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HABILITATION THESIS

River water quality modelling for river basin and water resources management with a focus on the Saale River, Germany

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Abstract

This thesis focuses on computer modelling issues such as i) uncertainty, including uncertainty in parameters, data input and model structure, ii) model complexity and how it affects uncertainty, iii) scale, as it pertains to scaling calibrated and validated models up or down to different spatial and temporal resolutions, and iv) transferability of a model to a site of the same scale. The discussion of these issues is well established in the fields of hydrology and hydrogeology but has found less application in river water quality modelling. This thesis contributes to transferring these ideas to river modelling and to discuss their utilization when simulating river water quality.

In order to provide a theoretical framework for the discussion of these topics several hypotheses have been adapted and extended. The basic principle is that model error decreases and sensitivity increases as a model becomes more complex. This behaviour is modified depending if the model is being upscaled or downscaled or is being transferred to a different application site.

A modelling exercise of the middle and lower Saale River in Germany provides a case study to test these hypotheses. The Saale is ideal since it has gained much attention as a test case for river basin management. It is heavily modified and regulated, has been overly polluted in the past and contains many contaminated sites. High demands are also placed on its water resources. To provide discussion of some important water management issues pertaining to the Saale River, modelling scenarios using the Saale models have been included to investigate the impact of a reduction in non-point nutrient loading and the removal and implementation of lock-and-weir systems on the river.

Keywords: complexity, eutrophication, heavily modified river, high level architecture (HLA), hydrodynamics, inorganic micro-pollutants, model coupling, morphology, Saale River, scale, sensitivity, substance transport, uncertainty, water quality, water resources management

Zusammenfassung

Diese Arbeit konzentriert sich auf Themen, die in der Computermodellierung vorkommen, wie z.B. i) Unsicherheiten, einschließlich Unsicherheiten in den Prozesskonstanten, Dateneingaben und Modellstrukturen, ii) Modellkomplexität und ihre Auswirkungen auf die Unsicherheiten, iii) Skalen, bezogen auf das Übertragen von kalibrierten und validierten Modellen auf kleinere oder größere Skalen mit unterschiedlichen räumlichen und zeitlichen Auflösungen, und iv) Übertragbarkeit eines Modells auf einem Gebiet der gleichen Skala. Diese Themen, die in der Hydrologie und Hydrogeologie häufig diskutiert werden, haben wenig Anwendung in der Fließgewässergütemodellierung gefunden. Diese Arbeit soll ein Beitrag leisten, diese Konzepte in die Flussmodellierung zu übertragen.

Um einen theoretischen Rahmen für die Diskussion dieser Themen zu stellen sind einige Hypothesen übernommen, verändert und ergänzt worden. Das Grundprinzip dieser Hypothesen ist dass bei ansteigender Komplexität des Modells, der Fehler zwischen Modellergebnissen und Messdaten verringert und die Gesamtsensitivität des Modells erhöht wird. Dieses Verhalten verändert und verschiebt sich entsprechend, wenn das Modell auf andere Skalen oder auf ein anderes Anwendungsgebiet der gleichen Skala übertragen wird.

Diese Hypothesen wurden mit einer Modellierung der mittleren und unteren Verläufe des Saale-Flusses geprüft. Die Saale ist als Fallstudie gut geeignet, da es viel Aufmerksamkeit als Testfall für Flussbassinmanagement gewonnen hat. Der Fluss ist mit vielen technischen Baumaßnahmen stark verändert worden, ist in der jüngeren Vergangenheit übermäßig beschmutzt worden, und enthält viele Altlasten. Von ihrer Wassserressourcen wird ein hoher Nutzungsgrad in Anspruch genommen. Um die Diskussion über einige wichtige Wassermanagement-Themen zu ergänzen sind Simulationsergebnisse von Szenarienberechnungen bereiht gestellt. Dazu gehören die Auswirkung einer Verringerung diffuser Nährstoffeinträge und den Bau von neuen Stauhaltungen und Rückbau existierende Staustufen.

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1 Introduction

1.1 River water quality modelling and the EU-WFD

In September 2000 the European Union (EU) passed a new water framework directive (WFD) with the goal of increasing and establishing a good ecological status on a long-term basis. Groundwater, surface waters and coastal waters are affected by this regulation making extensive management of rivers and their catchment areas indispensable. River basin management consists of co-ordinating all activities which can affect the water resources with the goal of maintaining good quality. Included in the management scheme are not only the water systems themselves but also the land surfaces in the river's catchment that affect these waters (Mostert, 1999, 2003).

The new EU-WFD requires that the management of water resources be politically organized and managed on the river catchment scale in hopes of retaining the present state of the water quality of our rivers or better, to attain an improvement in the quality of our water resources. River basin management is an interdisciplinary task and includes both components from both the natural sciences (hydrology, erosion and sediment transport, landscape assessment, hydrogeology, etc.) and social sciences (socio-economics, ecological economics, behavioural theory, etc.) (Rode, *et al*., 2002). This has given impetus to develop computer systems to support the management process (see Möltgen and Petry (2004) for an overview of integrated projects in Germany). An important component in the management of a river basin is the river itself since all the water resource activities that are carried out in the basin will have, in most cases, a direct impact on the ecological status of the river. Hence, we need to know the river's present ecological functioning and how the anthropogenic activities impact the quality of the water.

Water quality models are very useful in describing the ecological state of a river system and to predict the change in this state when certain boundary or initial conditions are altered. Such changes may be due to morphological modifications to the water body, such as straightening, and discharge regulations using control structures (weirs, dams, etc.), changes in the type (point or non-point), amount and location of pollutant loading into the system, and changes in meteorological inputs due to changing trends in climate. The degree of complexity in describing the ecological state varies from model to model. The complexity of deterministic models, the type investigated in this study, varies by the number and type of variables describing the state of the ecological system (e.g. concentration of chlorophyll-a and nutrients) and the parameters underlying the processes governing the kinetics of the system (e.g. rates of algal growth and nutrient uptake).

The new EU water framework directive has given a pulse of renewed interest in water quality modelling due to the directive's implementation of cost-covering and ecological-sound water resource

management on the river basin scale. Management options on the basin scale require a holistic approach of the basin's water resources, which include all components of the water cycle (roughly: precipitation - surface runoff - soil infiltration - percolation to groundwater - river channel discharge). In order to investigate the impact of management measures on the waters of the system several models must be implemented which cover all aspects of the source, transport and retention of water and substances important to the investigated river basin and coupled to a modelling system. Several projects are currently underway in Germany in which several methodologies are being developed and investigated in integrating these models into systems adapted to the characteristics of the river basins studied (e.g. Weiße Elster, Havel, Werra, Ems, etc.). In all these studies, the river model plays an important and integral role in these systems. The models must therefore be capable of simulating all effects in the river basin on the water quality of the river. This can be done using various levels of model complexity, depending on the stressors on the water resources and the scale of the application.

It is also important that hydrodynamic modelling compliment the water quality simulations. To carry out effective river basin management it is very important to receive accurate data on the discharges and flow velocities so that assertions on the substance concentrations and loadings and flooding effects can be made. This also applies to regulated rivers where weirs and dams have a major influence on the hydrodynamic regime and transport of pollutants. These include retentive properties through sedimentation during low flow conditions, which can be rapidly released during flooding and deposited onto floodplains. The current velocity is also a major component regulating the resuspension and deposition of sediment along the river bed. Determining velocity data for large rivers is very expensive and most measuring programs only include a sparse network of water level gages from which discharges and velocities can be determined. Also, the complexity of the currents through a regulated river does not allow analytical approaches to be applied with the accuracy required. Hence, hydrodynamic computer models, which can numerically simulate the currents along the entire course of the river, have become essential tools to simulate the velocities.

Although the treatment of waste water has significantly improved in Germany, it appears a limit has been reached in the degree of improvement that can be attained in river water quality. This is due to the high loads of nutrients still being emitted into the waters from non-point sources. Reduction of this source is slow and cumbersome and the pool of nutrients on land surfaces is still quite high. In particular to nitrogen, even if the supply of this nutrient pool is reduced, long lag times in its transport to the river cause minimal improvements in the water quality and only after significant time has passed. Another important factor that has limited the improvement of water quality is the heavy extent of discharge control by the construction of levies, dykes, weirs and locks and modifications by straightening river meanders. An additional objective of this contribution is to investigate the impact of these morphological river changes on water quality, especially on nitrate concentration.

Methodologically, the effect uncertainty of river hydrodynamic parameters have on the water quality output variables is explored.

This study includes excerpts from many articles published by the author in journals and book contributions. Key internationally reviewed articles include Lindenschmidt (2006), Lindenschmidt, Wodrich and Hesse (2006), Lindenschmidt, Hesser and Rode (2005), Lindenschmidt, Ollesch and Rode (2004), Lindenschmidt, Poser, and Rode (2005), Lindenschmidt, Rauberg, and Hesser (2005), Lindenschmidt, Schlehf, *et al*. (2005) and Lindenschmidt, Suhr, *et al*. (1998). An exhaustive list of all the author's articles pertaining to this research is given in the appendix. Additional information was drawn from eight Diploma theses all supervised by the author: Eckhardt (2004), Hesse (2004), Rauberg (2005), Refus (1997), Schlehf (2004), Sonnenschmidt (2002), von Saleski (2003) and Wodrich (2004). Groundwork for many of the concepts developed in this research stem from two projects that were acquired and managed by the author to successful completion:

- *Loading of solute and suspended solids from rural catchment areas flowing into Lake Victoria in Uganda*
  financed by the Canadian International Development Agency
- *Control and optimization of mobile and stationary aeration systems for Berlin surface waters*
  funded by the Berlin Senate.

This work makes a contribution in determining the ecological status of the Saale River and to investigate the transport and behaviour of pollutants in this river system. A computer modelling approach was pursued to fulfil this goal for a number of reasons:

- to provide a means of gathering and organizing data from several sources and sampling campaigns carried out on the Saale.
- to provide a more in-depth study of the functional interactions of processes within the ecosystem; there is a knowledge deficiency on the ecological functioning of the Saale,
- to give insight on the most crucial processes and functions in the ecosystem (sensitivity analysis, parameter identification)..
- to pinpoint deficiencies in data sampling and understanding of processes; future sampling programs can be steered to alleviate these deficiencies,
- to determine interrelationships between, for example, water pollution load and agricultural development (Braun *et al*., 2001, p. 22).

1.2 Modelling in water resources management

The amount of literature on computer modelling in water resources management is enormous. This study will give a survey of reviews and overviews that have been written on various aspects of the

subject. Such a survey may have different structures which focus on different facets of the field. Examples are:

- types of models (conceptual, deterministic, empirical, …)
- type of water body or hydrological component (coastal zone, estuaries, floodplains, groundwater, lakes, oceans, rivers, runoff, soil water, …)
- branches (agriculture, fisheries, forestry, water and wastewater treatment…)
- applications (e.g. climate change, soil erosion by water, irrigation, floods, reservoir operation, river water quality)

I have chosen to focus on the latter. The selection of applications is not exhaustive but gives a broad view of the many challenges faced by the water resources manager.

Climate change

An early review on modeling the effects of climate change on water resources is given by Leavesley (1994). In his review he identified many problem areas common to a variety of models applied, including parameter estimation, scale, model validation, climate scenario generation and data. He suggested at that time that research needs to address these problems included development of a more physically-based understanding of hydrological processes and their interactions, parameter measurement and estimation techniques for application over a range of spatial and temporal scales, quantitative measures of uncertainty in model parameters and model results, improved methodologies of climate scenario generation, detailed data sets in a variety of climatic and physiographic regions, and modular modeling tools to provide a framework to facilitate interdisciplinary research. Ten years later Varis, *et al*. (2004) published a review addressing the same subject. They state that improvements have been made in process descriptions and that uncertainty analyses have evolved to include risk assessment. Advances have also been made in statistical applications for climate scenario generation and in the description of regional weather patterns, such as ENSO (El Niño – Southern Oscillation) and NAO (North Atlantic Oscillation). Although climate models such as GCMs (Global Circulation Models) continue to evolve their outputs remain crude and are often inappropriate for basin scale hydrological analyses. The bridging techniques are evolving and are most prevalent in large-scale studies such as for the Rhine basin (Middelkoop, *et al*., 2001), the Nile basin (Conway, 1996) and Sweden (Rummukainen, *et al*., 2004). Other regional water resources studies based on climate change scenarios have been carried out such as on the Elbe basin (Krysanova, et al., 1999), south-western Bulgaria (Chang, et al., 2002), Britain (Arnell, 1998) and central Sweden (Xu, 2000).

Soil erosion by water

The management of water runoff has a significant effect on soil erosion. Models have become indispensable tools for the study of soil erosion processes and the quantification of sediment transport from hill slopes and river and stream basins. In his review on monitoring and modelling approaches in

quantifying soil erosion by water, Brazier (2004) indicates a shift in the research towards erosion modelling away from erosion monitoring. He suggests that data collection should concentrate on describing spatial heterogeneity of soil loss. Merritt, *et al*. (2003) review the different models used to study soil erosion and erosive processes focusing on those models which include sediment and sediment-associated nutrient transport. Lindenschmidt, Ollesch and Rode (2004) and Sharpley, *et al*. (2002) provide overviews of erosion models implemented to simulate phosphorus export. Other surveys of erosion models can be found in Deliman, *et al*. (1999) and ECOMatters (2002).

In their review on expected climate change impacts on soil erosion, Nearing, *et al*. (2004) predict that soil erosion rates will increase in many regions of the world due to the increase in the total rainfall and the frequency of high intensity rainfall events. This is also the case in areas where annual rainfall is expected to decrease since system feedbacks related to decreased biomass production can lead to greater susceptibility of the soil to erode. Reviews and research trends in tillage erosion and the impacts of erosion on land productivity are given by Lindstrom, *et al*. (2001) and Blaschke, *et al*. (2000), respectively. Borak and Bera (2003) provide an excellent overview of computer models used to quantify nonpoint pollution at the watershed scale.

Irrigation

The demand for irrigation water is steadily rising coinciding with accelerated competition for water and degradation of the environment. English, *et al*. (2002) speak of a paradigm shift in irrigatin management from irrigation management based on a biological objective (maximizing crop yields) to management based on economic objectives (e.g. maximization of net benefits). The former is relatively simple with a clear defined problem and a single objective. Maximizing benefits is a multi-objective problem and is far more complex requiring more detailed models and the relationships between water application, crop production, irrigation efficiency and economic factors. A review of models to simulate irrigation water values under different policies is provided by Conradie and Hoag (2004). Campos and Studart (2000) focus their review on charging for water and reallocation of water use through the water market. Mujumdar (2002) in his overview of mathematical tools for irrigation water management stresses the importance of addressing the interests of stakeholders when modelling irrigation system operation, crop water allocations and performance evaluation.

