplankton biomass (Chl a) on phosphate phosphorus loads (right). The experiments were performed using SWIM for the Saale river (gauge Groß Rosenburg) in the time period 1996-2003.

8.2 Discussion of the SWIM model applications in the Elbe basin

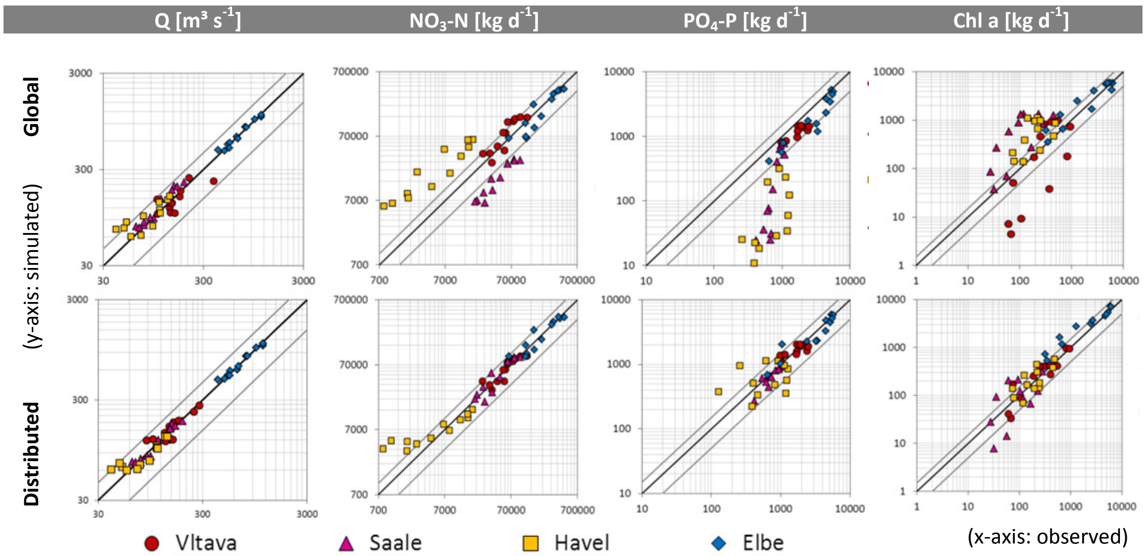
8.2.1 Water quality modelling with SWIM at different scales

In general, the ecohydrological model SWIM is a suitable tool for simulating water and nutrient flows in meso- to large-scale river catchments. The model applications in the Rhin (Chapters 3 and 4), Saale (Chapters 5 and 6) and entire Elbe river (Chapter 7) basins delivered sufficiently good calibration and validation results in regard to water quantity and quality, with model performances ranking in the good to very good categories. However, such calibration results could only be achieved by including new approaches in the standard SWIM model, especially in regard to representation of wetland processes in lowland rivers and implementation of nutrient retention and transformation in river reaches, as well as by using distributed input and calibration parameters in the large-scale model applications.

Generally, the water quality modelling is a challenging task in ecohydrological watershed modelling. For several reasons, such as diverse and transforming components, dependence on water flows, more complex description of processes (often by empirical equations), and rare or missing observations, the water quality modelling is more complex and involves higher uncertainty compared to the purely hydrological modelling. Nevertheless, numerous studies have demonstrated that semi-distributed process-based ecohydrological models are able to adequately represent hydrological, biogeochemical and vegetation growth processes at the catchment scale (Krysanova et al., 2009, 2015).

Depending on the scale of the modelled study area, different processes and data are dominating and define the necessary complexity of the model: soil and crop type, nutrient cycling and leaching are most important at the plot scale, hydrological processes dominate at the hillslope scale, and land use, rainfall and topography are important influences at the catchment scale (Drewry et al., 2006). It seems to be easier to achieve reasonable results for the river outlet of the larger basins than for the smaller ones, also with a lower model complexity. Problems arising due to missing consideration of nutrient retention could be evened out in the large-scale river basins, counterbalancing possible over- and underestimations of nutrient flows in the single tributary river reaches, and allowing getting satisfactory results at the basin outlet.

However, when model performance at intermediate gauges is checked in a large-scale case study (as for the entire Elbe river basin presented in Chapter 7), the basin-wide or "global" calibration parameters may not work. For example, the global calibration of the model delivered very good results for the most downstream Elbe river gauges (Neu Darchau and Schnackenburg), but results at gauges of the main tributaries were often quite poor (see Figure 8.3, upper row).



		Vltava (Vranany)		Saale (Calbe-Grizehne)		Havel (Havelberg)		Elbe (Neu Darchau)	
		global	*distributed*	*global*	*distributed*	*global*	*distributed*	*global*	*distributed*
Q	NSE	0.56	0.64	0.6	0.84	0.47	0.56	0.85	0.86
	DB	-16.8	-10.5	17.9	1.5	15.2	-1.5	-0.1	-0.5

		Vltava (Zelčin)		Saale (Groß Rosenburg)		Havel (Toppel)		Elbe (Schnackenburg)	
		global	*distributed*	*global*	*distributed*	*global*	*distributed*	*global*	*distributed*
NO_3-N	DB	34.1	-1.0	-64.1	10.0	265.9	-1.0	-10.5	-0.9
PO_4-P	DB	-31.1	-1.3	-62.4	-11.3	-87.7	-10.5	-28.3	-5.9
Chl a	DB	6.5	7.6	403.3	3.8	181.2	11.8	7.9	19.8

Figure 8.3 Comparison of the global and distributed calibration results for the long-term monthly averages of selected parameters (discharge (Q), nitrate nitrogen (NO_3-N), phosphate phosphorus (PO_4-P), chlorophyll *a* (Chl a)) in the Elbe river basin and three main tributaries (time period 2001-2010).

In general, the basin-wide constant calibrated parameters (e.g. for nutrient retention and decomposition) seem to be unrealistic in the large-scale water quality modelling. According to the geo-chemical conditions in soils, the intensity of denitrification or sorption processes, and consequently the residence time for nutrients in the lower and deeper soil profiles can vary. Similar to modelling experiments in this regard for the Saale river basin (Huang et al., 2009), it was not possible to find a smart solution to cope with this problem in the Elbe basin by including spatially-distributed calibration parameters based on soil properties or subbasin characteristics (e.g. sand content or river morphology). So, the large-scale calibration was performed in a "subcatch-mode" with individual combinations of the main calibration parameters in each of the main tributary catchments, improving model performances at the intermediate gauges (Figure 8.3, lower row). In fact, in this case, the calibration for the entire Elbe river basin was rather a combination of several meso-scale calibrations. Although a possibility to describe the large-scale catchment's heterogeneity by correlating the calibration parameters to the characteristics of their natural conditions would be a preferable solution, it could not be achieved in this study.

Another specific problem in water quality modelling and calibration is a distinction between nutrient loads and concentrations. A good watershed model should be able to provide both nutrient loads and concentrations, because pollutant loads provide valuable information on the impact potential of a river (to the receiving main stream or sea), whereas for a comparison with the water quality standards one needs nutrient concentrations. The concentration is a function of water discharge and nutrient amount, and therefore water quality modelling requires a well calibrated hydrological model. This is also essential because nutrient transport is always coupled to water flows. Thus, the water quality modelling is the second step in ecohydrological watershed model applications, and modelling efforts at this step are higher than for the hydrological modelling only.

In addition, the simulation of discharge and water in regulated lowland rivers is much more difficult compared to rivers in mountainous areas due to special characteristics of the former ones (e.g. water management and melioration activities or high percentage of wetland areas). This leads to problems in reproducing water flows and water quality by models. In the lowland Rhin case study these problems were partly solved by implementing all available data on water management in the model, which allowed achieving satisfactory results of model calibration (see Chapter 4). The simple wetland approach also helped to improve the calibration results here (compare Chapter 3 and Section 8.1.1).

Water quality modelling studies are often applied to get information on the amount and spatial distribution of nutrient pollution coming to river waters. The preliminary analysis and comparison of water discharge and nutrient concentration time series allows to determine the prevailing sources of nutrient pollution in a basin in advance. Increasing concentrations coming along with increasing discharge point to prevailing diffuse pollution sources, whereas decreasing concentrations during increasing discharge are a sign of predominantly point source pollution. The model application additionally helps to identify fractions of point and diffuse pollution, and areas of the highest diffuse pollution (as for the Rhin catchment presented in Chapter 4, and for the Saale catchment in Chapter 5).

The differentiation between point and diffuse nutrient pollution is an important step in water quality modelling, which is necessary for deriving appropriate measures to improve water quality. A reliable modelling of nutrient loads requires detailed fertilisation and effluent data, which was available only partly in all case studies presented in Chapters 4 to 7. The best availability of differentiated in time and space data was for the smallest case study, the meso-scale Rhin catchment (Chapter 4). This modelling was performed in close cooperation with the local environmental agency, and data could be delivered at short notice, and in a quite non-bureaucratic way.

In contrast, the SWIM model calibration on larger scales (Chapters 5 to 7) was often suffering from uncertain data taken from literature, assumptions or averaged input values on anthropogenic nutrient sources, hindering accurate model simulations. Averaging and homogenising increase the uncertainty of model results, and reduce their applicability in integrated water resources management. Data collection and homogenisation are even more difficult in transboundary river basins, which is relevant for the majority of the large-scale European rivers. Here, spatial and/or temporal discrepancies in available data exist in the most cases, often resulting in simplifying assumptions or spatially split model outputs in river catchments correspondent to the heterogeneity in data availability.

Several changes in the model codes were necessary for satisfying calibration and validation results in the investigated Elbe case study areas of increasing scale as described in Chapters 3 to 7. The calibration of nitrogen and phosphorus loads and concentrations using the standard SWIM model revealed that it would be beneficial to include phosphorus leaching through the soils (see Chapter 4) and nutrient retention and decomposition in the watershed and river reaches to reproduce observed seasonal variations and to achieve sufficient model performances. An additional water and nutrient retention process was implemented in SWIM by the simple wetland approach in the Rhin river case, which helped to reduce the overestimation of discharge and nitrate nitrogen loads in the summer months (Chapter 3, Figure 3.4).

However, this approach did not improve the results for phosphate phosphorus, which is mainly coming from point sources. As a first step in-stream retention and decomposition of the point source emissions was assumed by using the same retention equation as for the lateral flows in soils (Hattermann et al., 2006), which improved the results for PO_4-P, and allowed to get good model performance (Chapter 4).

Finally, the in-stream processes were implemented in SWIM (Chapter 5) to come closer to the real conditions in large basins with diverse sources of nutrient pollution. The calibration results for the Saale case study showed improved criteria of fit, especially for nutrient forms mainly originating from point sources. The main advantage of the in-stream approach with included phytoplankton growth and nutrient consumption by algae is in considering effects of algae on seasonal dynamics of nutrients during calibration, allowing to better fit the simulated monthly nutrient values (inversely correlated to the phytoplankton biomass) to observed loads and concentrations (Chapters 5 and 6 and Section 8.1.3).

Facilitated by the integration of several new methods and approaches to improve simulation of nutrient processes in river watersheds, the SWIM model applied to the Elbe river basin and its selected subcatchments was able to reproduce observed discharge, nutrient loads and concentrations well. After that, the calibrated SWIM model was prepared for the following model-based impact assessments, which will be discussed in the next section.

8.2.2 Impact assessment on water quality with SWIM

Model-based impact assessments in ecohydrology aim in projecting possible future developments of water quantity and quality in a case study under certain assumptions of changing climate, land use or other socio-economic conditions. A dynamic catchment model taking into account water and nutrient processes as functions of vegetation, land use and human impacts and driven by climate conditions, can provide a functional tool for this purpose. It can support the creation of river basin management plans to improve the ecological status of a watershed (as requested by the WFD). To increase the adaptation capacity of river basins to possible global change impacts, water management should be planned by considering potential climate and socio-economic changes, which the basin could be confronted with in future. The impact assessment studies using ecohydrological watershed models allow to virtually test the suitability of adaptation measures in advance.

The ecohydrological model SWIM can be used for this purpose, too, and it was done in this study by applying different scenario approaches. For the meso-scale Rhin catchment (Chapter 4) as well as for the Saale basin (Chapter 5) climate and management change sensitivity experiments were conducted, aiming in identification of the catchment's sensitivity to single land use or climate parameter variations. For the entire Elbe catchment, the climate change impact assessment was performed using a multi-model approach and applying an ensemble of dynamic climate scenario data covering two future periods (2021-2050 and 2071-2098) (Chapter 7). The land use change experiments for the Elbe basin applied in Chapter 7 were not dynamic and similar to those of the Chapters 4 and 5. In Chapter 4 two selected realisations of the statistical climate model STAR (dry and wet in regard to the climatic water balance to cover the uncertainty range) were additionally applied mainly confirming the results achieved with the simple climate sensitivity analysis.

The climate change impact assessment with SWIM is one of the most useful SWIM model applications for integrated water resources management. The model can be easily used for climate sensitivity experiments to test the simple effects of reduced or increased temperatures or precipitations (as shown in Chapters 4 and 5). This application can be helpful to account for the main climate processes influencing the resulting water quality parameters at the outlet of the basin and their predominant dependence on specific climate parameters.

Though, a simple climate sensitivity experiment cannot say something about the probability of certain climate changes in future. For that, climate scenario data are necessary, either statistically developed as used in Chapter 4, or produced by a set of several GCM/RCM combinations. Climate scenario data of the latter type were applied for the large-scale Elbe river basin and the advantages of such model applications were discussed in detail in the corresponding scientific publication (Chapter 7). Application of a set of several climate scenarios allows quantifying the uncertainty ranges in future climate and subsequent water quality changes, which increases the reliability of the impact assessment results. It is worth to mention that a discussion started in the meantime about the general suitability of statistical models as STARS to produce climate scenarios (Wechsung & Wechsung, 2014 and 2015).

Just as the complexity of the water quality calibration approaches is increasing following the publication sequence of this thesis from Chapter 3 to Chapter 7, the same is true for the climate change impact assessment approaches. The climate sensitivity experiments are the simplest form of impact assessment, and running the model driven by the wettest and driest realisations of a climate scenario data set is a possible next step, but impact assessment using an ensemble of multiple scenario data delivers results more respected by the scientific community. However, such approach requires higher computation efforts and skills in data management and analysis, and it is thus more time consuming.

Nevertheless, scenario projections never include a guaranty for being true and for showing what will certainly happen. This can be easily seen by calculating the climate change signals of 19 different scenarios included in the climate scenario ensemble set (see Chapter 7, Table 7.8). A wide range of possible changes can be found, even in opposite directions concerning precipitation and radiation, and nobody knows which scenario is the most realistic.

There are some methods (e.g. Kling et al., 2012) to find the "best-fitting scenario" in the scenario set by comparing the single scenarios with historically measured real climate data, which could be done for several climate stations representing different geophysical subregions. But there is no guaranty that the best scenario for the past would perform similarly good in the future.

Therefore, it was preferred to show the scenario results as averages of all simulations with uncertainty ranges, without saying anything about their probability. It was also decided not to use bias correction for the climate impact assessment conducted in Chapter 7, and to compare average simulations driven by 19 RCMs between the future and reference periods instead, in order to simply detect trends and the relative changes caused by climate change.

The variation between the climate change signals of scenarios using different downscaling methods can even be larger than within one scenario set. For example, the climate projections of the statistical approach STARS suggest a distinct decrease in precipitation on average, and increasing drought problems for the central German part of the Elbe river basin (Gerstengarbe & Werner, 2005), whereas the ENSEMBLES data project an increasing precipitation on average (Chapter 7). This should be kept in mind when comparing the results of Chapters 4 and 7. The two model runs driven by the selected wet and dry realisations of the STARS applied for the Rhin catchment (Chapter 4) represent a kind of uncertainty range of potential changes, which are not always similar (especially for future discharge projections) to those detected by applying the whole multi-model ENSEMBLES climate scenario set to the other cases (Chapter 7) for the first future period (Figure 8.4).