Increased water demand is not the only problem facing irrigation practice. The negative effects on soil and environment also need to be addressed. These include water logging, soil salinization and water quality degradation. Reviews on alleviating detrimental effects on the soils and irrigation water include subjects such as improving drainage designs (Guitjens, *et al*., 1997), using subsurface drip irrigation (Camp, 1998), managing soil physical properties such as increasing infiltrations rates and stabilizing macropores (Jayawardane and Chan, 1994), ameliorating saline soils (Qadir, *et al*., 2000)

and remediating irrigation water with a high salt content (Oster, 1997). The implications of new technologies such as GIS applications (Know and Weatherfield, 1997) and remote sensing (Ambast, *et al*., 2002; Van Niel, *et al*., 2004) are increasingly being advanced to aid crop identification, regional yield forecasting and on-farm productivity monitoring and management.

This area of water resources management is not untouched by the effects of climate change. In their review on drainage developments around the world, De Wrachien and Feddes (2004) call for a re-examination of planning principles, design driteria and operating rules than can adapt to rapid shifts in climate. A United States perspective disagrees finding no threat to North American agriculture due to climate change and little inducement for diverting agricultural adaptation resources to efforts in slowing or halting the climate change process (Easterling, 1996). Water scarcity will, however, continue to be a growing concern and is addressed with reviews regarding progress in irrigation management (Pereira, *et al*., 2002) and plant genetic improvement and general management response to climate (Inman-Bamber and Smith, 2005).

Floods

Currently, many countries have engaged in research activities to develop catchment-wide flood management programs. Flood management plans in a modelling and decision support framework are now being prepared for all 80 catchments in England and Wales (Evans, *et al*. 2002). In 2005, the German Federal Ministry of Education and Research followed suite and began funding over 30 large projects for flood management and mitigation in large river basins in Germany (http://www.rimax-hochwasser.de). The EU project "FloodSite" involves many countries in Europe covering physical, environmental, ecological and socio-economic aspects of floods from rivers, estuaries and the sea. Transnational cooperations have also commenced to strengthen relations between countries sharing common river basins. One such project is the transnational INTERREG III B Project to develop joint strategies on spatial planning in the Elbe catchment area (http://www.ella-interreg.org). The CRUE network has been set up to consolidate existing European flood research programmes, promote best practice and identify gaps and opportunities for collaboration on future programme content. (http://www.crue-eranet.net).

Extensive reports have also been provided giving synopses of large floods in i) recent times: for example, the Elbe river (DKKV, 2004), Oder river (Erlich, *et al*., 2004), Red River, Canada (Simonovic and Carson, 2003) and Mississippi River (Changnon, 1998); and ii) the past: for example, central Europe (Mudelsee, *et al*., 2004) and USA (Burian, *et al*., 1999).

Much progress has been achieved in implementing new technologies in flood management. This includes the field of remote sensing along with geographic information systems (Sanyal and Lu,

2004), radar estimates of rainfall (Collier, 2002) and satellite monitoring (Grigorev and Kondratev, 1997; Smith, 1997). Advances in the hydrological and meteorological aspects of floods are reviewed by Bacchi and Ranzi (2003). The intensification of flooding due to climate, land-use and environmental change has been reviewed by Bronstert (2003), Bronstert, et al. (2002), Fleming (2002) and Poesen and Hooke (1997).

A paradigm shift has occurred in recent years in flood sciences from flood management to flood risk management. Merz (2005) provides an extensive work on the subject. The concept of risk contains the assessment of damage due to floods – reviews are provided by Blong (2003), Smith (1994) and Viljoen, *et al*. (2001).

Reservoir operation

Many of the reviews in reservoir management focus on the optimisation of reservoir operation. This is due to the complexity of the many demands on the stored water, such as drinking water supply, hydroelectric power generation, water quality, recreation and irrigation, which require high water stages in the reservoir. These demands conflict with flood control measures for which lower stage levels are necessary to buffer peak discharges from the upstream catchment areas. Labadie (2004) gives an excellent review of the state-of-the-art in optimal operation of multireservoir systems. Applications of heuristic programming methods using evolutionary and genetic algorithms are described, along with applications of neutral networks and fuzzy rule-based systems for inferring reservoir system operating rules. Overviews are also found in the literature on optimising techniques using specific computational methods such as stochastic modelling (Srinivasan and Simonovic, 1999), genetic algorithms (Sharif and Wardlaw, 2000) and fuzzy logic (Tilmant, *et al*., 2002).

The incorporation of hydrologic models into the optimising techniques is reviewed by Yang, *et al*. (1995). Decision models may also be included into the optimisation to integrate simultaneously all relevant aspects in reservoir operation, such as physical, hydrological, technological, financial and socioeconomic characteristics (Cunha, 2003). In their review, Lund and Guzman (1999) summarise a variety of derived operating policies for reservoirs in series and in parallel. Overviews on reservoir release policies and real-time reservoir operations specific for irrigation are given by Mujumdar and Ramesh (1997) and Sahoo, *et al*. (2001). Reservoir operation optimisation has followed suite with many other water management fields in incorporating risk analyses (Ouarda and Labadie, 2001), to include concepts such as reliability, resilience and vulnerability in characterising operation practices.

River water quality

River water quality modelling has gained impetus in recent years due to increased political awareness of river quality issues. New environmental policies such as the EU Water Framework Directive and

the US Total Maximum Daily Load concept require these modelling tools to evaluate river water quality and to assess management practices for the improvement of aquatic health and functioning. (Horn, *et al.*, 2004). River qater quality models are also a critical link to other processes in the river basin in many river basin management systems (Saleth, 2004). Interest in water quality modelling is also evident among social scientists and socio-economists, who draw additional information from the model results important for decision makers (Korfmacher, 1998). Trepel and Kluge (2002) give an excellent review of models they find applicable for the implementation of the EU Water Framework Directive.

Traditionally, river water quality models have focused on predicting dissolved oxygen concentrations in the river and, later, on plankton-nutrient dynamics in river eutrophication problems. Cox (2003a, 2003b) gives exhaustive overviews of river water quality models and their applications in simulating dissolved oxygen in lowland rivers. This tradition still forms an important foundation for ecological assessments and Smith (2003) reviews recent advances in algae-related eutrophication research. He points to gaps in our understanding of river and stream eutrophication such as the hysteresis effect of nutrient loading on suspended algae growth, inhibitory effects of high concentrations of inorganic suspended solids on algal growth and cyanobacterial dominance of phytoplankton worldwide. Phosphorus is most often the limiting nutrient in eutrophication models and a review of phosphorus retention studies in streams is given by Reddy, *et al*. (1999). McIntyre and Wheater (2004) point to the need for more research required in uncertainty estimation of these types of models.

Many river water quality models are complimented with the description of macrophyte-nutrient dynamics, particularly for smaller streams. Barendregt and Bio (2003) review modelling studies simulating the effect of water quantity and quality on macrophytes on the regional, local and site scales. In light of the new and growing field of ecohydrology (Zalewski, 2002, 2004), the importance of the effect macrophytes have on hydrodynamics (flow resistance) has gained recognition (Tabacchi, *et al*., 2000; Green, 2005). Aquatic invertebrate fauna are increasingly being incorporated in river quality modelling (Clarke, *et al*., 2003). The biology of zebra mussels as it relates to water quality problems in rivers is reviewed by Effler, *et al*. (1996). Ward, *et al*. (1998) give an overview of metazoans associated within the interstices of the stream bed and their effect on lotic ecosystems.

Apart from dissolved oxygen and nutrient modelling, other pollution-causing substances have been given increasing attention. Yapa and Shen (1994) review studies on major oil spills that have occurred in rivers and show the state-of-the-art in river oil spill modelling. Petit, *et al*. (1995) provide a review of strategies for modelling the environmental fate of pesticides discharged into riverine systems. Cao and Carling (2002) give an overview of the current status of research in modelling the transport of suspended sediments in rivers and conclude that the models are still far from being mature in giving

reliable predictions. In their paper, Monte, et al. (2005) summarise the development of models used for predicting the migration of radionuclides through rivers. Håkanson (2004) points to the value and new insights radionuclide simulations give in understanding river ecology.

The effect of a river's morphology on its aquatic ecology has also gained awareness. Wagenschein, Lindenschmidt and Rode (2005) show differences in nitrogen retention in naturally-meandering and channelized sections of the same stream. Doyle, et al. (2003) review hydrogeomorphic controls on phosphorus retention in streams. Mosselman (1995) gives an overview of mathematical models used to predict planform changes in rivers.

The biogeochemical processes within the upper few centimetres of river sediments (hyporheic zone) has a profound effect on aquatic chemistry and much current research has been focused in this field (Sophocleous, 2002). In their book, Jones and Mulholland (2000) give an excellent overview on the subject. Further reviews of incorporating the hyporheic zone in water quality modelling are given by Runkel, *et al*. (2003) and Supriyasilp, *et al*. (2003).

Like many other components of the water system, river aquatic ecosystems are affected by climate change in regards to their ecosystem functioning and health. Meyer, *et al*. (1999) review models that could be used to explore potential effects of climate change on freshwater ecosystems. These include models of instream flow, bioenergetics, nutrient spiralling and riverine food webs.

1.3 Modelling issues in hydrology applied to river water quality modelling

Important issues in modelling for water resources management are model uncertainty, complexity, scale and transferability. These issues are more established in the field of hydrology but still need to be applied and investigated in river water quality modelling. The next subsections give an introduction to each of these issues.

Uncertainty analysis

An important consideration when modelling is the uncertainty in the model results due to errors in sampled data and model structure. Sources of error include: i) errors in the data used as initial and boundary conditions in the model, ii) errors in the data used to calibrate and validate the model results, and iii) errors due to the structure of the model which includes the equations, solutions and parameters used for the simulations. A literature search indicates that uncertainty analyses have been carried out on a number of water quality modelling studies, such as the transport of organic (Giri *et al*., 2001) and inorganic (Carroll and Warwick, 2001) pollutants, simple Streeter-Phelps oxygen dynamics (Warwick *et al*., 1997; Maihot and Villeneuve, 2003), phytoplankton - nutrient dynamics using QUAL2E (McIntyre *et al*., 2003) and the Biebrza river model (van der Perk and Bierkens, 1997) and solute

transport (Whelan *et al*., 1999). However, all these modelling exercises were run assuming steady state flow and concentrated on the uncertainty in the water quality parameters, not on hydrodynamic parameters. Sincock *et al*. (2003) conducted an uncertainty analysis with hydrodynamic parameters in a river water quality model under unsteady flow conditions but they used a simplified routing approach based on the kinematic wave with a lag-cascade model extension. The parameters that they incorporated in their analysis were the storage coefficient and a corresponding flow exponent. The model used in this study, DYNHYD, a module in the WASP5 simulation package (Ambrose, *et al*., 1993), uses the full dynamic wave equation and Manning's equation to simulate river flow for which the roughness and weir overflow coefficients become important for parameter uncertainty.

One aim of this research was to simulate the hydrodynamics and water quality of the regulated river Saale (Germany) and to conduct an uncertainty analysis of the parameters and input data on the output state variables. Highlighted in this study is not only to see the effect water quality parameters have on its state variables but also to see how hydrodynamic parameters affect the water quality variables. Hence, the influence of the morphological status of the river, which is described by the hydrodynamic parameters, on the water quality can be derived.

Another important source of uncertainty in river water quality modelling is that found in model structure (Radwan *et al*., 2004). In this study, the structure of the model is understood to be the algorithms and equations used to describe and calculate the processes. Structural uncertainty is very difficult to quantify and only a few attempts are found in the literature. For example, Engeland *et al*. (2005) calculated both total and parameter uncertainty in a hydrological model and found that “the uncertainties in the simulated stream flow due to parameter uncertainty are less important than uncertainties originating from other sources”. Reference is made to model structure as one of the sources of uncertainty but it was not explicitly calculated. Todd *et al*. (2001) investigated the effect different demographic equations have on calculating the population dynamics of the eastern barred bandicoot, a small marsupial endemic to south-eastern Australia. However, each equation has a different set of parameters which needs to be calibrated; hence a strict division of parameter and structural uncertainty cannot be quantified. This, too, is the case in Håkanson’s (2000) uncertainty analysis of lake eutrophication models. van der Peck (1997) implemented eight different equations of increasing complexity to simulate orthophosphate concentrations as a function of distance along a river. Here, too, attention is given to the uncertainty of the parameter sets used in the equations and less on the uncertainty due to the equations themselves. Hence, another important goal for this work is to differentiate more distinctly between uncertainty stemming from parameters, boundary conditions and model structure.

Another important issue to the development of modeling systems is the propagation of errors as simulation output from models are transferred to other models as input. The author is unaware of research specifically focused on “cross-model” uncertainty analysis. This is a necessary step for the advancement of the development of integrated modeling systems for river basin management to determine how the uncertainties of parameter values and boundary and initial condition values affect variables globally in the system environment. Also from the perspective of the decision maker, who is to use the system for decision support, an assessment of the largest uncertainty in the system to be managed is required in order to judge the risks involved in the various management schemes. It can be argued that if many models are incorporated into one large model the propagated errors through the model chain are the same as in the large conglomerated model. This is not necessarily so since interdependencies may exist between variables and parameters in the conglomeration that may not exist if the variables and parameters are found in separate models. In other words, the sum of the uncertainties of each coupled model is not necessarily equal to the total uncertainty of the modeling system.

Model complexity

A key question in choosing or developing a water quality model is how complex the model structure should be to suit the needs in evaluating the management measures to be implemented. Increased complexity means that more processes will be represented in the system potentially reducing the error in the simulation results. The downside is that increasing the model complexity increases the number of degrees of freedom within the model (more parameters and variables) which can be expressed as the total increase in model sensitivity on output results. This makes calibration more difficult and reduces the predictive power of the model.

A hypothesis has been proposed by Snowling and Kramer (2001) which relates the uncertainty of a simulation model with respect to model complexity, sensitivity and error. The hypothesis is illustrated in Figure 1. “Model sensitivity increases with model complexity due to the larger number of degrees of freedom and the structure of the interactions between parameters and state variables. Modelling error decreases with increasing model complexity as the more complex models are able to better simulate reality with more processes included and fewer simplifying assumptions” (Snowling and Kramer, 2001, p. 21). Also, with increasing model complexity identification of the model parameters becomes poorer meaning that the parameters become increasingly correlated (van der Perk, 1997).

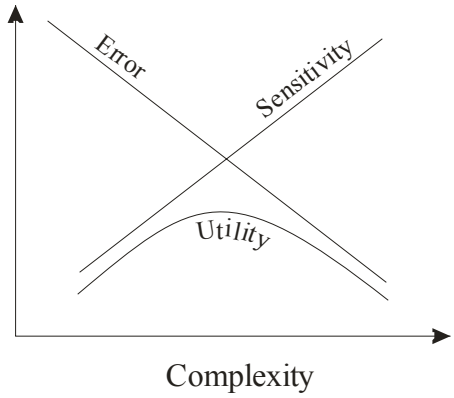


Figure 1: Uncertainty (error and sensitivity) and model utility as a function of complexity.