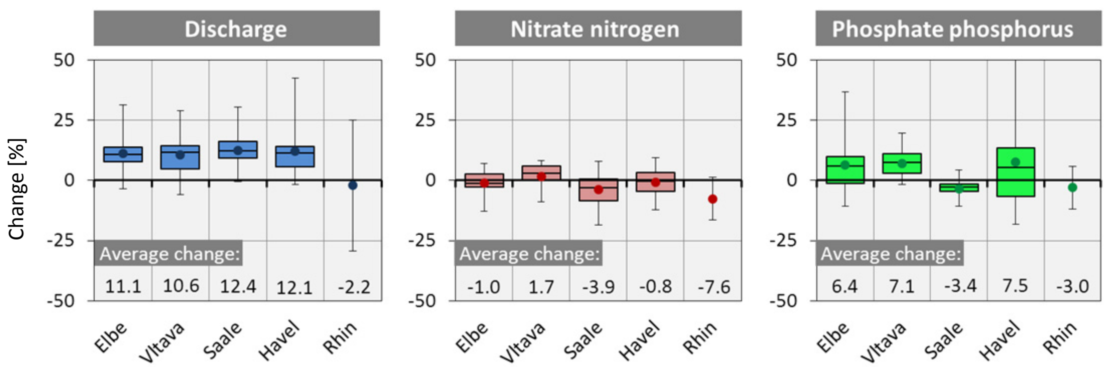


Figure 8.4 Comparison of the average percental changes (dots and numbers) and ranges of individual changes (boxes and whiskers) in river discharge as well as NO_3-N and PO_4-P loads for the total Elbe river basin and selected subbasins as simulated in two of the presented studies (Chapters 4 and 7), either under an ensemble of 19 dynamic climate scenarios (future period 2021-2050 compared to the reference period 1971-2000 of the same scenario; Elbe, Vltava, Saale and Havel catchments) or using the driest and wettest realisation of a statistical model (period 2016-2025 compared to reference period 1991-2000 of the same realisation; Rhin catchment).

Summarising the results of the climate sensitivity experiments in publications presented in this study, it can be seen that the projected nutrient loads under climate change often correspond to the precipitation change signals, especially when the standard SWIM model using a simple routing of nutrients through the river network is applied (Chapter 4). The increased precipitation causes higher nitrogen (and partly phosphorus) leaching through soils as well as higher phosphorus erosion rates with surface flow to the river network. Both processes increase nutrient loading to the river waters. This simple linear relationship between the precipitation change signal and the final nutrient load can be "disturbed" and modified by including the in-stream and algal processes in the ecohydrological model, due to transformation and ingestion of nutrients by algae in the river network (Chapter 5). In the new SWIM model with implemented in-stream processes mainly based on water temperature, the algal processes are to a large extent temperature and radiation dependent, which can overlay and hidden the simple precipitation dependence of nutrient load changes (Chapters 5 and 7).

Additionally, the problem of water quality parameter description by loads or concentrations already described above in Section 8.2.1 gets a special importance in climate change impact assessment. Reduced nutrient loads under climate change do not necessarily mean reduced nutrient concentrations and an improved water quality. This is due to often also reduced discharge under climate change, which acts as nutrient enrichment factor. Such and also the opposite behaviour and connections between discharge, load and concentration can be clearly seen in the climate experiments and the wet and dry scenarios conducted for the Rhin catchment (Chapter 4). It was less pronounced in the Saale catchment (Chapter 5), probably due to the superimposing effects of the implemented in-stream processes, but also to seasonally differentiated precipitation changes. The climate change impact assessment for the Elbe basin presented in Chapter 7 did not include analysis of impacts on nutrient concentrations. Therefore, results presented in this publication can be used mainly for assessment of possibility to reduce the impact potential to the receiving sea.

Concerning the management change experiments applied in Chapters 4, 5 and 7 of this study, it can be seen that single measures often do not have the capability to remarkably improve river water quality for all nutrient substances under study. To achieve this, the combination of several management measures has to be recommended. This is mainly due to the fact that the nitrogen and phosphorus nutrient forms behave quite differently in regard to retention potential and leaching rates. The composition of the nutrient loads coming from point or diffuse sources is also important in this respect. So, it is not surprising that measures to reduce the diffuse nutrient pollution (as lower fertilisation rates or cultivation of high nitrogen demanding crops) mainly act in reducing the nitrate nitrogen loads, whereas the reduction of effluents coming from point sources mainly reduces phosphorus pollution.

Changes in land use composition (such as enlargement of grassland instead of agricultural acreages around river courses or in mountainous regions) mostly affect the diffuse pollution. This is due to lower total fertiliser amounts per area and, consequently, it improves water quality (Chapters 4 and 7). Variations in land use structure (e.g. deciduous forests instead of coniferous ones or larger areas with perennial vegetation) can also influence the hydrological cycle in a watershed due to a changed evapotranspiration, and subsequently affect water quality. Higher annual evapotranspiration decreases river discharge and vice versa, resulting in changes of nutrient concentrations by dilution or enrichment processes (e.g. see the forest experiment in Chapter 4). The composition of crop types within a watershed can also have influences on discharge and resulting nutrient loads in the rivers due to the crop type specific water and nutrient consumption (Figure 8.5). However, such effects are indirect and smoothed by soil retention processes, and they are not very high. However, changes in fertilisation regime and, especially, point source emissions can have much higher influence on the resulting nutrient concentrations, as they act more directly on the nutrient loads.

The water management measures according to the requirements of the WFD often include changes in the river's hydromorphology (e.g. reconnection of abandoned channel parts, enlargement of floodplain areas or removal of dams and weirs) to improve its structural quality and ecological status. Some of such potential effects can also be investigated with SWIM by changing the hydromorphological characteristics of a river course (e.g. channel length and width), and they were tested in Chapter 5. It could be seen that changes in the channel width had almost no influence on the observed nutrient concentrations in the river, whereas increases in the channel length resulted in a remarkable decrease of nutrient concentrations (accompanied by an increase in phytoplankton biomass benefiting from lower flow velocity).

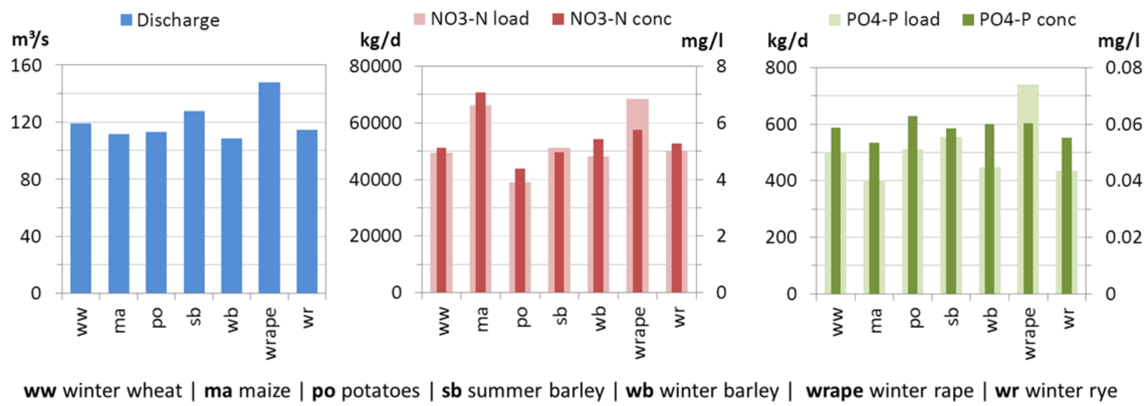


Figure 8.5 Experimental model run to test the impact of different crops (each cultivated with the same fertilisation) on river discharge and on nitrate nitrogen (NO_3-N) and phosphate phosphorus (PO_4-P) concentrations and loads for the Saale river basin in the period 1996-2003.