Snowling and Kramer (2001) tested their hypothesis on two models: i) a sorption model for radioactive zinc onto sediments in solution (LeBeuf, 1992 cited in Snowling and Kramer, 2001) and ii) the transport of a groundwater tracer plume. In the first model the complexity was changed by varying the sorption process (equilibrium or kinetic) and the number of solute and sorbed phases. For this model their hypothesis was verified in which increased complexity caused an increase in parameter sensitivity and a decrease in model error. The complexity of the second model was changed by varying the sorption process (equilibrium or kinetic), degradation processes (zero or first order) and isotherms (linear, non-linear and Monod – in order of increasing complexity). In this case, the hypothesis could only be verified in part. Sensitivity does increase with increasing complexity but no relation was evident between error and complexity. Ideally, the best model is one in which both sensitivity and error are minimised. Here, a utility function was implemented to evaluate which complexity is best suited for the characteristics of the study site.

In this study the hypothesis is tested on a water quality model developed for the Saale River (see also Lindenschmidt, 2006). The model EUTRO, a module in the WASP5 simulation package (Ambrose, *et al*., 1993) which describes the phytoplankton-nutrient-oxygen dynamics in a water body, was implemented. The complexity of the model can be easily increased by enabling more state variables, parameters and functions used for the simulation. Increasing the number of variables also increases the number of processes interacting between the variables for which additional parameters are required to control these processes. TOXI, another module in WASP5 for simulating sediment and micro-pollutant transport, is also applied in the framework of this hypothesis using increasing degrees of complexity in describing the sorption kinetics between suspended solids and heavy metals (see also Lindenschmidt, Wodrich and Hesse, 2006).

Scale issues considering complexity and uncertainty

Most studies on scale issues in the water sciences, in which model results across different scales are compared, are found in the field of hydrology (see for example Kalma (1995), Sposito (1998) and Sivapalan, *et al*. (2004)). These mostly consider processes occurring on or in the land surfaces of

catchment areas. The focus is mainly on water fluxes although some studies do include substance transport, for example erosion (Kandel, 2004), nitrate leaching (Hosang, 1998) and dissolved organic carbon (Aitkenhead, *et al*., 1999). Few studies consider scaling issues of processes of substance transport in the stream or river. Examples of such cross-scale studies include the influence of the riparian zone on stream water chemistry (Smart *et al*., 2001), the effect hydrological conditions have on stream water acidity (Wade, *et al*., 1999) and the relationship between soil organic carbon pools on dissolved organic carbon in stream water (Aitkenhead, *et al*., 1999). These studies have a focus on the stream but with the perspective from processes occurring on or in the land surfaces connected to the stream or river network. The authors are not aware of investigation focusing on instream processes on the transport of substances in stream water at different scales. Hence, this study should give new insight on scale comparisons, shifting the focus from river catchments and their land surfaces ("area" scale) to transport mechanisms within the stream itself ("line" scale).

Many studies are also found in the literature which explore the effect model complexity has on model uncertainty. Elert, *et al*. (1999) compiled the results of 13 different modelling exercises from seven research teams investigating the transport of surface contamination of a pasture soil using three different radionuclides. No simple relationship was found between model uncertainty and complexity.

Lindenschmidt, Wodrich and Hesse (2006) propose a hypothesis stating that there will be a shift in the complexity versus uncertainty relationship when implementing the same model for studies of different scale (see Figure 2). For example, when reducing both the temporal and spatial scales, processes become more dynamic and quick-lived (Blöschl and Sivapalan, 1995) and increased model complexity is required to obtain the same reduction in model error. Additional processes which may be dampened or deemed less significant at the large scale need now to be included in the small-scale model description to achieve better accuracy in model output. This increase in complexity also increases the overall model sensitivity since the inclusion of additional processes bring with it additional parameters and data input.

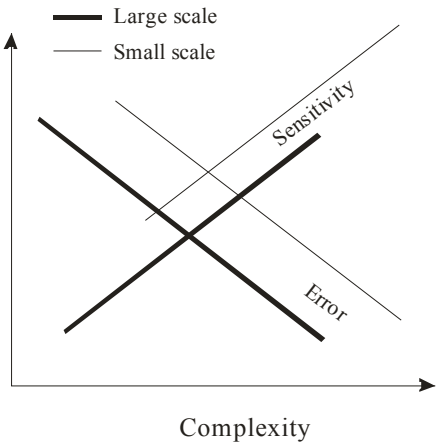


Figure 2: Model uncertainty versus complexity at different scales.

A goal of this study is to test this hypothesis using a water quality model on two sections of the river Saale, Germany, representing two different scales. The transport of suspended solids and inorganic pollutants were simulated once on the large-scale model of a 90 km reach with a discretization of 500 m segments and a simulation time step of one day, and again on the small scale of a lock-and-weir system on the same river using a segmentation of 100 m and a time step of one hour. Care was taken that both temporal and spatial resolutions were made finer when downscaling (see Blöschl and Sivapalan (1995)). The effect of locks and weirs on the transport of substances at different scales is also highlighted.

Model transferability

Transferability can be defined as a model's ability to capture the hydrological regimes in different climatic and physiographic regions at the relevant spatial and temporal scales without requiring changes in model structure or physical parameterizations (Devonec and Barros, 2002). Many studies show that model performance drops when models and model parameters are transferred both spatially and temporally. Even when transferred within the same region with similar climatic and basin characteristics a re-calibration of parameters is often unavoidable to retain accuracy and predictability. Devonec and Barros (2002) found that model transferability in hydrology is very sensitive on the hydroclimatic variability between different regions and time periods. This dependency may not be as strong for river water quality modelling. Heuvelmans, *et al*. (2004) evaluate the transferability of the main controlling parameters of a semi-distributed hydrology model (SWAT). The results indicate that there is a decline in model performance when parameters are transferred in time and space and care should be taken when exchanging parameter values between regions with a different topography, soil and land use.

For sediment and nutrient transport Lindenschmidt, Ollesch, *et al*. (2003) showed that generalities can be made between two adjacent-lying catchments in Uganda, since they have identical climates and have similar soils but only to a limited extend. A slight change or addition in land-use type (e.g.

presence of wetlands) can have a marked effect on the outcome of a substance regime as is clearly shown in their study by the difference in phosphorus behaviour between the two basins (each catchment area ≈ 25 km^2). The sensitivity to certain parameters and basin characteristics require the description of different processes dominating in different basins which must be defined quite precisely in order to increase accuracy when transferring or aggregating data across catchments. León, *et al*. (2001) also state that the transferability of model parameters to other watersheds, especially those in remote areas without enough data for calibration, is a major problem in diffuse modelling. Drawing on additional GIS data improved model portability.

Transferability becomes increasingly difficult in ecological models (e.g. Leftwich, *et al*. (1997) and Guay, *et al*. (2003) for fish habitat models). More success is shown in models of larger scale (e.g. Lettenmaier (2001)). The author is unaware of specific transferability studies for river water quality models. Hence, an interesting goal that will additionally be pursued is to investigate to what extent parameter sets calibrated on data from a particular stretch of a river (e.g. most downstream lowland course) can be adopted to other stretches of the river (e.g. middle reaches). He proposes an extension of the hypothesis of Snowling and Kramer (2001) to test the transferability of a model on a different river or river section of the same scale. Figure 3 shows the behaviour of the error and sensitivity curves of a model being transferred to a different study area. If the error remains relatively the same or decreases with model complexity (error curve shifts to the left or downward) the model is said to be transferable. For sensitivity, the shape of the curve is important. If sensitivity continuously increases with complexity, transferability is assured. However, if a plateau arises in which sensitivity remains constant then the model is less reactive to the parameter setting and the transfer has deprived the model of its predictive strength. This hypothesis extension is to be tested by comparing complexity versus uncertainty behaviour between modelling exercises of the lower and middle courses of the Saale River, which are of the same scale.

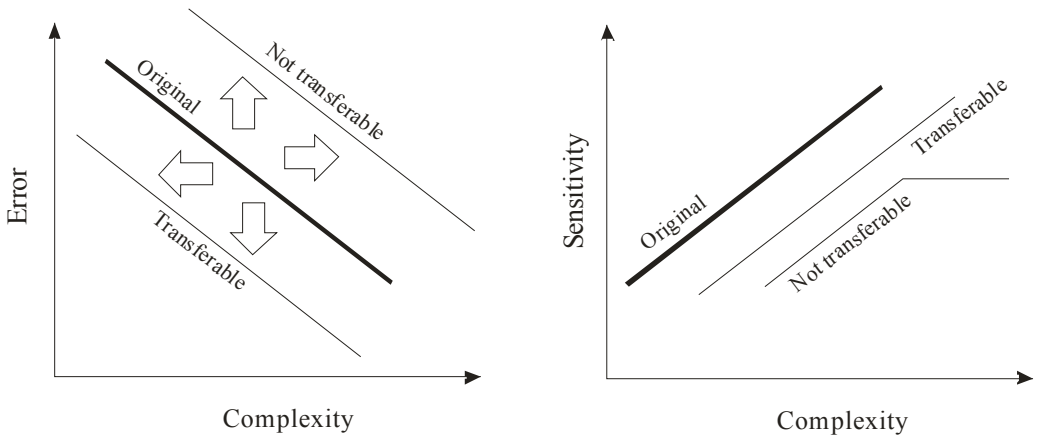


Figure 3: Possible behaviour of error (left) and sensitivity (right) when the model is transferred to another river or river section.

2 Method of solution approach: simulation modeling

2.1 Why WASP5 (Water quality Analysis Simulation Program)?

An own model development was considered but the time required for such a development is extensive and would exceed the time duration planned for the Saale project. The project required an up-and-running model of the Saale within two years. Also, the processes used in deterministic models do not vary greatly and it is not justified to develop a new model with perhaps a slightly different configuration of process descriptions. The source code of the model was available to make adaptations specific to the Saale River. Furthermore, a large portion of this research was to concentrate on other aspects and problems specific to modeling exercises such as uncertainty analysis, scaling problems and model coupling. These topics would all have come too short had an own model development been pursued.

A comparison of general characteristics of several models is given in Table 1. Additional information can be found in Trepel and Kluge (2002). An important criterion for choosing a water quality model was the accessibility of the program source code. This is required for the integration of the models into a modelling system for river basin management. Hence, only the first three models listed in the table are suitable: QUAL2E, WASP5 and CE-QUAL-RIV1. QUAL2E was disregarded because it is a steady state model with no hydrodynamic component. CE-QUAL-RIV1 was also not considered because it does not simulate branched river systems and embayments appendaged to rivers. WASP5 was the best choice for implementation into the modelling system. The program executables, source codes and user manuals for WASP5 are freely accessible via the Internet. The existence of good documentation is also an important criterion that should not be underestimated.

The model is also an appropriate tool for the implementation of the WFD. The goal of the WFD is to attain a good ecological and chemical status of a water body. Nutrients are not included in evaluating the chemical status but are a physical-chemical component in the assessment of the ecological condition. The WFD also gives equal weighting to point and non-point pollution loading in which nutrients play an important role for both. Exemplary for nitrogen, the LAWA, a consortium responsible for the implementation of the WFD in Germany, has set the standard for surface water bodies to be: total nitrogen <= 3 mg N/L; nitrate <= 2.5 mg N/L; ammonium <= 0.3 mg N/L. The mean concentrations of the lower Saale River are still above these values.

2.2 Past studies with WASP5

WASP5 has been implemented for many water quality studies and many open water bodies. An overview for rivers and estuaries is given in Table 2:

Table 1: Comparison of selected water quality models

Table extented from Rauch et al. (1998)
(i) Brown & Barnwell (1987)
(ii) Ambrose et al. (1993)
(iii) Cerco & Cole (1995)
(iv) ATV (1996)
(v) DHI (1992)
(vi) Kirchesch & Schöl (1999)

		QUAL2E (i)	WASP5 (ii)	CE-QUAL-RIV1 (iii)	ATV (iv)	MIKE11 (v)	QSIM (vi)	QualSim/Jabron (vii)
source code	accessible	y	y	y	n	n	n	n
documentation	available	y	y	y	y	y	n	y
water quantity	simulated	n	y	y	y	y	y	y
	control structures	n	e	y	y	y	y	y
	advection	y	y	y	y	y	y	y
	dispersion	y	y	y	y	y	y	y
	flooding	n	e	n	n	y	n	y
water quality	sediment	n	y	n	y	y	y	y
	temperature	y	n	y	y	y	y	y
	nitrifiers	n	n	n	y	y	y	n
	O_2-BSB	y	y	y	y	y	y	y
	nitrogen	y	y	y	y	y	y	y
	phosphorus	y	y	y	y	y	y	y
	silicon	n	e	n	y	y	y	y
	phytoplankton	y	y	y	y	y	y	y
	zooplankton	n	n	n	y	y	y	y
	bentic algae	n	e	n	y	y	y	y
structure	embayments	n	y	n	n	n	n	n
	non-point loading	y	y	n	y	y	n	y

e - extended; y - yes; n - no

- Hajda and Novotny (1996) conducted a study to evaluate the impact of the absence and presence of a dam on the Milwaukee River in Wisconsin, USA. They found that removing the dam alleviated the effects of eutrophication. Phytoplankton growth increased due to improved light conditions and benthic decomposition reduced. These factors improved the oxygen balance in the water.

- Rehfus, Lindenschmidt and Hegemann (1997) and Lindenschmidt and Wagenschein (2004) used WASP5 to optimize the operation of an aeration ship on the flowing waters within the city of Berlin, Germany. The ship is used to supplement the water with liquid oxygen during periods of high oxygen demand, particularly after heavy storm events. The emitted pollution loading from storm runoff rapidly consumes the dissolved oxygen which can lead to large fish kills. They found that injecting oxygen at a stationary point upstream from the affected area was more effective than distributing the oxygen in the water by driving the ship up and down the waterway.

Table 2: Summary of WASP5 modelling exercises applied to rivers and estuaries.

Site	Application	Flow	Variables	Results	Reference
Rivers					
Milwaukee River Wisconsin, USA	effect of damm removal	steady state	DO - BOD Chl-a, N, P	damm removal causes: Chl-a >, DO >, P & N >, SOD <	Hajda & Novotny (1996)
Spree Berlin, Germany	optimizing operation of aeration ship	dynamic	DO - BOD	point rather than distributive application of liquid O_2 increases DO in river	Refus, Lindenschmidt & Hegemann (1997)
Black River Washington, USA	Total max. daily load for DO > 8 mg/l	water balance	DO - BOD, Cl^- Chl-a, N, P	TP should be < 0.05 mg/l at low flow	Pickett (1997)
Lower Truckee River Nevada, USA	effects of groundwater & agriculture on w.q.	dynamic + weirs	DO - BOD periphyton, N, P	strong impact of groundwater nitrate on water quality	Warwick *et al*. (1999)
Carson River Nevada, USA	estimates non-point pollution sources	steady state	DO - BOD periphyton, N, P	reduce TP by 97% or total load (CBOD + TP + TN) by 70%	Warwick *et al*. (1997)
Carson River Nevada, USA	estimates bank erosion rate of Hg	steady state	sediment Hg^{2+} ? CH_3Hg	bulk of Hg transported by suspended load, not bedload; bank erosion = *f* (long. slope)	Heim & Warwick (1997) Carroll & Warwick (2001)
Estuaries					
Scheldt Estuary Netherlands	PCB distribution	dynamic	salinity, SS PCB (12 isomers)	tides, SS transport & hydrophic sorption regulate PCB distribution	Vuksanovic *et al*. (1996)
Scheldt Estuary Netherlands	heavy metal behaviour	dynamic	salinity, SS Cr, Cu, Ni, Pb, Zn	tides, SS transport & metal sorption to SS regulate heavy metal behaviour	De Smedt *et al*. (1998)
Venice lagoon & channel system	calculate residence times	dynamic	salinity	classification of channel system into vivid, medium and restricted channel dynamics	Umgiesser *et al*. (2001)

- WASP5 has also been used for Total Maximum Daily Load (TMDL) studies such as for the Black River in Washington State, USA (Pickett (1997). The middle stretch of the river is burdened with low oxygen conditions, especially during low flow. To prevent eutrophic conditions to persist, the total phosphorus *TP* load to the river should not exceed 0.05 mg/L.

- Warwick *et al*. (1999) made the first modifications to DYNHYD by incorporating weirs into the model. Water was diverted by the weirs for irrigation and returned to the river as surface point and ground water non-point return-flow. They showed the strong impact of nitrate leaching on the water quality of the river. von Saleski, *et al*. (2004) adapted the extended model for large lock-and-weir systems on the Saale River.

- Many modelling studies have been carried out on the Carson River in Nevada, USA (Carroll, *et al*. (2004); Carroll, *et al*. (2000); Carrol and Warwick (2001); Heim and Warwick (1997); Warwick, *et al*. (1997)). Aside from eutrophication studies the transport of mercury has also been investigated. Large deposits of mine tailings are found along the river's banks emitting large amounts of mercury into the water, especially from bank erosion during flood events. This was simulated using an extended version of TOXI.

- The Scheldt Estuary has also received modelling attention using WASP5 (De Smedt, *et al*. (1998); Vuksanovic, *et al* (1996)). DYNHYD incorporates tidal flows in its hydrodynamic simulations and, hence, the transport of sediments and selected inorganic and organic micro-pollutants in the estuary could be investigated. They found that the pollutants accumulate in the zone of the turbidity maximum and only a small amount actually reaches the sea. Another application on an estuary is by Umgiesser and Zampato (2001), in which DYNHYD simulated the flow through the channel network of Venice and was coupled to a 2-D model of the Venice Lagoon.

Due to their three-dimensional configuration, the WASP5 modules, EUTRO and TOXI, can also be implemented for large basin water bodies. Studies include applications on coastal areas (Wang, *et al*., 1999), lakes (James, *et al*., 1997; Jin, *et al*., 1998; Kellershohn and Tsanis, 1999; Rygwelski, *et al*., 1999) and reservoirs (Kao, *et al*., 1998; Tufford and McKellar, 1999; Wu, *et al*., 1996).

2.3 Model comparison: WASP5 vs. QSIM

Although QSIM does not qualify as a water quality model for our purposes, a comparative study was carried out using the model to test the performance of WASP5. A detailed comparison of the two models with results is given in Lindenschmidt and Wagenschein (2004) and Lindenschmidt, Schlehf, Suhr, *et al*. (2005). Table 1 gives a comparative overview of the two models' capabilities.

For a discharge of up to approximately twice the mean flow both WASP5 and QSIM are capable of depicting the hydrodynamics comparatively well. The Kalinin-Miljukov technique, an approach based on storage coefficients, is used for the hydraulic simulations in QSIM, which is not suited for higher flows and floods. If flood management is an issue for the studied river basin, the St. Venant approach, which solves the momentum and continuity equations of a dynamic wave, is a better alternative, which is the method implemented in WASP5. A new version of QSIM in which the St. Venant equations are implemented is currently being tested (V. Kirchesch, pers. comm., Dec. 2003).

There are marked differences in the functionality of the two models in regards to water quality simulations. Temperature and pH are not simulated in WASP5, they are input as time-varying functions. QSIM is able to simulated two algal groups, green algae and diatoms, whereas the original version of WASP5 sums the two together into one class. Due to the differentiation of the algal groups, QSIM includes silicon to its simulated nutrient spectrum. James *et al*. (1997) extended the WASP5 code to include the differentiation of three algae groups (greens, diatoms and blue-greens) and the silicon cycle and applied it successfully to simulate the water quality of Lake Okeechobee in Florida, USA. Zooplankton is a state variable in QSIM, it is an input time-varying function in WASP5. Both models simulate sediment transport and periphyton, the WASP5 extension developed by Shanahan (2001). An important advantage of WASP5 is its capability to model the transport and fate of organic and inorganic micro-pollutants. WASP5 also has more flexibility in the discretization of the river network compared to QSIM. Embayments and floodplains may be discretized separately from the main channel and branched and braided rivers can also be represented. The processes depicted in WASP5 are also not restricted to the water column but also apply to the sediment layers. An additional file representing the emissions of non-point pollution may also be coupled to the model.

Figure 4 compiles the mean goodness-of-fit of selected variables between all the simulated and measured values for both WASP5 and QSIM using a likelihood function from Beven (2001, p. 249), which lies in the range between 1 (perfect fit) and 0 (no fit). Some of the nutrient variables do not correspond exactly between the two models. However for comparison sake similar variables were grouped together so that dissolved phosphorus *DP* , total phosphorus *TP* and total nitrogen *TN* from QSIM are grouped together respectively with total inorganic phosphorus *TIP*, total organic phosphorus *TOP* and total organic nitrogen *TON* from WASP5. Generally, both models measured similar likelihood values. WASP5 results are slightly better since the simulations underwent a more rigorous calibration process. Ammonium *NH4-N* has the worst fit between simulated results and measured values for both models due to the aforementioned uncertainty in the surge from the combined sewerage overflow at Halle. The error for nitrate *NO3-N*, dissolved or inorganic phosphorus and chlorophyll-a *Chl-a* increases along the river flow and is due to the higher variability in the chlorophyll-a values sampled in the lower reach of the studied river course. Both (dissolved) calcium

Ca^{2+} and (particulate) suspended solids *SS* were simulated in WASP5 using the TOXI submodule and included here for comparison sake. WASP5 performed better in simulating the transport of suspended solids perhaps due to its more accurate description of the hydrodynamics (St. Venant approach in WASP5, Kalinin-Miljukov approach in QSIM; see Lindenschmidt and Wagenschein (2004) for a comparison). Calcium was simulated with the least error to measurements for both models. Good agreement between the model and samples was achieved for oxygen O_2. The agreement is slightly less for the total or organic fractions of the nutrients, reflecting the uncertainty in the phytoplankton dynamics.

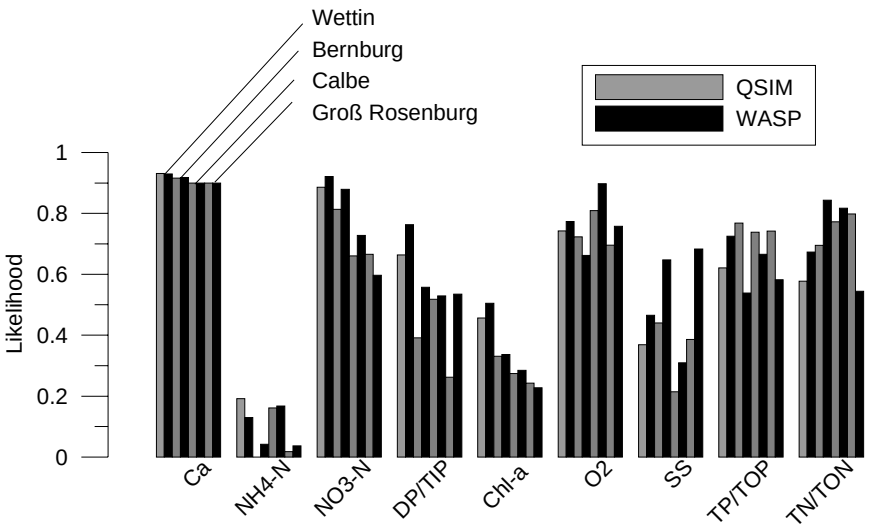


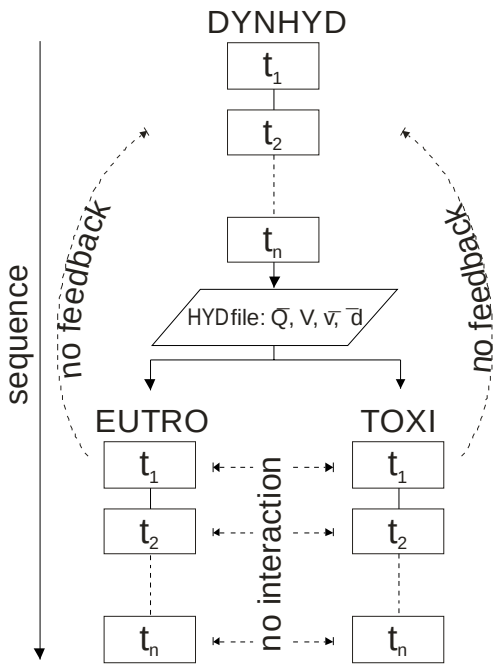
Figure 4: Summary of the goodness-of-fit (likelihood) between measured values and simulated results for both QSIM and WASP5.
(from Lindenschmidt, Schlehf, et al., 2005)

This comparative study allowed important conclusions to be made and gave a high degree of confidence in using WASP5. Both models, QSIM and WASP5, were able to simulate the state of the river system for the two week sampling program and the river stretch under investigation. The simulation results between the two models for the variables that corresponded directly between them were in good agreement with one another. The largest deviations resulted in the state variable ammonium and may have resulted in the difference in modelling approaches. QSIM uses the growth dynamics of nitrifier bacteria whereas WASP5 uses first-order kinetics to model nitrification. The higher complexity in QSIM does not lead to more accuracy. The variability found in the output, such as chlorophyll-a, was not captured even with higher model complexity.

2.4 The WASP5 modeling system

The modeling package used for the simulation of the river water quality is WASP5, developed by the US Environmental Protection Agency (Ambrose, *et al*. 1993). It is written in the FORTRAN programming language and consists of three models: i) DYNHYD - calculates the hydrodynamics of a

water body, ii) EUTRO - simulates phytoplankton and nutrient dynamics and iii) TOXI - computes sediment and micro-pollutant transport. Figure 5 illustrates the typical sequence of the dynamic (varying with time) simulations. In the original version of WASP5 a simulation of the hydrodynamics is first run for *T* days (t_1, t_2, … t_n). The output from DYNHYD is stored in a file which is later retrieved from EUTRO and TOXI for their simulations of *T* days. In the original version there is no interaction between EUTRO and TOXI and no feedback from these models to DYNHYD. These capabilities have been added in this work as described in subsection 2.5: *Model Coupling with HLA (High Level Architecture)*



(from Lindenschmidt, Hesser, et al., 2005)

Figure 5: Simulation sequence of DYNHYD, EUTRO and TOXI in the original WASP5 package-

A mass balance equation is used accounting for all material entering and leaving the system by point and non-point loading, advective and dispersive transport and physical, chemical and biological transformations:

$$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x}(U_x C) - \frac{\partial}{\partial y}(U_y C) - \frac{\partial}{\partial z}(U_z C) + \frac{\partial}{\partial x}\left(E_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(E_y \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(E_z \frac{\partial C}{\partial z}\right) + S_B + S_K + S_L$$

where C is the substance concentration with $\partial C / \partial t$ representing its change with respect to time *t*, E_x , E_y and E_z are the longitudinal, lateral and vertical diffusion coefficients (only the first was implemented here), S_B , S_K and S_L are the rates for boundary loading, kinetic transformations and

loading from point and non-point sources, respectively, and U_x , U_y and U_z are the longitudinal, lateral and vertical advective velocities (only the first is required for our one-dimensional case). The velocities are provided by the DYNHYD hydrodynamic simulations.

2.4.1 DYNHYD

DYNHYD solves the St. Venant equations, which includes the momentum equation for the momentum balance:

$$\frac{\partial U}{\partial t} = -U\frac{\partial U}{dx} + a_g + a_f$$

and the continuity equation for the mass balance:

$$\frac{\partial Q}{\partial x} + \frac{1}{B}\frac{\partial H}{\partial t} = 0$$

where: a_f - frictional acceleration; a_g - gravitational acceleration = $-g \cdot \partial H / \partial x$; B - river width; g - gravitational acceleration; H - water surface elevation or head; Q - volume discharge; U - velocity along the river longitudinal axis; x - distance along the river longitudinal axis and increasing upstream. Manning's equation is used for the frictional acceleration:

$$a_f = \frac{g \cdot n^2}{R^{4/3}} \bullet U \bullet |U|$$

where: n - Manning's roughness coefficient; R - hydraulic radius (cross-sectional area / wetted perimeter). $|U|$ ensures that friction always opposes the flow direction. The roughness coefficient depends on the characteristics of the river bottom and is used for calibration.

These equations are integrated numerically on a discretized network of the river course. A “link-node” approach is used to solve the equations at the respective grid points. At each time step the momentum equation is solved using the links giving the required velocities and the continuity equation is solved via the nodes giving the water levels and volumes of each unit of discretization.

Warwick (1999) extended the model to include weirs. The discharge *Q* over a weir is based on the Bernoulli equation, which assumes the streamlines of the flow are straight and there are no energy losses:

$$Q = \left(\frac{2}{3}\right)^{\frac{3}{2}} \cdot g^{\frac{1}{2}} \cdot b \cdot h^{\frac{3}{2}}$$

where: b - breadth of weir crest; g - gravitational acceleration; h - height between weir crest and water level upstream of the weir. A modification to the equation is the Poleni equation which

integrates a weir discharge coefficient μ in order to allow differentiation between various construction types of weirs:

$$Q = \frac{2}{3} \cdot \mu \cdot \sqrt{2g} \cdot b \cdot h^{\frac{3}{2}}$$

which can be simplified to:

$$Q = \alpha \cdot b \cdot h^{\beta}$$

which serves as the basis for the weir discharge in DYNHYD. The coefficient α was set originally to 3.5 to represent small weirs in an irrigation network. α is expected to range between 1.6 and 2.0 for the weirs along the Saale. The exponent coefficient β is set to 1.5 and is not altered.