This points to a general problem in explaining the impact assessment results using SWIM with implemented in-stream processes: due to the influence of the phytoplankton biomass on the nutrients in river waters, it is often difficult to distinguish between the primary impacts on soil nutrient processes and river loads caused by certain land use or water management changes, and the secondary impacts due to altered chlorophyll *a* concentrations and a resulting change in nutrient uptake rates in the water body. The in-stream processes include a complex dynamics of nutrients with a high number of interactions and feedbacks with the algae population. The simulated effect on nutrient loads due to climate and socio-economic changes is always influenced by the phytoplankton population, and vice versa. Therefore, the obtained land use change impacts described in Chapters 5 and 7 have to be treated with caution, as they are not only caused by the land use and management changes, but also indirectly influenced by the subsequently changed phytoplankton conditions in the river water.

The SWIM driven land use change impact assessments applied in this study do not represent the “full” set of potential future land use changes in the watersheds, and only the effects of single measures connected to nutrient sources and agricultural practices on water quantity and quality were tested. Many other changes, also in combinations, are possible and even more probable (e.g. with regard to urbanisation or population development). Thus, the results of the management change impact assessments should be seen as a first step to find suitable methods for adaptation to projected climate change impacts.

Models like SWIM are useful for impact assessment studies, but there are still limits and restrictions: not all land use changes that are of interest to water managers can be easily implemented in the model, and not all easily modelled scenarios can be realised in an inhabited region. The land use change can be considered for analysis of climate change impacts on water quality, and the combined climate and land use change scenarios may be helpful in land use planning in order to increase the adaptive capacity of river basins (Krysanova et al., 2015). Climate change impacts cannot be neglected in socio-economic impact assessments, because climate change affects the status of water bodies, and it affects the effectiveness of measures to manage the water environment and meet policy objectives (Arnell et al., 2015).

Following this suggestion, the land use change scenarios were run alone as well as in combination with climate change scenarios for the entire Elbe river basin (Chapter 7). It could be seen that water discharge was most sensitive to climate change impacts, and land use change measures had only a little influence on runoff. It is difficult to derive such general conclusion regarding the main impacts on water quality. However, with this approach it was possible to detect some management changes, which would be intensified or reversed by the projected climate changes (see Section 7.4.4). This could be very helpful to derive feasible and necessary measure for adaptation to climate change.

The model-based impact assessments using SWIM in the Elbe river basin confirmed the importance of physical boundary conditions (climate, river morphology and land use pattern) on concentrations and loads of nutrients in rivers. Unfortunately, changing the river shape and the boundary conditions are measures, which are almost impossible to realise for the local agencies (e.g. climate variations), or they require application of complex and costly intervention measures, e.g., extension of floodplains by dike relocation or re-meandering of river courses. Taking this into account, it is recommended to focus on reduction of nutrient emissions, namely: application of lower rates of fertilisers adjusted to the plant requirements to reduce nitrate concentrations in water, and lower input from point sources to reduce phosphate and ammonium contamination in the rivers.

However, the results of the impact assessments presented here are region-specific, as they depend on physiographic setting and anthropogenic influences, and the transferability to other regions is limited. Even within the Elbe river basin, a high variability of projections could be detected when comparing results for several tributaries (Chapter 7, Figure 7.7). Taking the spatial heterogeneity of the climate change signals and of the resulting impacts into account, the advantages or disadvantages of the different impact assessment approaches should be compared when applying them to catchments of different sizes. The reasonability of the application of dynamic climate scenario data produced by GCM/RCM downscaling for the small scale is questionable, due to the spatial heterogeneity within the scenario projections. This heterogeneity can be better balanced at the large scale basins. In contrast, the application of static management change experiments is more reasonable for smaller scales, as such measures cannot be implemented for a large-scale watershed. They are rather designed for the local scale.

Nevertheless, despite all the questionable points mentioned in the overarching discussion of the matter in this section, impact assessment using a process-based semi-distributed watershed model enables to provide useful results for integrated water resources management. They can also help to derive valuable and necessary adaptation measures to possible threats and stresses caused by global changes.

8.3 Uncertainties

As usual in hydrological or ecohydrological watershed modelling and model-based impact assessment, all approaches go along with a certain degree of uncertainty, and it cannot be expected that the model calibration and climate or socio-economic impact assessment deliver valid and strict results, as well as that the projected impacts will be realised in future in case the scenario assumptions would be fulfilled. The results of model applications for different case study areas located within the Elbe river basin and presented in this dissertation come along with some uncertainty, which should be kept in mind when they are analysed and interpreted. The uncertainties were already partly mentioned in the discussions of results in previous chapters, and these scattered mentioning will be merged here for an overall summary and compilation of main sources of uncertainties.

The uncertainties are due to a wide range of possible problems, and can be categorised into three main sources, which will be shortly discussed below. They are related to:

a) data availability and quality for the watershed model setup, calibration, and validation,

b) model ability to reproduce the simulated interrelated processes in the watersheds, and

c) reliability of the climate / socio-economic scenarios applied for the impact assessment.

Data-related uncertainty. A hydrological or ecohydrological model used for impact assessment should be parametrised based on a full set of necessary input data, and properly calibrated and validated in advance. Relating to the SWIM model, this means that appropriate homogeneous and complete spatial datasets (DEM, land use and soil maps) and time series (daily climate parameters and regularly observed discharge and nutrient concentrations) are necessary for a successful model setup and calibration/validation. However, almost in all model applications – especially at the large-scale and in transboundary basins – some data are missing, or data coverage in time and/or space is problematic.

The observed water quality data and data on point and diffuse sources, in particular, are often insufficient in spatial and temporal dimensions in order to properly calibrate the SWIM model for water quality characteristics. For example, problems could arise by using partly short and often not overlapping time series (e.g. for climate and discharge, or for discharge and nitrogen, or for discharge at different gauges), missing data sets for some parameters, data sets with different origin, low temporal resolution in regard to point source emission data, or data sets with trends. Therefore, model calibration for water flows and – especially – water quality variables is often very complicated and always associated with a certain degree of uncertainty.

Nevertheless, despite of some data gaps also in the Elbe case studies presented here, SWIM was calibrated and validated with satisfactory, good or very good results, what enabled application of the model for climate and land use change impact assessment.

Model-related uncertainty. A model is always a simplification of reality, and natural processes taking place in soils, water bodies and vegetation, as well as interrelations between them, are represented in models with a certain degree of accuracy. This is due to a restricted memory of computers and computation time, as well as simply due to a limited human knowledge and understanding of processes. The computer-based models are always characterised by some level of abstraction. They are never – and cannot be – a full copy of an eco- or hydrological system.

The hydrological and ecohydrological watershed models can reproduce observed river discharge and nutrient loads/concentrations quite well, but they also have limitations. Different models come with different model uncertainties regarding representation of processes (structural model uncertainty). In general, the model uncertainty rises with the rising model complexity, and goes along with rising calibration efforts (compare Chapter 6), and this should be taken into account when a model is extended by adding new processes.

The SWIM model extended by in-stream processes seems to be characterised by a quite high level of uncertainty, simply due to the number of processes taken into account, and the increased number of calibration parameters (uncertainty related to model parametrisation). The mathematical description of some processes could not be confirmed by real in-situ measurements, and some parameters are based on values taken from literature. Therefore, as suggested above, the in-stream module should be activated and used for case studies, where it is really needed, e.g. in large-scale watersheds with extended floodplains. Besides, the complex process-based watershed models should be applied for water quality modelling by experienced modellers in order to deliver meaningful model results.

To overcome the limitations and weaknesses of a single hydrological or ecohydrological model, it could be also useful to apply several models with the same input parameter sets (model intercomparison) for a more comprehensive assessment of uncertainties and for an elicitation of more robust outputs (Warszawski et al., 2013; Schewe et al., 2013; Krysanova and Hattermann, 2017).

Scenario-related uncertainty. A further large uncertainty is connected to the scenarios applied for impact assessments. Different models come along with different scenarios, and nobody knows the most probable future climate and socio-economic development in a region, or at the national level, as they are influenced by several unpredictable factors.