2.4.2 EUTRO

The water quality was simulated using the computer model EUTRO, which is a module of the WASP5 package. Water quality pertains to the oxygen balance in a river and can be simulated using six varying degrees of complexity. Only the first five were implemented and are summarized in Table 3. Petersen matrices and input data descriptions are given in the appendix. The complexities vary from simple Streeter-Phelps dissolved oxygen – biological oxygen demand description to more complex nutrient limited phytoplankton growth dynamics and are described as follows:

Table 3: The state variables and number of parameters for each model complexity in EUTRO. *(from Lindenschmidt, 2006)*

	Complexity					
	1	2	3	4 (P-limited)	4 (N-limited)	5
Variable name:						
Ammonium		*NBOD*	NH_4^+-*N*		NH_4^+-*N*	NH_4^+-*N*
Nitrate			NO_3^--*N*		NO_3^--*N*	NO_3^--*N*
Inorganic Phosphorus				*IP*		*IP*
Phytoplankton				*PHYT*	*PHYT*	*PHYT*
Biological Oxygen Demand	*TBOD*	*CBOD*	*CBOD*	*CBOD*	*CBOD*	*CBOD*
Dissolved Oxygen	*DO*	*DO*	*DO*	*DO*	*DO*	*DO*
Organic Nitrogen			*ON*		*ON*	*ON*
Organic Phosphorus				*OP*		*OP*
Number of parameters:						
Total	3	5	12	19	19	32
Used for calibration	1	2	6	12	12	21

Complexity 1: Streeter-Phelps with $TBOD_{max}$ and SOD

This is the simplest complexity and is based on the Streeter and Phelps (1925, cited in Chapra, 1997) approach in which the oxygen consumption is characterised in the water column using the total maximum biological oxygen demand ($TBOD_{max}$). A portion of the $TBOD_{max}$ is allowed to settle from the water column, which is particularly pronounced immediately downstream from sewage treatment plant outfalls (see Chapra, 1997, p.355f).

Oxygen is also consumed in the sediments, which is described in the model by the sediment oxygen demand (*SOD*). Sediment cores were taken at selected sites along the river and incubated at 20°C for 41 days. Lindenschmidt (2006) shows several oxygen consumption curves which range between 0.9 and 3.0 g/m²/day. A value of 1.0 g/m²/day for the entire stretch was determined in the calibration which conforms to values determined from other modelling studies of regulated rivers in Germany (Haag, 2003).

An important source of oxygen into the water body is reaeration via the water surface from the atmosphere. Here, three different equations, according to O'Connor-Dobbins, Owen-Gibbs and Churchill, are used depending on the depth and mean flow velocity of the water. Parameters include the total deoxygenation rate and the settling velocity of organic matter. The former is temperature dependent; hence temperature is an input function in the model.

Complexity 2: Modified Streeter-Phelps with $NBOD_{max}$

An important modification in this complexity is the separation of the $TBOD_{max}$ into its carbonaceous and nitrogenous components, $CBOD_{max}$ and $NBOD_{max}$, respectively. Both components have individual deoxygenation and settling rates. *SOD* remains the same but is supplemented with a temperature dependency. Karlsruhe bottle experiments with and without nitrification inhibitor allowed the differentiation of the two. Lindenschmidt (2006) gives an example of such an experiment in which $TBOD_{max}$ (without inhibitor) and $CBOD_{max}$ (with inhibitor) are determined. The difference between the two equals $NBOD_{max}$. The initial rates of increase gives an indication of the deoxygenation rates of each component. The parameter *k* and the BOD_{max} variables were fit using (Thomann and Mueller, 1987, p. 271f):

$$BOD = BOD_{\max}\left(1 - \exp(-k \cdot t)\right)$$

where *BOD* is the oxygen consumed at time *t*.

Complexity 3: Linear DO balance with nitrification

Complexity is increased at this level by separating the bulk variable $NBOD_{max}$ into its nitrogen components: total organic nitrogen (*ON*), ammonium (NH_4^+-*N*) and nitrate (NO_3^--*N*). The nitrogenous deoxygenation rate is also differentiated into the rates for mineralization ($ON \rightarrow NH_4^+$-*N*) and nitrification (NH_4^+-$N \rightarrow NO_3^-$-*N*). Settling of the nitrogenous matter is restricted to *ON*. Nitrite

concentrations are considered minute and are added to NO_3^--N. An additional oxygen source and sink are phytoplankton photosynthesis and respiration, respectively. Phytoplankton is, however, not a simulated variable in this complexity level but an input function in the model. At low oxygen concentrations, the denitrification process can be included in the simulation and both carbonaceous deoxygenation and nitrification are oxygen limited.

Complexity 4: Simple eutrophication

At this complexity, phytoplankton is a simulated variable which can be nutrient limited. Inorganic nitrogen (NH_4^+-N + NO_3^--N) and inorganic phosphorus (*IP*) are the limiting nutrients described using Monod kinetics. A preference factor for NH_4^+-N or NO_3^--N is utilized. Organic phosphorus (*OP*) is also included in the dynamics and undergoes mineralization and settling. Phytoplankton growth is also light limited and is adjusted with a temperature coefficient. Phytoplankton loss rate is governed by respiration, death, settling and zooplankton grazing.

Complexity 5: Intermediate eutrophication

DO and *BOD* dynamics of Complexity 1, phytoplankton photosynthesis and respiration from Complexity 3 and nutrient and light limited phytoplankton growth from Complexity 4 are combined in Complexity 5. Additional processes with corresponding parameters are required to couple the *DO*-*BOD* and phytoplankton-nutrient cycles. A Petersen matrix of the processes and their stoichiometric affects on the variables are given for each complexity in the appendix. A description of the variables, parameters and functions are included.

2.4.3 TOXI

The transport of salts, suspended solids and heavy metals was simulated using the computer model TOXI. The substances transported are any combination of three dissolved and three particulate substances. Most salts can be modeled as conservative substances hence, no reaction terms S_K are required. The transport of suspended solids *SS* requires additional sink and source terms to describe the movement of particles to and from the bottom sediments. Settling, deposition and resuspension rates are described by velocities and surface areas. The sedimentation rate v_{sed} is set within the range of Stoke's velocities corresponding to the suspended particle size distribution. This rate is multiplied by a probability of deposition to obtain the deposition rate. The probability of deposition depends upon the shear stress on the benthic surface and the suspended sediment size and cohesiveness. Likewise, the resuspension rate v_{res} depends upon the shear stress, the bed sediment size and cohesiveness and the state of consolidation of surficial benthic deposits (Ambrose, *et al*. 1993). Diffusion of dissolved substances from the bottom sediments into the water column is driven by the gradient of the substance

concentration in the sediments c_{sed} and the overlying water. The rate is controlled by the diffusion coefficient D_y.

Sorption processes must also be included in the reaction term when the transport of heavy metals is simulated. Sorption is the bonding of dissolved chemicals to the particulate solid material in suspension or in the sediments. The process is described using a partition coefficient K_D which represents the fraction of dissolved and particulate fractions of the heavy metals in relation to the concentration of suspended solids. Sorption is the most sensitive parameter (details upcoming in Section 6: "Results"), hence its complexity was varied as follows and summarised in Table 4:

Table 4: Sorption partitioning function of various complexity in TOXI.
(from Lindenschmidt, Wodrich and Hesse, 2006)

Complexity	Sorption process
1	conservative transport
2	$K_D = f(f_{OC})$
3	$K_D = f(C_{dis}, C_{part}, SS)$
4	$K_D = f(C_{dis}, C_{part}, SS, time)$

Complexity 1: Conservative transport (no sorption)
In the simplest complexity all substances, both particulate and dissolved fractions, are transported conservatively without any sorption reactions between the phases or with different substances.

Complexity 2: Dependency on organic carbon
The complexity of heavy metal transport is increased by considering the organic carbon content in the sorption kinetics. Many metals have an affinity to sorb either to the fraction of organic carbon f_{OC} of the particulate matter or to bind with the dissolved organic carbon *DOC* fraction to form colloids. *DOC* remained fairly constant in the flow direction whereas a large variability in f_{OC} was observed. Hence, the dependence of the partition coefficient K_D on f_{OC} was explored:

$$K_D = f_{OC} \cdot K_{OC}$$

where K_{OC} is a constant and represents the organic carbon partition coefficient and is calibrated for each heavy metal separately.

Complexity 3: Equilibrium sorption
In this complexity sorption reactions are fast relative to other reactive terms and are assumed to be in equilibrium in which the transfer rates of metals from the dissolved to the solid phase and vice versa

are equal. The partition coefficient K_D is a constant and relates the concentrations of the metal phases and the suspended solids as:

$$K_D = \frac{C_{part}}{C_{dis} \cdot SS}$$

where C_{dis} and C_{part} are the dissolved and particulate fractions of the heavy metal, respectively, and SS is the concentration of suspended solids.

Complexity 4: Dynamic sorption

In this complexity the partition coefficient K_D is allowed to increase or decrease in the flow direction at a particular rate. This spatial (and temporal) dependency of the phase partitioning is important when sorption does not occur quicker than other reaction processes. This is particularly the case when large loads of dissolved heavy metals are emitted into a river causing a large increase in the metal concentrations in the river. This is the case for the tributary Schlenze which drains large amounts of copper, lead and zinc from a large abandoned underground mine (details in Section 5: Model set-up).

2.5 Model Coupling with HLA (High Level Architecture)

The models of the WASP5 package were imbedded in a coupling system in order to improve interactive transfer of information between the models. The aim is to investigate how uncertainty of parameters and input data propagate through a chain of models and models that interact with one another as they simulate in parallel. More control of information transfer between time steps also allows improved analysis of model system dynamics. Lindenschmidt, Ollesch and Rode (2004) also show that coupling models allow variables to be exchanged so that a more even sensitivity of all the parameters can be sought.

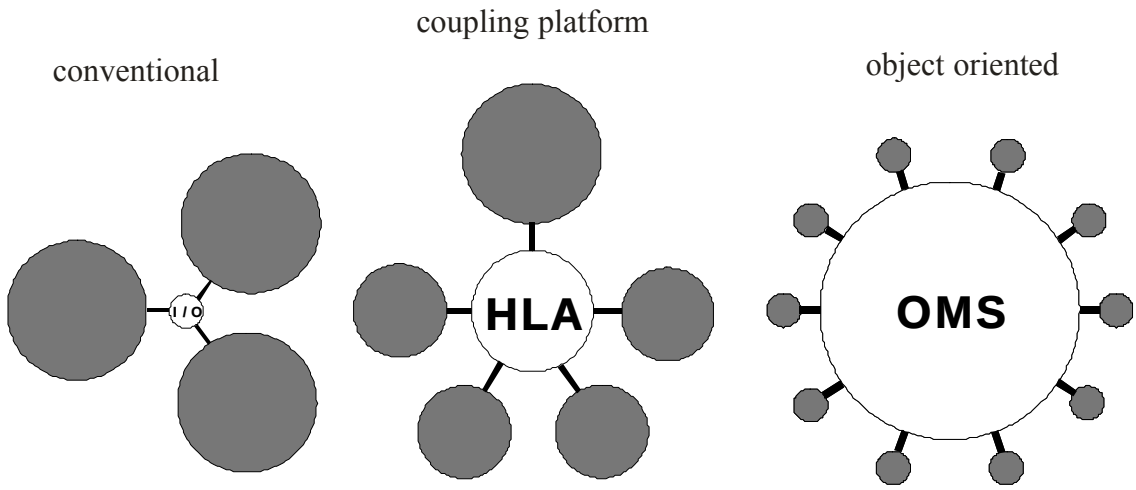


Figure 6: Model coupling approaches for model system development.

There are three basic approaches to model coupling (Lindenschmidt, Hesser and Rode, 2005) which are summarized in Figure 6:

conventional – models are loosely coupled, in that information is transferred from one model to another by file storage and retrieval. Additional programming in the model source codes is not necessary. Sequence control is managed by batch files or an external program. For an application example, see Lindenschmidt, Ollesch and Rode (2004).

coupling platform – an example of such a platform is HLA (High Level Architecture) in which entire models are easily and rapidly integrated into the simulation environment, but efficiency may be compromised since the execution of service and support routines that are similar in several coupled models need to be repeated. Programming in the source code is required to include HLA functionality, which eliminates the need for buffer storage of data for model interaction. For an application example, see Lindenschmidt, Rauberg and Hesser (2005).

object oriented – in the open source project OMS (Object Modeling System) (David, 1997; Hesser and Kralisch, 2003; http://oms.ars.usda.gov/) models are refracted to single processes and only called when required for simulating a particular modelling exercise. The processes act on single represented objects called entities. A central kernel controls iteration in time and space and the data exchange is realised by global variables without the aid of buffer storage files. The time required for integrating new components is low but is extensive for the development of the entire system. Flexibility in the configuration of the modelling exercise is high.

Table 5 give a summary of the attributes of each coupling approach. OMS advances the decomposition approach to integrated modeling system development in which only those modeling components from a model are adapted and integrated into the OMS environment which are needed for the specific problem and study site. This has the advantage of having low-level program descriptions of single processes that can user-interactively be included or excluded into the simulation, depending on the management scenario, scale or issue under investigation. Hence, it is a simple matter to test new process approaches and hypotheses. Another advantage is that repeatability of computer code of universally required processes is avoided. Examples are algorithms for evaporation which are a requirement for numerous models.

Table 5: Attributes of the various coupling approaches for model system development.