Regarding the climate scenarios, a common method to overcome these problems is to use different RCMs or combined GCMs and RCMs to produce an ensemble of scenarios. The ensemble of scenarios is used to drive a hydrological or ecohydrological model for impact assessment. This approach allows investigating the range of uncertainty related to climate scenarios, as was also done in this dissertation for the entire Elbe case study presented in Chapter 7. This method is preferable in comparison with applying just one climate scenario as driver (Giorgi et al., 2001; Tebaldi & Knutti, 2007).

On the other hand, the uncertainty of future socio-economic pathways also hinders obtaining robust regional hydrological and water quality projections, so that they are still highly uncertain (Wilby, 2010). For the Elbe case study and its tributaries investigated in this dissertation, the management change scenarios were just optional and often unrealistic with regard to their generalisation and application to the entire case study areas. To reduce this uncertainty, it would be favourable to apply the socio-economic scenarios with ranges and with a spatial distribution of measures. This would support a more comprehensive assessment of uncertainties related to the socio-economic assumptions.

Due to lack of more detailed information on case-specific observations and measurements, not all possible methods to reduce uncertainties could be applied in this study. Furthermore, the climate scenario uncertainty seems to be unavoidable in the current stage of climate research. However, the climate and land use change impact assessments presented in the scientific publications included in this thesis, deliver first results and evaluation of probable future developments in the Elbe basin.

Despite all uncertainties involved in ecohydrological modelling, the water quality models are very important tools to support water managers and policy makers in implementing integrated management measures. It would be impossible to evaluate the effectiveness of land management measures and impacts of changes in land use and climate on water quality without using modelling tools. Considering the uncertainties and constraints, models have the power to provide insights in water quality processes, to support water management, and to facilitate communication with experts and stakeholders. But the modelling results have to be critically interpreted and a detailed communication and explanation to local experts and stakeholders is accordingly important (Krysanova et al., 2009).

8.4 Overall conclusions and outlook

An ecohydrological water quality model considering hydrological processes, vegetation and nutrient cycles within a watershed and driven by climate and management practices, can be a helpful tool for integrated water resources management. It allows to analyse nutrient fluxes and processes and to estimate possible future developments under changing climate, land use and management. The water quality models help to understand the behaviour of a river system, to identify the fractions of point and diffuse pollution coming to the streams, and to localise areas of the highest diffuse pollution in catchments. The scenario driven model applications allow to find reasonable measures for improving the ecological status of a river ecosystem for the implementation of the Water Framework Directive. The Soil and Water Integrated Model (SWIM) is one of such useful models for the regional scale.

However, the majority of water quality models available so far are suffering from incomplete representation of nutrient processes, and are thus subject to a steady further development. Sometimes also special catchment conditions and/or research questions require additional model adaptations to enable the models applicability for impact assessments. In regard to experiences gained with the SWIM model simulations in the Elbe river subcatchments, it could be detected that especially nutrients introduced to the river network by point sources should not only be routed, but also influenced by retention and decomposition processes in the rivers. This could be successfully implemented in the model code, and led to enhanced model performance.

The newly implemented approaches in SWIM presented in this study are an important contribution to improve the representation of nutrient cycling and their in-stream retention and transformation processes in the model. Furthermore, inclusion of the phytoplankton biomass in SWIM increases its usability for deriving conclusions on the ecological status of river water bodies based on biological indicators.

Improving the SWIM model in this respect, a sound base was developed for the reliable model-based impact assessments regarding possible future changes in climatic and socio-economic conditions, and also combinations of both, in order to derive suitable adaptation measures and to support preparation of the river basin management plans requested by the WFD.

Ecohydrological model calibration and impact assessment for the Elbe river basin using the new implemented in-stream module driven by a set of 19 climate scenarios resulted in a clear increasing trend in discharge and spatially variable projections for future nutrient loads of the rivers mainly due to the high heterogeneity of natural condition within the large-scale catchment, but also due to numerous of interrelated processes included with a high dependence on temperature, phytoplankton growth and nutrient consumption.

The inclusion of additional nutrient processes in the SWIM model increased its complexity quite significantly by bringing a set of new, sometimes interdependent, parameters. Thus, the uncertainty of the water quality modelling has increased, too, due to the structural changes and additional parametrisation requirements. But testing some less complex approaches to represent the in-stream retention and decomposition processes in river reaches could not result in the recommendation to use such simplifications.

However, the question, which level of complexity is really necessary to answer the specific research question and to achieve useful model results with minimal efforts, should be responded in every case study, and the experience described in this dissertation could be useful for that.

SWIM with the in-stream module should be used for water quality modelling in large watersheds with phytoplankton dominated rivers, as well as when the evaluation of the ecological status of a stream is needed. On the other hand, the in-stream processes can be neglected for nitrate nitrogen modelling only or for the analysis of diffuse emission from agriculture. The minimisation of model error as well as model sensitivity (to avoid over-parametrisation) should always be the aim to get the most useful model applications and realistic model results, which can be mostly achieved at a level of intermediate complexity.

Future applications of the ecohydrological model SWIM for water quality modelling in the Elbe river basin or in similar European large-scale river catchments can be based on the experiences and results presented in this thesis. Nevertheless, some points should be taken into account for potential further improvements of the SWIM model approaches and applications. They are related to a) model calibration, b) process descriptions, and c) management implications for integrated water quality modelling.

An intensive model calibration and validation is the main base for reliable model applications and results. Model calibration can only be successfully applied based on a complete set of spatial and temporal data and time series of an adequate duration, supplemented by the implementation of essential management measures (e.g. reservoirs or crop rotations). In the model set-ups presented here data on diffuse or point nutrient sources were only marginally accurate due to missing information. Modelling transboundary river basins is also often characterised by a large heterogeneity in available data. The harmonisation of observations and data preparation methods would be advantageous in international river basin management. It should also be well chosen in advance, which model complexity and spatial resolution of calibration parameters to use (e.g. whether to represent lock and weir systems in river reaches or spatially distribution according to soil properties, or not) in order to provide the most effective way to get useful model results at the large scale.

In view of following climate change impact assessments, SWIM model calibration should be especially focused on a careful calibration in similar climate conditions as expected in the future. The overall climate change signal could be considered already during the model calibration, e.g. if precipitation is expected to increase, it would be helpful to check the model performance in a wet subperiod in the past to get more reliable water quality projections for the future periods. In a changing world with overall increasing temperatures such careful checking and calibration of model processes are particularly needed for the temperature related processes newly included in SWIM (e.g. the ammonium cycle in soil or the in-stream algae processes) to avoid the projection of unrealistic high nutrient transformation rates in future.

A reliable water quality modelling needs a lot of transformation processes, boundary conditions and feedbacks being taken into account, as all are influencing the resulting water quality of the river system. This is often hard to be realised and neglecting or simplifying some processes is necessary to avoid overparametrisation or ineffective computation times. However, some aspects (e.g. more detailed nutrient input by erosion or benthic sediment processes) could be additionally implemented in the code to come closer to real conditions in the river waters and their catchments.

The main benefit of the newly developed in-stream SWIM module is its ability to consider biological processes (mainly in regard to the biological indicators requested by the WFD). But the phytoplankton biomass is not the only indicator usually used to evaluate the biological status of a surface water system. Also zooplankton, macrophytes and macro-invertebrates or fish are investigated and used for this purpose, too, and models to assess the impacts of future changes on the water quality should also be able to additionally consider such indicators, which would need further efforts in model development.

Model applications for impact assessments could benefit from the availability of better and more reliable climate and land use scenarios. Regarding climate scenarios, the ensembles of up-to-date projections of GCMs or RCMs should be used. In view of land use, representation of dynamic changes in time would be useful to come closer to real conditions. However, as climate change can strengthen, revoke or inverse land use change impacts, these changes and their impacts should be preferably investigated together to deliver more sound future projections. Additionally, the model intercomparison using several ecohydrological models for simulating water quality within the Elbe river catchment (or in other catchments) would help to identify uncertainty ranges of nutrient outputs in future projections.

Model-based impact assessments are useful for integrated water resources management considering possible future developments and threats. The modelled nutrient concentrations in the rivers could be used for the comparison with the thresholds of water quality classes. It would be a valuable next step to generate such model outputs and to produce maps presenting the expected ecological status of the river network under future scenarios. Such spatially differentiated information would be highly appreciated by water managers and stakeholders, and would improve the suitability of the model outputs for their local management decisions.

In general, a close collaboration between researchers, modellers and decision makers is needed. On the one hand, the special knowledge of local stakeholders and managers on natural conditions and anthropogenic impacts in a case study area could help to properly set up, test and calibrate the model. On the other hand, impact assessment results could be directly discussed and considered in upcoming management decisions. This would support not only the implementation of the WFD aimed in reaching the good ecological status of the river waters, but also be useful for other management decisions, as, for example, reducing nitrate pollution of the groundwater (which is also urgently needed, e.g. in view of the pending action of the EC against Germany based on the requirements of the nitrate directive (EC, 1991)), and to improve the earth's water quality for further generations.

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List of Abbreviations

(except for the terms used in mathematical equations and tables and explained immediately)

Δμ	Balance measure (relative bias of the mean annual observed and simulated values)
Δσ	Amplitude from the lowest to the highest monthly values
AMP	Active mineral phosphorus
ANIMO	Soil and nutrient leaching model
Arge-Elbe	Working Group to Control the Environmental Pollution of the Elbe
BGR	Federal Institute for Geosciences and Natural Resources
BOD	Biological oxygen demand
BÜK1000	General German soil map
CBOD	Carbonaceous biological oxygen demand
CCLM	COSMO-Climate Limited-area Modelling
CENTURY	model simulating the dynamics of carbon, nitrogen, phosphorus, and sulfur for different plant-soil systems
Chla	Chlorophyll *a*
CLC	CORINE Land Cover
DB (B)	Relative deviation in balance
DEM	Digital Elevation Model
DLR	German Aerospace Center
DOX (DO)	Dissolved oxygen
DWD	German Weather Service
EC	European Commission
EEA	European Environment Agency
EEC	European Economic Community
ENSEMBLES	EU-funded project to develop an ensemble prediction system for climate change
ESDB	European Soil Database
ESWAT	Extended SWAT
EU FP	The European Union's Research and Innovation funding programme
EU	European Union
FAO	Food and Agricultural Organization of the United Nations
FGG-Elbe	River Basin Community Elbe
GAP	Good Agricultural Practices
GCM	General Circulation Model
GIS	Geographic Information System
GWP	Global Water Partnership
HBV-NP	Hydrologiska Byråns Vattenbalansavdelning model with integrated nitrogen and phosphorus processes
HRU	Hydrological Response Units
HYPE	Model named Hydrological Predictions for the Environment
IKSE	International Commission for the Protection of the Elbe River
INCA	Integrated Catchment Model
IPCC	Intergovernmental Panel on Climate Change
ISI-MIP	Inter-Sectoral Impact Model Intercomparison Project
IWRM	Integrated Water Resources Management
LAI	Leaf Area Index
LAWA	German Working Group on Water Issues
LBGR	Brandenburg State Office of Mining, Geology and Resources
LHW	State Office of Flood Protection and Water Management Saxony-Anhalt

LP	Labile phosphorus
LUA	Brandenburg State Office of Environment
LUFA	Agricultural Analytic and Research Institute Saxony-Anhalt
MATSALU	Water quality model of the Estonian Matsalu bay
MESAW	statistical model for source apportionment of the riverine transport of pollutants
MIKE11	model that simulates flow, water quality and sediment transport in inland water bodies
MLUR	Brandenburg Ministry of Agriculture, Environmental Protection and Land Use Planning
MONERIS	MOdelling Nutrient Emissions in RIver Systems
N	Nitrogen
NASA	US National Aeronautics and Space Administration
NBL	Map of the hydrological units of the German Democratic Republic
NeWater	European project “New Approaches to Adaptive Water Management under Uncertainty”
NH4-N	Ammonium nitrogen
NO3-N	Nitrate nitrogen
NSE (E)	Nash-and-Sutcliffe-Efficiency
P	Phosphorus
PBIAS	Percent bias
PEST	Model Independent Parameter Estimation
PO4-P	Phosphate phosphorus
PRTR	Pollutant Release and Transfer Register
Q	River water discharge
QUAL2E	Enhanced Stream Water Quality Model
r	Pearson’s correlation coefficient
R^2	Coefficient of determination
RCM	Regional Circulation Model
RCP	Representative Concentration Pathways
REMO	Regional Modelling
RIKS	Research Institute for Knowledge Systems
RMSE	Root Mean Square Error
RSR	RMSE-observations standard deviation ratio
SCS	US Soil Conservation Service
SMP	Stabile mineral phosphorus
SRTM	Shuttle Radar Topographic Mission
STARS	Statistical Analogue Resampling Scheme
SWAT	Soil and Water Assessment Tool
SWIM	Soil and Water Integrated Model
TLL	Thuringian Regional Office for Agriculture
TMLNU	Thuringian Ministry of Agriculture, Nature Protection and Environment
TN	Total nitrogen
TP	Total phosphorus
T_{wat}	Water temperature
UBA	German Environmental Agency (Umweltbundesamt)
UNESCO	United Nations Educational, Scientific and Cultural Organization
WAVE	Model for simulating water and agrochemicals in the soil and vadose environment
WETTREG	Weather conditions based regionalisation method
WFD	European Water Framework Directive

Appendixes

Table A5.1 Ammonium cycle in soil – Mathematical descriptions derived from Neitsch et al. (2002a) and Voß (2007) to simulate ammonium processes in soil

Erosion and Leaching

$E_{amm} = (0.001 \times E_{sed} \times Amm_{i=1} \times er) / Ah_{sub}$

$L_{amm} = (0.01 \times Amm_i \times W_{tot}) / RSW_{amm}$

Nitrification / Volatilisation

$NitVol_i = Amm_i \times (1 - \exp(-(\eta_{temp} \times \eta_{swat}) - (\eta_{temp} \times \eta_{dep})))$

$frNit_i = 1 - \exp(-(\eta_{temp} \times \eta_{swat}))$

$frVol_i = 1 - \exp(-(\eta_{temp} \times \eta_{dep}))$

$Nit_i = frNit_i / (frNit_i + frVol_i) \times NitVol_i$

$Vol_i = frVol_i / (frNit_i + frVol_i) \times NitVol_i$

$\eta_{temp} = 0.41 \times (T_{soil,I} - 5) / 10$

$\eta_{swat} = (SW_i - WP_i) / (0.25 \times (FC_i - WP_i))$ *if* $SW_i - WP_i < 0.25 \times (FC_i - WP_i)$

$= 1$ *if* $SW_i - WP_i \geq 0.25 \times (FC_i - WP_i)$

$\eta_{dep} = 1 - z_i / (z_i + \exp(4.706 - 0.0305 \times z_i))$

Table A5.2 Ammonium cycle in soil – List of abbreviations

Parameter	description	Unit
Ah_{sub}	area of the subbasin	ha
Amm_i	ammonium concentration in soil layer i	g t^{-1}
$Amm_{i=1}$	amount of ammonium in the first soil layer	g t^{-1}
E_{amm}	ammonium reduction by erosion	kg ha^{-1}
er	enrichment ratio for the subbasin	-
E_{sed}	reduction of sediment by erosion	t
FC_i	amount of water in soil layer i at field capacity	mm
$frNit_i$	fraction of nitrified ammonium in the soil layer i	-
$frVol_i$	fraction of volatilised ammonium in the soil layer i	-
L_{amm}	amount of ammonium leaving the soil layer i	kg ha^{-1}
Nit_i	transformation amount by nitrification in the soil layer i	kg ha^{-1}
$NitVol_i$	ammonium transformation amount in soil layer i	kg ha^{-1}
RSW_{amm}	ratio between ammonium concentration in the soil to that in soil water	m^3 t^{-1}
SW_i	soil water content of layer i on a given day	mm
$T_{soil,i}$	soil temperature in soil layer i	°C
Vol_i	transformation amount by volatilisation in soil layer i	kg ha^{-1}
WP_i	amount of water in the layer i at wilting point	mm
W_{tot}	total amount of leaving water	mm
z_i	depth from the soil surface to the middle of the layer i	mm
η_{dep}	soil depth coefficient	-
η_{swat}	soil water coefficient	-
η_{temp}	soil temperature coefficient	-