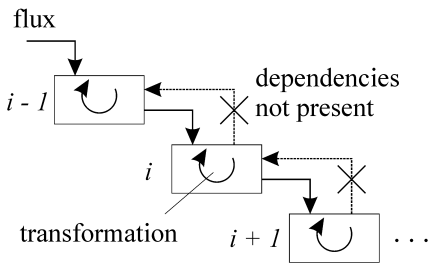
Attributes	**Coupling approach**		
	I/O	HLA	OMS
Coupling and interaction			
Component types	model	model	model & modules
Model codes	no restrictions	source code	source code
Flexibility (small granularity)	low	medium	high
Exchange opportunities	low	medium	high
Feedback mechanisms	no	yes	yes
Extension opportunities	low	medium	high
Performance and costs			
Distributed computing	no	yes	yes
Computing time	moderate	low	high
Platform development costs	low	none	very high
Implementation cost	high	moderate	very high

An important disadvantage to this approach is its (still) limited applicability to models requiring a "cascade" approach to its solution (see Figure 7(a)). This is distinctive in hydrological modeling and, to a large extent, substance transport modeling from land surfaces in which water and substances are transported downhill and the mass balance at any position is dependent on the transformations at that position and the flux uphill from that position (not the downhill flux). Each flux represents one equation with one unknown and the equations in the matrix can be solved successively in a feed forward manner. This situation is, however, different for river hydrodynamics and groundwater flow, in which the transport of water in a reach is dependent on the volume and velocity of water both upstream and downstream (in a global sense) from the reach. Here, a "control volume" approach is required (see Figure 7(b)) in which each discretized unit is dependent on both the upstream and downstream fluxes from all adjacent cells. Each corresponding equation has at least two unknowns, hence, the solution needs to be determined iteratively using a matrix solver. Decomposing such a model, which in principle would be required for the implementation in OMS, becomes difficult because the solver must consider the modeled system in its entirety. It should be noted that OMS will be equipped with the capability of "matrix" solvers but only in the long term.

a) Cascade approach (each equation is solved successively)

$$\begin{bmatrix} \cdot & \cdot & \cdot & 0 & 0 & 0 & 0 \\ \cdot & \cdot & 0 & 0 & 0 & 0 & 0 \\ \cdot & a_{i-1,i-2} & a_{i-1,i-1} & 0 & 0 & 0 & 0 \\ 0 & 0 & a_{i,i-1} & a_{i,i} & 0 & 0 & 0 \\ 0 & 0 & 0 & a_{i+1,i} & a_{i+1,i+1} & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & \cdot & \cdot & \cdot \end{bmatrix} \begin{Bmatrix} \cdot \\ \cdot \\ c_{i-1} \\ c_i \\ c_{i+1} \\ \cdot \\ \cdot \end{Bmatrix} = \begin{Bmatrix} \cdot \\ \cdot \\ W_{i-1} \\ W_i \\ W_{i+1} \\ \cdot \\ \cdot \end{Bmatrix}$$

response matrix *unknowns* *loads/ boundaries*



b) control volume approach (requires iterative solution)

$$\begin{bmatrix} \cdot & \cdot & \cdot & 0 & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & 0 & 0 & 0 & 0 \\ \cdot & a_{i-1,i-2} & a_{i-1,i-1} & a_{i-1,i} & 0 & 0 & 0 \\ 0 & 0 & a_{i,i-1} & a_{i,i} & a_{i,i+1} & 0 & 0 \\ 0 & 0 & 0 & a_{i+1,i} & a_{i+1,i+1} & a_{i+1,i+2} & \cdot \\ 0 & 0 & 0 & 0 & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & \cdot & \cdot & \cdot \end{bmatrix} \begin{Bmatrix} \cdot \\ \cdot \\ c_{i-1} \\ c_i \\ c_{i+1} \\ \cdot \\ \cdot \end{Bmatrix} = \begin{Bmatrix} \cdot \\ \cdot \\ W_{i-1} \\ W_i \\ W_{i+1} \\ \cdot \\ \cdot \end{Bmatrix}$$

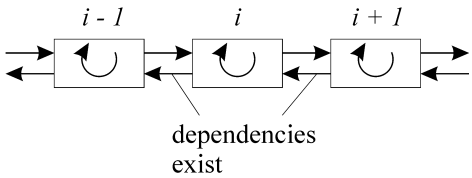
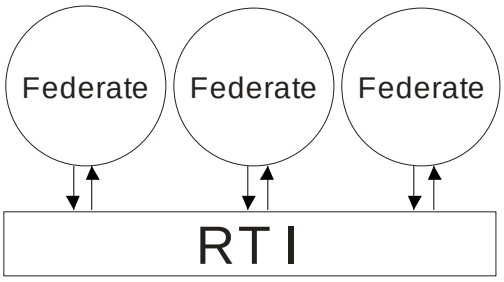


Figure 7: Numerical solution approaches for (a) hydrological models using cascades in sequence and (b) hydrodynamic models using interactive control volumes.

Decomposing models into single process components requires a high time expenditure in the development phase. The time saving comes later in the implementation phase when new processes can be added very simply to the overall system. The same is also true for the case when amalgamating many smaller models into one large model. However, for quick coupling and testing of existing models, decomposition or amalgamation is not very efficient, especially if models need to be added or exchanged rapidly in river basin management systems. Hence, a platform is also required which can quickly interconnect existing models into one conglomerate system. HLA is such a platform and was chosen for the coupling of the WASP5 modules.

HLA (High Level Architecture) is computer architecture for constructing distributed simulations. It facilitates interoperability among different simulations and simulation types and promotes reuse of simulation software modules (Kuhl *et al.*, 1999). HLA can support virtual, constructive, and live simulations from a variety of application domains. The core of the HLA is the RTI (Run-Time Infrastructure) which implements a set of services that precisely specifies the interoperability-related actions that a simulation may perform, or be asked to perform, during a simulation execution. The RTI starts and stops a simulation execution, transfers data between interoperating simulations, controls the amount and routing of data that is passed, and co-ordinates the passage of simulated time among the

simulations. Within the HLA, a set of collaborating simulations is called a federation, each of the collaborating simulations is a federate, and a simulation run is called a federation execution. Figure 8 provides a conceptual view of a HLA federation. Federates that adhere to the rules can exchange data defined using an object model template; those services are provided at run-time by the RTI (Petty, 2002). HLA has been implemented for a broad spectrum of applications. For example, developing multi-agent systems for applications in mobile robotics (Das and Reyes, 2002), providing online/real-time location information of streetcars for the public transportation company in Magdeburg, Germany (Klein, 2000) and designing simulation environments for human training (esp. military personnel) (Maamar, 2003). The author is not aware of any HLA applications in the field of water resources management.



(adapted from Petty, 2002)
Figure 8: The High Level Architecture (HLA) environment.

Figure 9 and Figure 10 show the sequence reconfiguration of the WASP5 simulations in HLA. The hydrodynamic output data from DYNHYD is not stored in a file but is transferred immediately after each time step for consecutive simulations of the same time step in EUTRO and TOXI. The process is repeated for the next time step until t_n is completed. Since the WASP5 modeling system is written in FORTRAN and the HLA is written in C++, a wrapper for each model DYNHYD, EUTRO and TOXI needed to be implemented in order for the RTI functions to be transmitted between the models and the RTI. The wrapper is a dynamic link library (DLL) written in the C++ programming language and contains the calls for the RTI functions. The WASP5 models, which are written in the FORTRAN programming language, can read the compiled versions of these calls found in the DLL. The models can now communicate with one another via the RTI.

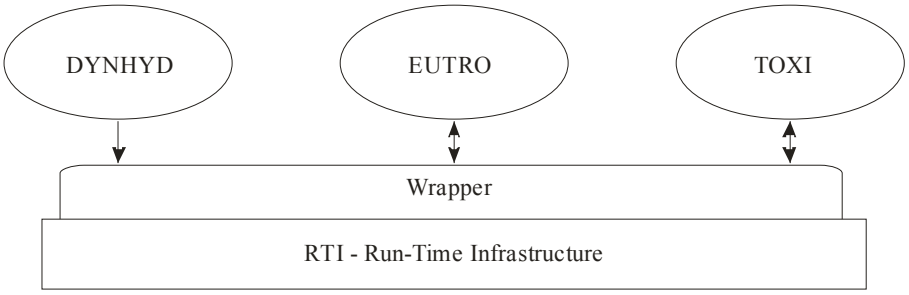


Figure 9: The models from the WASP5 package embedded in HLA.

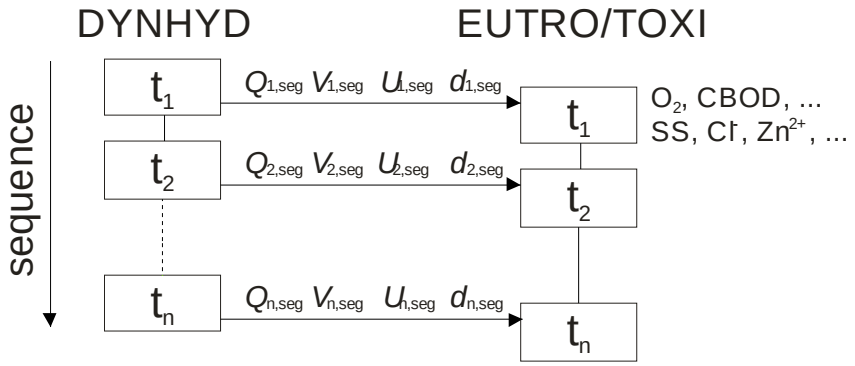


Figure 10: DYNHYD simulation time-steps synchronised with those from EUTRO and TOXI.
(adapted from Lindenschmidt, Hesser and Rode, 2005 and Lindenschmidt, Rauberg and Hesser, 2005)

Figure 11 shows how the MOCA is implemented in WASP5 using the HLA environment. Shown exemplary is the variation in a parameters set *a* and error deviation set ε. *N* sets of these parameters are comprised by randomly selecting values from the distribution. The sequence is then repeated *N* times using the corresponding parameter sets. The repeated DYNHYD simulation induces a variability in the output values *V, U* and *d* which are transferred to EUTRO and TOXI. This variability is propagated through the EUTRO and TOXI simulations and their outputs (e.g. oxygen in EUTRO and suspended solids in TOXI) will also comply with a particular probability distribution. This MOCA analysis was repeated to include the variation in the hydrodynamic boundary conditions, which are the flow discharges of the tributaries and the inflow and outflow of a river.

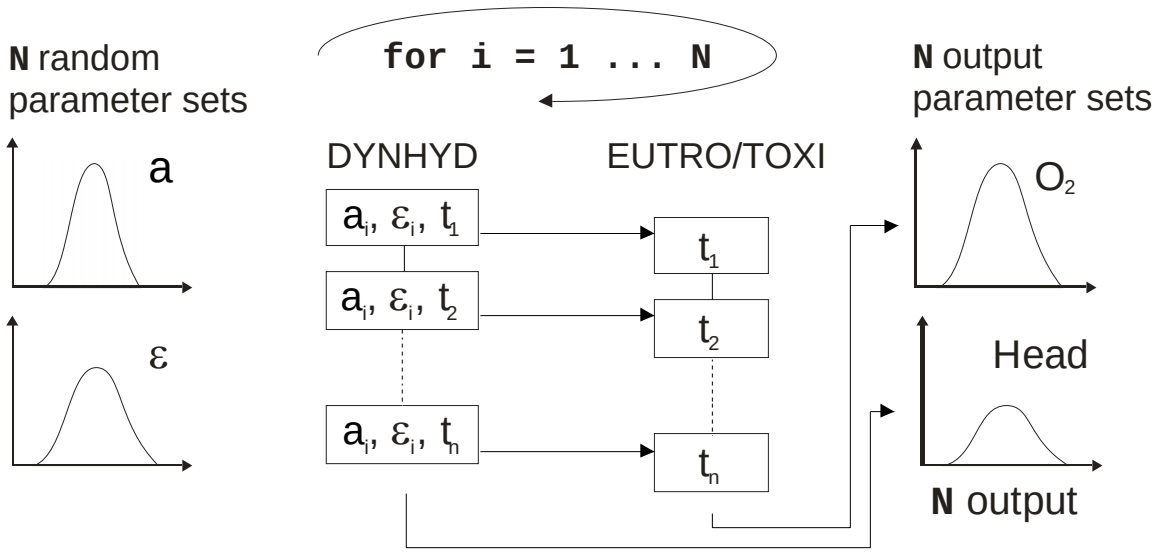


Figure 11: Monte-Carlo Analysis of the WASP5 federation.
(adapted from Lindenschmidt, Hesser and Rode, 2005)

3 Additional methods for uncertainty analysis

In this study the Monte Carlo Analysis was used to investigate the uncertainties in the utilized models. This method is based on the implementation of many thousands of simulations with parameters and input data chosen randomly from a given probability distribution. Other methods were also explored such as Predictive Analysis by Doherty (2001) and Doherty and Johnston (2003) (implemented in Lindenschmidt, von Saleski, *et al*., 2005; von Saleski, *et al*., 2004) and *GLUE* (Generalized Likelihood Uncertainty Analysis) by Beven and Binley (2001) (implemented in Lindenschmidt, Poser and Rode, 2005; Rode, *et al*., 2004). Additional methods were required to compliment the analyses, which are described below.

3.1 Local sensitivity

The sensitivity s of the input parameter values P on model output values O was calculated using:

$$s = \frac{\partial O}{\partial P} \cdot \frac{P}{O}$$

First, a base run is simulated with the parameter setting P_{base} to give O_{base}. A parameter is then increased or decreased by a certain fraction x designated as P_x which gives the resulting O_x. The sensitivity then becomes:

$$s \approx \frac{\Delta O}{\Delta P} \cdot \frac{P}{O} = \frac{\left(O_x - O_{base}\right)}{\left(P_x - P_{base}\right)} \cdot \frac{P_{base}}{O_{base}}$$

Since $P_x = \left(1 + x\right) \cdot P_{base}$ the equation reduces to:

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

x was typically set to 0.1 (= 10% difference).

3.2 Global sensitivity

The sensitivity analysis according to Reichert and Vanrolleghem (2001) was implemented. In this technique a sensitivity measure is given for each parameter used in the model but the measure indicates how sensitive each parameter is on the system globally, i.e. how small changes in the parameter affects all the state variables. First, a sensitivity function must be defined:

$$\mathrm{s}_{\mathrm{i,j}} = \frac{\Delta\theta_{\mathrm{j}}}{\mathrm{sc}_{\mathrm{i}}} \cdot \frac{\partial \mathrm{y}_{\mathrm{i}}}{\partial \theta_{\mathrm{j}}}$$

where θ is the parameter value with its corresponding number *j* and Δθ is its range of uncertainty. *y* is the value of an output variable with its corresponding number *i* and ∂y is the change in the output variable due to the change in the parameter setting ∂θ. *sc* is a characteristic scaling factor to make the order of magnitude between the different model outputs numerically comparable with one another. The sensitivity of each parameter δ is:

$$\delta_j = \sqrt{\frac{1}{N_i}\sum_{i=1}^{N_i} s_{i,j}^2}$$

where N_i is the total number of output variable values. The total sensitivity of the model of a certain complexity δ_{total} was taken as the sum of the sensitivities of all parameters N_j normalised to the maximum value of all parameter values:

$$\delta_{total} = \frac{1}{\max(\delta_j)}\sum_{j=1}^{N_j}\delta_j$$

3.3 Error

The error ε between model results and sampled data was calculated using:

$$\varepsilon = 1 - e^{(-\sigma)}$$

which is an adaptation of a likelihood function from Beven (2001, p. 249). σ is a normalised error variance between the measurements x_m and simulated x_s values normalised to the average of the measured values $\overline{x}_m$:

$$\sigma = \frac{1}{\overline{x}_m}\sqrt{\sum\left(x_m - x_s\right)^2}$$

Taking the exponent of σ allows the error to lie in the range between 1 (perfect fit) and 0 (no fit).