Table A5.3 In-stream processes – Mathematical descriptions derived from Neitsch et al. (2002a) to simulate in-stream processes in the river network

Algae

algae	=	$algcon + (\mu_a \times algcon - \rho_a \times algcon - \sigma_1/depth \times algcon) \times TT$
chla	=	$\alpha_0 \times algae$
μ_a	=	$\mu_{max} \times FL \times \min(FN,FP) \times 1.047$^$(T_{wat}-20)$
ρ_a	=	$\rho_{a,20} \times 1.047$^$(T_{wat}-20)$
σ_1	=	$\sigma_{1,20} \times 1.024$^$(T_{wat}-20)$
FL	=	$0.92 \times DL/24 \times 1/(k_1 \times depth) \times \ln((K_L + (fr_{phosyn} \times H_{day})/DL) /$ $(K_L + (fr_{phosyn} \times H_{day})/DL \times \exp(-k_1 \times depth)))$
FN	=	$(C_{NO3} + C_{NH4}) / ((C_{NO3} + C_{NH4}) + K_N)$
FP	=	$C_{solP} / (C_{solP} + K_P)$
k_1	=	$k_{1,0} + k_{1,1} \times \alpha_0 \times algcon + k_{1,2} \times (\alpha_0 \times algcon)$^$2/3$

Nitrogen cycle

orgN	=	$orgNcon + (\alpha_1 \times \rho_a \times algcon - \beta_{N,3} \times orgNcon - \sigma_4 \times orgNcon) \times TT$
nh4	=	$nh4con + (\beta_{N,3} \times orgNcon - \beta_{N,1} \times nh4con + \sigma_3/(1000 \times depth) - fr_{NH4} \times \alpha_1 \times \mu_a \times algcon) \times TT$
no2	=	$no2con + (\beta_{N,1} \times nh4con - \beta_{N,2} \times no2con) \times TT$
no3	=	$no3con + (\beta_{N,2} \times no2con - (1-fr_{NH4}) \times \alpha_1 \times \mu_a \times algcon) \times TT$
$\beta_{N,3}$	=	$\beta_{N,3,20} \times 1.047$^$(T_{wat}-20)$
σ_4	=	$\sigma_{4,20} \times 1.024$^$(T_{wat}-20)$
$\beta_{N,1}$	=	$\beta_{N,1,20} \times (1 - \exp(-0.6 \times oxcon)) \times 1.083$^$(T_{wat}-20)$
σ_3	=	$\sigma_{3,20} \times 1.074$^$(T_{wat}-20)$
fr_{NH4}	=	$(pref_{NH4} \times nh4con) / (pref_{NH4} \times nh4con + (1-pref_{NH4}) \times no3con)$
$\beta_{N,2}$	=	$\beta_{N,2,20} \times (1-\exp(-0.6 \times oxcon)) \times 1.083$^$(T_{wat}-20)$

Phosphorus cycle

orgP	=	$orgPcon + (\alpha_2 \times \rho_a \times algcon - \beta_{P,4} \times orgPcon - \sigma_5 \times orgPcon) \times TT$
po4	=	$po4con + (\beta_{P,4} \times orgPcon + \sigma_2/(1000 \times depth) - \alpha_2 \times \mu_a \times algcon) \times TT$
$\beta_{P,4}$	=	$\beta_{P,4,20} \times 1.047$^$(T_{wat}-20)$
σ_5	=	$\sigma_{5,20} \times 1.024$^$(T_{wat}-20)$
σ_2	=	$\sigma_{2,20} \times 1.074$^$(T_{wat}-20)$

CBOD

cbod	=	$cbodcon - (\kappa_1 \times cbodcon + \kappa_3 \times cbodcon) \times TT$
κ_1	=	$\kappa_{1,20} \times 1.047$^$(T_{wat}-20)$
κ_3	=	$\kappa_{3,20} \times 1.024$^$(T_{wat}-20)$

Dissolved oxygen

Ox_{dis}	=	$oxcon + (\kappa_2 \times (Ox_{sat} - oxcon) + (\alpha_3 \times \mu_a - \alpha_4 \times \rho_a) \times algcon - \kappa_1 \times cbodcon - \kappa_4/(1000 \times depth)$ $- \alpha_5 \times \beta_{N,1} \times nh4con - \alpha_6 \times \beta_{N,2} \times no2con) \times TT$
κ_2	=	$\kappa_{2,20} \times 1.024$^$(T_{wat}-20)$
κ_4	=	$\kappa_{4,20} \times 1.060$^$(T_{wat}-20)$

Table A5.4 In-stream processes – List of abbreviations

Parameter	description	Unit
algae	algal biomass concentration at the end of day	mg L^{-1}
algcon	algal biomass concentration at the beginning of the day	mg L^{-1}
cbod	CBOD concentration at the end of day	mg L^{-1}
cbodcon	CBOD concentration at the beginning of the day	mg L^{-1}
chla	chlorophyll *a* concentration	µg L^{-1}
C_{NH4}	concentration of ammonium nitrogen in the reach	mg L^{-1}
C_{NO3}	concentration of nitrate nitrogen in the reach	mg L^{-1}
C_{solP}	concentration of phosphate phosphorus in the reach	mg L^{-1}
depth	depth of water in the channel	m
DL	day length	hr
FL	algal growth attenuation factor for light	-
FN	algal growth limitation factor for nitrogen	-
FP	algal growth limitation factor for phosphorus	-
fr_{NH4}	fraction of algal nitrogen uptake from ammonium pool	-
fr_{phosyn}	fraction of solar radiation that is photosynthetically active	-
H_{day}	solar radiation reaching the water surface in a given day	MJ m^{-2}
K_L	half-saturation coefficient for light	kJ $(m^2 \cdot min)^{-1}$
k_l	light extinction coefficient	m^{-1}
$k_{l,0}$	non-algal portion of the light extinction coefficient	m^{-1}
$k_{l,1}$	linear algal self-shading coefficient	$m^{-1} \cdot (\mu g\ L^{-1})^{-1}$
$k_{l,2}$	nonlinear algal self-shading coefficient	$m^{-1} \cdot (\mu g\ L^{-1})^{-2/3}$
K_N	half-saturation constant for nitrogen	mg L^{-1}
K_P	half-saturation constant for phosphorus	mg L^{-1}
nh4	concentration of ammonium nitrogen at the end of the day	mg L^{-1}
nh4con	concentration of ammonium nitrogen at the beginning of the day	mg L^{-1}
no2	nitrite concentration at end of day	mg L^{-1}
no2con	concentration of nitrite nitrogen at the beginning of the day	mg L^{-1}
no3	nitrate nitrogen concentration at the end of day	mg L^{-1}
no3con	nitrate nitrogen concentration at the beginning of the day	mg L^{-1}
orgN	concentration of organic nitrogen at end of the day	mg L^{-1}
orgNcon	concentration of organic nitrogen at the beginning of the day	mg L^{-1}
orgP	concentration of organic phosphorus at the end of day	mg L^{-1}
orgPcon	concentration of organic phosphorus at the beginning of the day	mg L^{-1}
oxcon	concentration of dissolved oxygen in the stream	mg L^{-1}
Ox_{dis}	dissolved oxygen concentration at end of day	mg L^{-1}
Ox_{sat}	saturation oxygen concentration	mg L^{-1}
po4	concentration of soluble phosphate phosphorus at the end of the day	mg L^{-1}
po4con	concentration of phosphate phosphorus at the beginning of the day	mg L^{-1}
$pref_{NH4}$	algal preference factor for ammonia	-
TT	flow travel time in the reach segment	day
α_0	ratio of chlorophyll *a* to algal biomass	µg mg^{-1}
α_1	fraction of algal biomass that is nitrogen	mg mg^{-1}
α_2	fraction of algal biomass that is phosphorus	mg mg^{-1}
α_3	rate of oxygen production per unit of algal photosynthesis	mg mg^{-1}
α_4	rate of oxygen uptake per unit of algal respiration	mg mg^{-1}
α_5	rate of oxygen uptake per unit of NH_4-N oxidation	mg mg^{-1}
α_6	rate of oxygen uptake per unit of NO_2-N oxidation	mg mg^{-1}
$\beta_{N,1}$	rate constant for biological oxidation of NH_4 to NO_2	day^{-1}
$\beta_{N,1,20}$	rate constant for biological oxidation of NH_4 to NO_2 at 20°C	day^{-1}

$\beta_{N,2}$	rate constant for biological oxidation of NO_2 to NO_3	day^{-1}
$\beta_{N,2,20}$	rate constant for biological oxidation of NO_2 to NO_3 at 20°C	day^{-1}
$\beta_{N,3}$	rate constant for hydrolysis of organic nitrogen to NH_4	day^{-1}
$\beta_{N,3,20}$	rate constant for hydrolysis of organic nitrogen to NH_4 at 20°C	day^{-1}
$\beta_{P,4}$	rate constant for mineralisation of organic phosphorus to PO_4	day^{-1}
$\beta_{P,4,20}$	rate constant for mineralisation of organic phosphorus to PO_4 at 20°C	day^{-1}
κ_1	CBOD deoxygenation rate	day^{-1}
$\kappa_{1,20}$	CBOD deoxygenation rate in the reach at 20°C	day^{-1}
κ_2	oxygen reaeration rate	day^{-1}
$\kappa_{2,20}$	oxygen reaeration rate in the reach at 20°C	day^{-1}
κ_3	rate of loss of CBOD due to settling	day^{-1}
$\kappa_{3,20}$	rate of loss of CBOD due to settling in the reach at 20°C	day^{-1}
κ_4	benthic oxygen demand rate	mg (m^2 day)$^{-1}$
$\kappa_{4,20}$	benthic oxygen demand rate in the reach at 20°C	mg (m^2 day)$^{-1}$
μ_a	local specific growth rate of algae	day^{-1}
μ_{max}	maximum specific algal growth rate	day^{-1}
ρ_a	local respiration or death rate of algae	day^{-1}
$\rho_{a,20}$	local algal respiration or death rate at 20°C	day^{-1}
σ_1	local settling rate of algae	m day^{-1}
$\sigma_{1,20}$	local algal settling rate in the reach at 20°C	m day^{-1}
σ_2	benthic source rate for soluble phosphorus	mg (m^2 day)$^{-1}$
$\sigma_{2,20}$	benthic source rate for soluble phosphorus in the reach at 20°C	mg (m^2 day)$^{-1}$
σ_3	benthic source rate for ammonium	mg (m^2 day)$^{-1}$
$\sigma_{3,20}$	benthic source rate for ammonium in the reach at 20°C	mg (m^2 day)$^{-1}$
σ_4	rate coefficient for organic nitrogen settling	day^{-1}
$\sigma_{4,20}$	rate coefficient for organic N settling in the reach at 20°C	day^{-1}
σ_5	rate coefficient for organic phosphorus settling	day^{-1}
$\sigma_{5,20}$	rate coefficient for organic P settling in the reach at 20°C	day^{-1}

The author's contribution to the individual papers

Hydrological Sciences Journal 53(5), 2008, 1001-1012 (Chapter 3):

The paper on modelling of wetland processes in regional applications was planned in succession of a SWAT conference in Potsdam by ***Fred Hattermann*** and ***Valentina Krysanova*** for the HSJ Special Issue "Advances in ecohydrological modelling with SWAT" and deals with a comparison of two approaches of different complexity to implement the special behaviour of wetlands regarding consumption of water and nutrients in ecohydrological modelling. While ***Fred Hattermann*** applied, tested and described the more complex approach for the Nuthe river basin, ***Cornelia Hesse*** ran and analysed several experiments using the simple wetland approach in the Rhin river basin, wrote the associated parts of the paper and prepared the corresponding figures. Final editing of the text as well as the addition of the Introduction and Discussion parts were done by ***Fred Hattermann*** and ***Valentina Krysanova***.

Ecological Modelling 218, 2008, 135-148 (Chapter 4):

SWIM model application simulating the water quality in the Rhin river catchment evolved in collaboration with the environmental authority of the German federal state Brandenburg (LUA) as a result of the stakeholder process within the European project NeWater (New Approaches to Adaptive Water Management under Uncertainty, contract number 511179 of the 6th framework program of the European Commission). ***Cornelia Hesse*** prepared the SWIM project, slightly adjusted the model code, calibrated and validated the model, analysed the different nutrient sources in the basin, run and interpreted the land use and climate experiments, and prepared the text, figures and tables for the publication. Together with his colleagues of the LUA, ***Jens Päzolt*** delivered all requested monitoring data of the study area for model setup. He additionally discussed the results and commented on the manuscript. ***Fred Hattermann*** was involved in the stakeholder process with the LUA, discussed model results and commented on the manuscript, too. ***Valentina Krysanova*** guided and supervised the entire process, checked the drafted paper and helped to improve its scientific relevance and linguistic style.

Environmental Modelling & Assessment 17(6), 2012, 589-611 (Chapter 5):

Implementing in-stream processes in the SWIM model was one of several tasks in the generally planned further development of the ecohydrological model SWIM within the SWIM user community in the Potsdam-Institute for Climate Impact research (PIK) leaded by ***Valentina Krysanova***. ***Cornelia Hesse*** adapted the model code based on the SWAT approach as well as on former work and experiences of ***Anja Voß*** regarding implementation of ammonium nitrogen in soils supplemented by own ideas. ***Cornelia Hesse*** prepared the input data for the model application, set up the SWIM project for the Saale river basin, calibrated and validated the model, run several management and climate experiments and analysed the results. ***Cornelia Hesse*** also prepared the tables and figures for the publication, wrote the text and formatted the paper. ***Valentina Krysanova*** supervised the whole process, discussed the results, and commented and edited the manuscript.

Ecological Modelling 269, 2013, 70-85 (Chapter 6):

The research question about the usefulness of differently complex methods to simulate nutrient retention in river catchments arose from the large parameter uncertainty in the former application of the extended by in-stream processes SWIM model in the Saale river basin. ***Cornelia Hesse*** prepared and calibrated the SWIM project for the Saale river basin with implemented landscape and in-stream processes, included some additional simpler approaches for nutrient retention in the river network in the SWIM code, and planned the simulation experiments. ***Tobias Vetter*** found in literature and included in the SWIM code the additional equation for the simple nutrient retention in rivers as a function of water temperature. ***Julia Reinhardt*** started and analysed several PEST runs for automatically calibration of different SWIM versions. ***Cornelia Hesse*** finalised the PEST runs and output analyses for all retention approaches with SWIM, prepared the tables and figures for the publication, wrote the text and formatted the paper. ***Valentina Krysanova*** debated the research questions and possible approaches in advance, discussed results during their application, and edited the manuscript.

Water 8, 2016, 40 (Chapter 7):

For modelling climate and management change impacts on water quantity and quality in the entire Elbe river basin ***Cornelia Hesse*** planned the whole simulation project, set up, adjusted and calibrated the extended SWIM model with included in-stream processes, ran the climate and land use change scenarios and analysed the temporal and spatial scenario output data. ***Cornelia Hesse*** also prepared the tables and figures for the publication, wrote the text and formatted the paper. ***Valentina Krysanova*** guided and supervised the whole process, discussed results during the modelling study, and edited the manuscript.

Curriculum vitae

Diese Seite enthält persönliche Daten und ist daher kein Bestandteil der Online-Veröffentlichung.

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Erklärung

Hiermit erkläre ich, dass die Arbeit an keiner anderen Hochschule eingereicht sowie selbstständig und nur mit den angegebenen Mitteln angefertigt wurde.

Potsdam, den 08.06.2018 (Cornelia Hesse)

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