3.4 Model utility

Both the sensitivity and the error values can be used to evaluate the "best" model for a particular application, in terms of an index of utility U_m for model *m* (Snowling and Kramer, 2001):

$$U_m = 1 - \sqrt{\frac{w_S \cdot \hat{s}_{total,m}^2 + w_E \cdot \hat{\varepsilon}_{total,m}^2}{w_S + w_E}}$$

where $\hat{s}_{total,m}$ and $\hat{\varepsilon}_{total,m}$ are the sensitivity and error of each model normalized to 1. w_S and w_E are weighting factors for sensitivity and error and both equal 1 for no preference. Increasing one factor emphasises that particular characteristic. The aim is to maximise U_m by decreasing both sensitivity and error.

4 The Saale River

4.1 Overview

The Saale River is the second largest tributary, in regards to length and discharge, of the Elbe river (Reimann and Seiert, 2001). Its source lies in the Fichtelgebirge near the German-Czech border and it flows 413 km northward to its confluence into the Elbe. Its catchment area is approximately 23 770 km^2 with land use that is predominantly agriculturally based (68.3%) and 23% of the land is forested. The river was chosen as a test case because of its particular challenge for river basin management due to the numerous problems and conflicts regarding the basin's water resources (Rode, 2001). The river itself is still heavily loaded with nutrients of which the largest fraction is from non-point sources (Behrendt, *et al*., 2001). The river is also heavily modified with a series of five reservoirs (of which one is the largest in Germany by volume) in the upper course and numerous weirs along its entire extent. In the lower reach, locks have been constructed to make the river navigable. All these regulatory measures have a large impact on the water quality and hydrological regime of the river. The effects of these measures on the riverine biocenosis are numerous and can be divided into the areas of water quality, flow regime, structural diversity, sediment regime, water network and ground water regime (Rode, *et al*. 2002). Although the river is heavily modified it still has numerous sections that are near-natural or semi-natural and have a large potential for natural recovery. The Saale basin has also been subject to rapid economic and social change since German reunification and therefore, makes special demands on the forecast of future usage claims and their effect on the waters in regards to quantity and quality. In this study only the lower and middle courses of the Saale are examined, between Saaleck and the confluence (see Figure 12).

4.2 Hydrological characteristics

There are eleven main tributaries flowing into this portion of the Saale - Unstrut, Wethau, Rippach, Luppe, Laucha, Weiße Elster,Salza, Schlenze, Wipper, Fuhne and Bode. The hydrological characteristics of each and selected points along the Saale are given in Table 6. There are 19 weir systems, one each at Saaleck, Bad Kösen, Öblitz, Bad Dürrenberg, Rischmühle, Meuschau, Planena, Wettin, Rothenburg, Alsleben, Bernburg and Calbe, three in Weißenfels (Beuditz, Brückenmühle and Herrenmühle) and four in Halle (Böllberg, Halle-Stadt, Gimritz and Trotha). Figure 13 shows the water levels at mean discharge along the regulated course of the national waterway. The most downstream reach between Calbe and the confluence is still too steep to allow year-round passage of ships weighing 1000 tonnes or more. Hence, the construction of an additional lock-and-weir system (labelled “Schleuse”) or a diversion channel has been proposed.

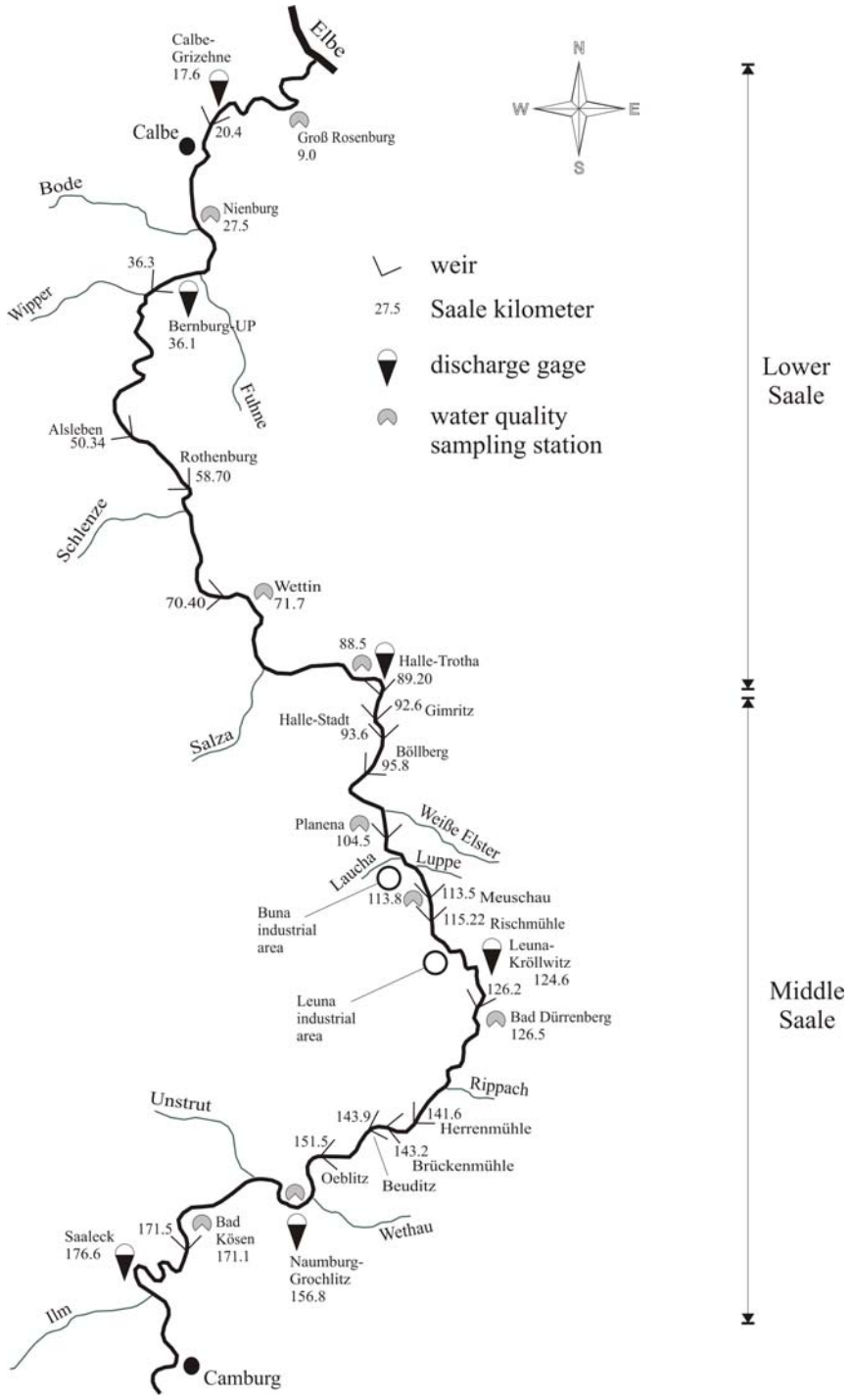


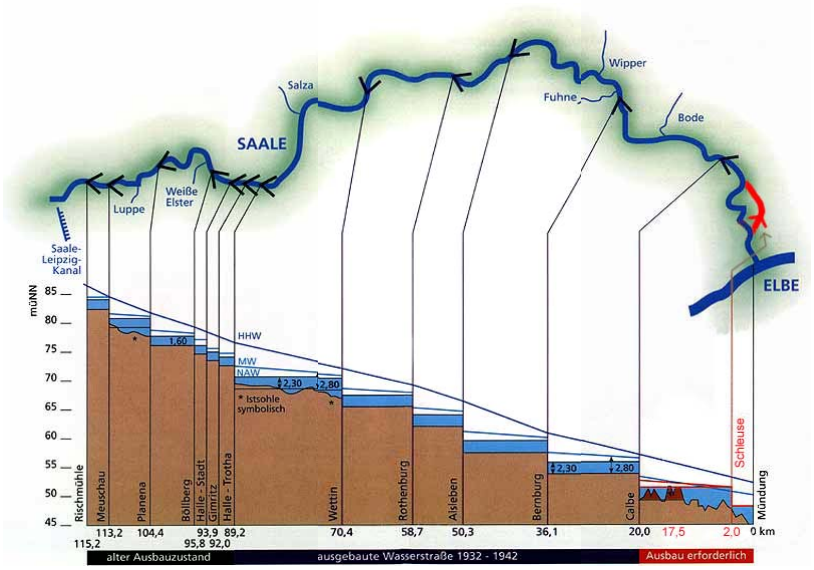
Figure 12: The middle and lower courses of the Saale River.

Due to its leeside position to the Harz Mountains (west of the study area), the lower Saale basin is relatively dry (average yearly precipitation ≈ 490 mm) causing relatively low flows in the summer months. This hinders ship navigation and water abstraction for industry and agriculture. Water regulation through weirs and reservoirs does not always cover the water deficit in summer and measures are planned and being taken to flood abandoned open-pit mines for use as a water supply supplement (Reimann and Seiert, 2001). There is a seasonality within the yearly course of the discharge cycle, shown in Figure 14 plotted using long-term monthly averages of the discharges.

Snowmelt in the Harz and Erz Mountains cause the high discharges in March and April. The discharges steadily decrease to its lowest values in August and September.

Table 6: Discharge characteristics at discharge gages along the Saale and its tributaries (italic).

				Discharge (m^3/sec)				
Gage	River	Saale km	Series	NQ (Date)	MNQ	MQ	MHQ	HQ (Date)
Saaleck	Saale	176.6	1965 - 1998	7.6 (25.08.93)	15.6	41.5	176	558 (14.04.94)
Naumburg-Grochlitz	Saale	156.8	1934 - 2001	8.6 (15.07.34)	26	67.6	245	695 (15.04.94)
Laucha	*Unstrut*	*161.8*	1946 - 2001	4.6 (29.06.60)	10.7	30.5	104	360 (12.02.46)
Mertensdorf	*Wethau*	*155.5*	1963 - 2000	0.15 (17.09.64)	0.39	1.06	9.76	30.6 (13.04.94)
Rippach	*Rippach*	*136.7*	1993 - 1998	0.06 (06.08.94)	0.09	0.28	2.82	4.38 (15.04.94)
Leuna-Kröllwitz	Saale	124.6	1995 - 1998	18 (16.08.98)	24.5	71.5	270	377 (02.02.95)
Schkopau	*Laucha*	*108.9*	1998 - 1998	0.082 (09.11.97)	0.082	0.191	0.653	0.653 (08.07.98)
Oberthau	*Weiße Elster*	*102.7*	1973 -2000	7.52 (04.01.93)	10.4	25.3	121	226 (29.04.80)
Trotha	Saale	89.2	1955 - 2000	21	39.4	99.2	352	796
Zappendorf	*Salza*	*79.2*	1982 - 1998	0.21 (11.07.88)	0.34	1	3.75	7.56 (28.02.87)
Friedeburg	*Schlenze*	*62.9*	1967 - 1998	0.01 (14.07.94)	0.07	0.18	4.81	20.3 (07.05.69)
Groß Schierstedt	*Wipper*	*37.7*	1961/2000	0.36 (04.09.64)	0.67	2.45	16.4	92 (14.04.94)
Bernburg	Saale	36.1	1957 - 2000	23	41.8	101	313	671
Baalberge	*Fuhne*	*33.7*	1970 - 1999	0.03 (31.07.76)	0.36	1.13	3.67	6.93 (15.04.94)
Hadmersleben	*Bode*	*27.6*	1931 - 2000	0.6 (02.10.49)	3.96	14.3	56.6	124 (16.04.94)
Calbe-Grizehne	Saale	17.6	1932 - 2002	11.5	44	115	374	716



(source: www.wsa-magdeburg.de)

Figure 13: The regulated national waterway along the Saale River

The discharge regulation of the reservoirs in the upper course of the Saale has a marked impact on the discharge of the lower course. One application during the GDR regime was to dilute high salt concentrated water in the lower course of the Saale with less polluted water from the reservoirs. The Unstrut tributary is a heavy loader of salts into the Saale River which accentuated during low-flow conditions so that the water could not be used for industrial purposes. Flushing water from the reservoirs through the Saale diluted the salt concentrations to values acceptable for industrial abstraction.

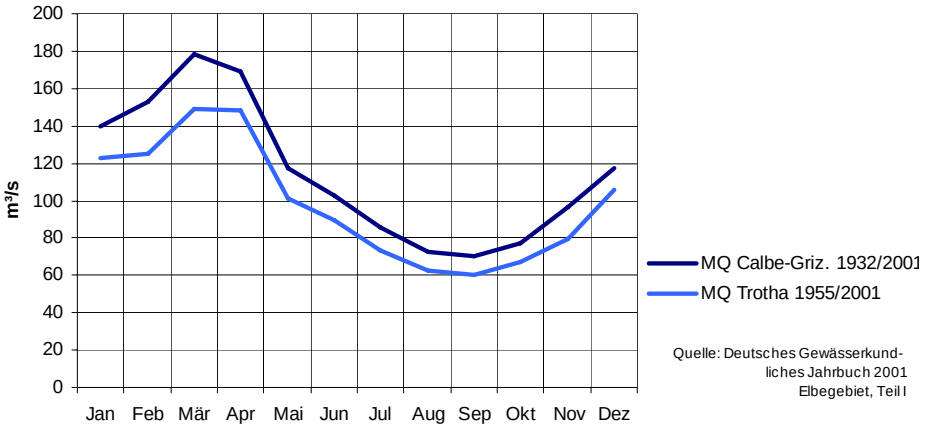


Figure 14: Long-term monthly means of discharge (MQ) at Halle-Trotha und Calbe-Grizehne.

4.3 Nutrients, dissolved oxygen and chlorophyll-a

The Saale was at the time of German reunification a very eutrophied water body. In the years 1989 and 1990 the water quality of 10% of the water course was classified as III-IV (very heavily polluted); 40% was classified as III (heavily polluted), 30% as II-III (critically polluted) and 20% as II (moderately polluted) (Theile, 2001). This was attributed to the emissions from industrial and

communal wastewater treatment plants which operated very poorly with outdated equipment and to the high input of fertilizers in agriculture. Due to the closure of industrial plants, upgrading of wastewater treatment facilities and reduction in fertilizer applications the Saale's water quality has progressively improved so that currently, 50% of the Saale's river course is classified as II-III (critically polluted) and 50% as II (moderately polluted) (Theile, 2001).

Figure 15 shows the annual mean concentrations of total phosphorus and ammonium. Since German reunification the phosphorus concentrations have halved. The ammonium concentrations have also reduced markedly. Nitrate also follows this same pattern (data not shown). In the short-term there is still potential for considerable reductions in ammonium loadings; however in the long-term total nitrogen concentration are not expected to decrease significantly (Theile, 2001). There is still an increasing trend in the nutrient concentrations in the flow direction. This trend is attributed more to emissions in the middle Saale (between Bad Kösen and Halle) and less so within the lower course of the river (between Halle and Groß Rosenburg).

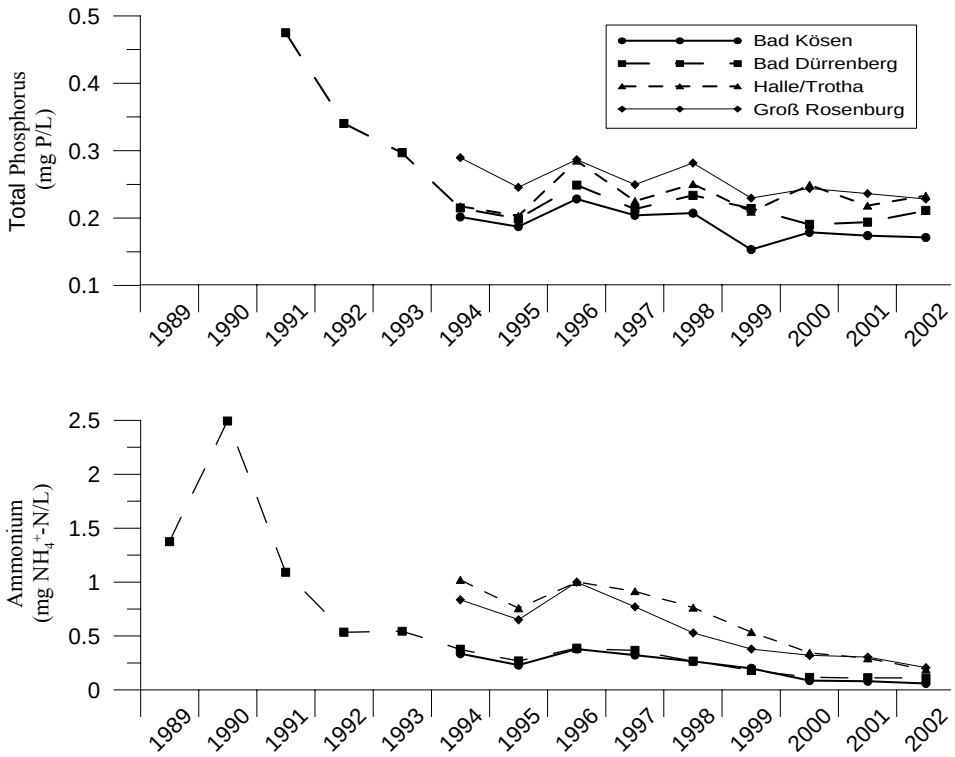


Figure 15: Development of total phosphorus and ammonium since German reunification at selected locations along the Saale River.

Figure 16 shows the annual mean concentrations of dissolved oxygen and chlorophyll-a. Within the past ten years dissolved oxygen has been on an increasing trend at Bad Kösen whereas the values from Groß Rosenburg have remained fairly steady. There is a large variability of dissolved oxygen at the stations in between (Bad Dürrenberg and Halle/Trotha). Chlorophyll-a concentrations have been

variable at Bad Kösen during the last decade whereas all other stations report a decreasing trend of this pigment. These results confirm the improved water quality situation in the Saale. In addition, for the last reported years, 2001 and 2002, both the oxygen and chlorophyll-a contents in the water have remained relatively steady along the course of the river. This may indicate that the production and consumption processes of oxygen have come to a steady state condition.

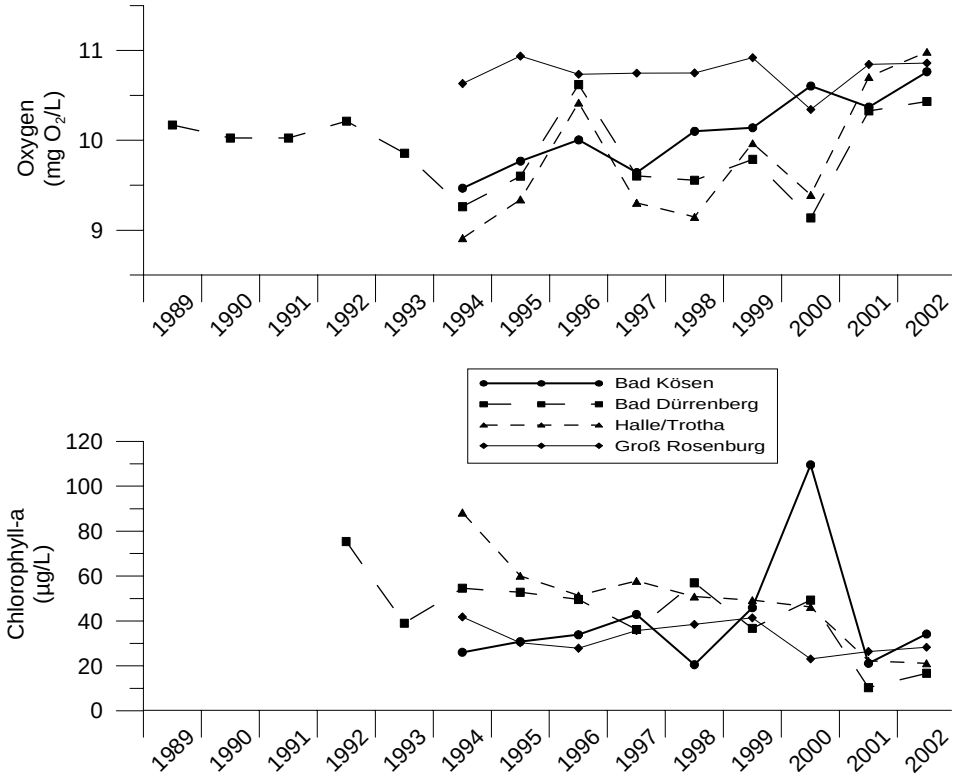


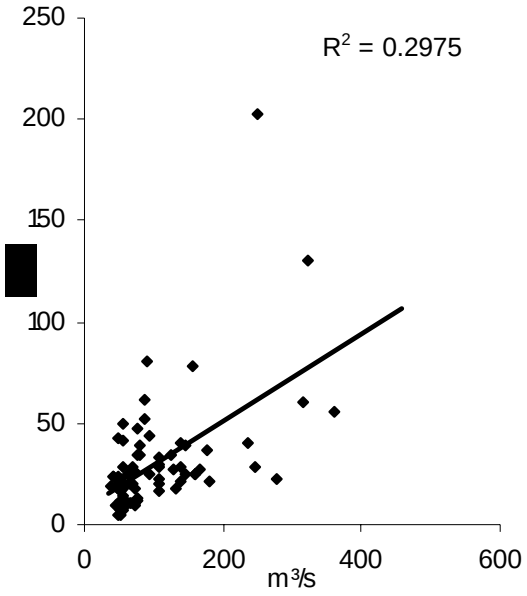
Figure 16: Development of dissolved oxygen and chlorophyll-a since German reunification at selected locations along the Saale River.

4.4 Sediments and micro-pollutants

Of all its tributaries, the Saale has the largest impact on the sediment regime of the Elbe river (Vetter, 2003). Figure 17 shows the correlation between discharge and suspended sediment concentrations, which is poor. Generally, high discharges lead to higher sediment loading but there are numerous exceptions. This is due to the many factors influencing sediment transport such as the seasonal cycle of phytoplankton growth, erosion in the catchment and sedimentation and flushing of sediment in the backwaters of the lock-and-weir systems.

Figure 18 gives a comparison of the chloride concentrations at the confluences of selected large rivers of Germany, of which the Saale River has the highest concentrations. Although the geogenic source of the Saale's salt loading is higher than in other river basins, the majority of the loading stems from anthropogenic sources. These include tailings from current and abandoned potash and salt mines, soda ash production, salt refineries and copper mining activities. Since German reunification salt emissions

have steadily reduced. The anthropogenic : geogenic ratio of chloride is currently 1:4 at Leuna but has been as high as 1:1 for the Unstrut during the GDR regime (Theile, 1996).



(source: Hesse, 2004)

Figure 17: Correlation between discharge at Calbe-Grizehne (m^3/sec) and suspended sediment concentrations (mg/L) at Groß Rosenburg using bi-weekly samples from 1999 to 2001.

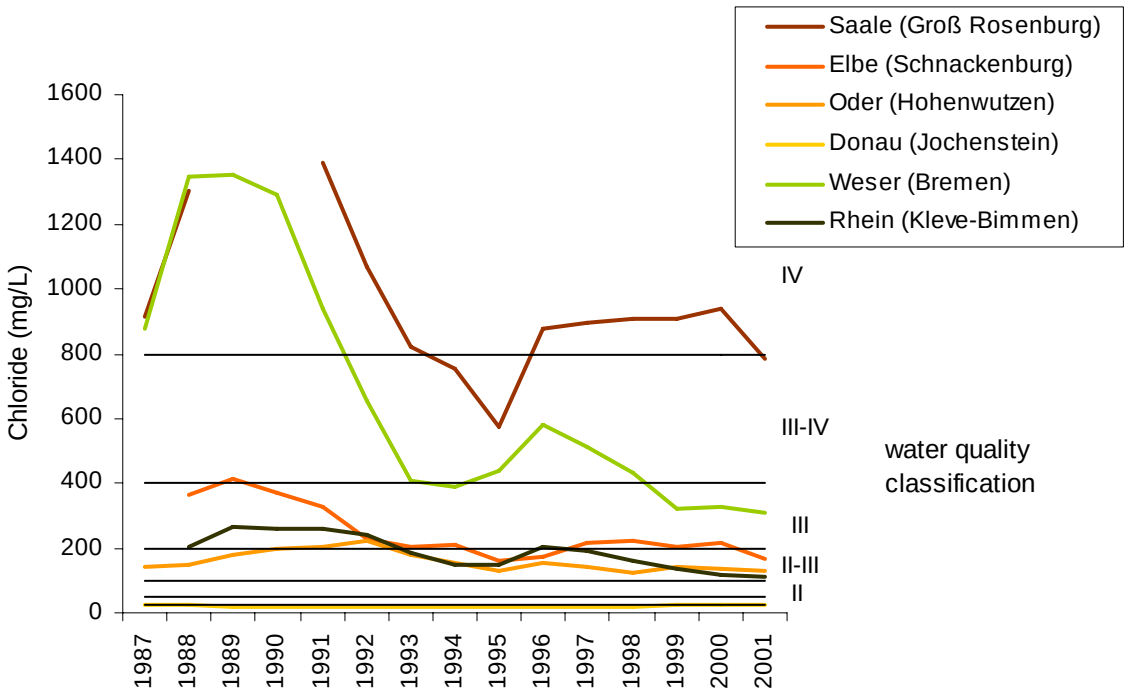
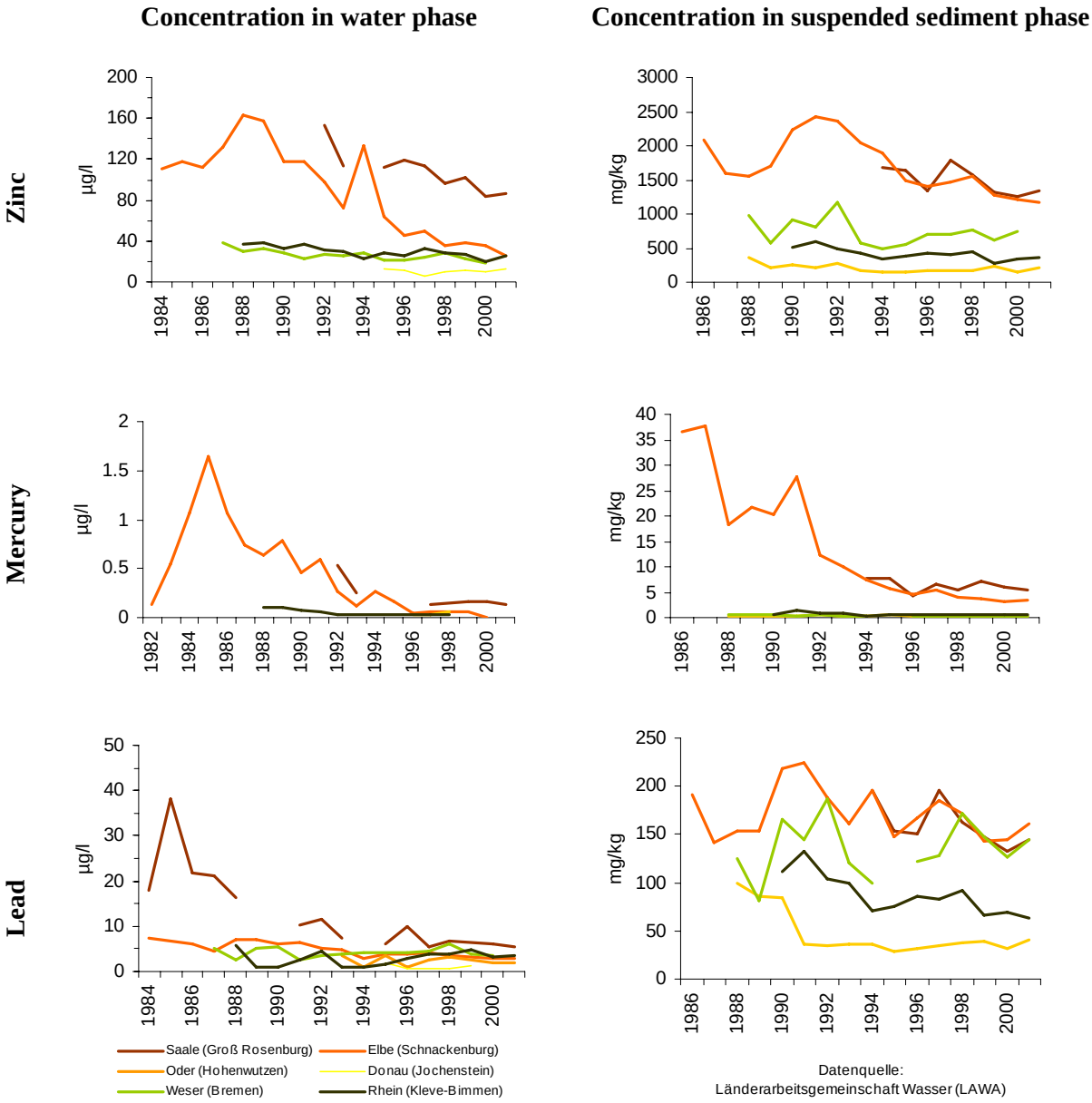


Figure 18: Comparison of chloride concentrations of large rivers in Germany.

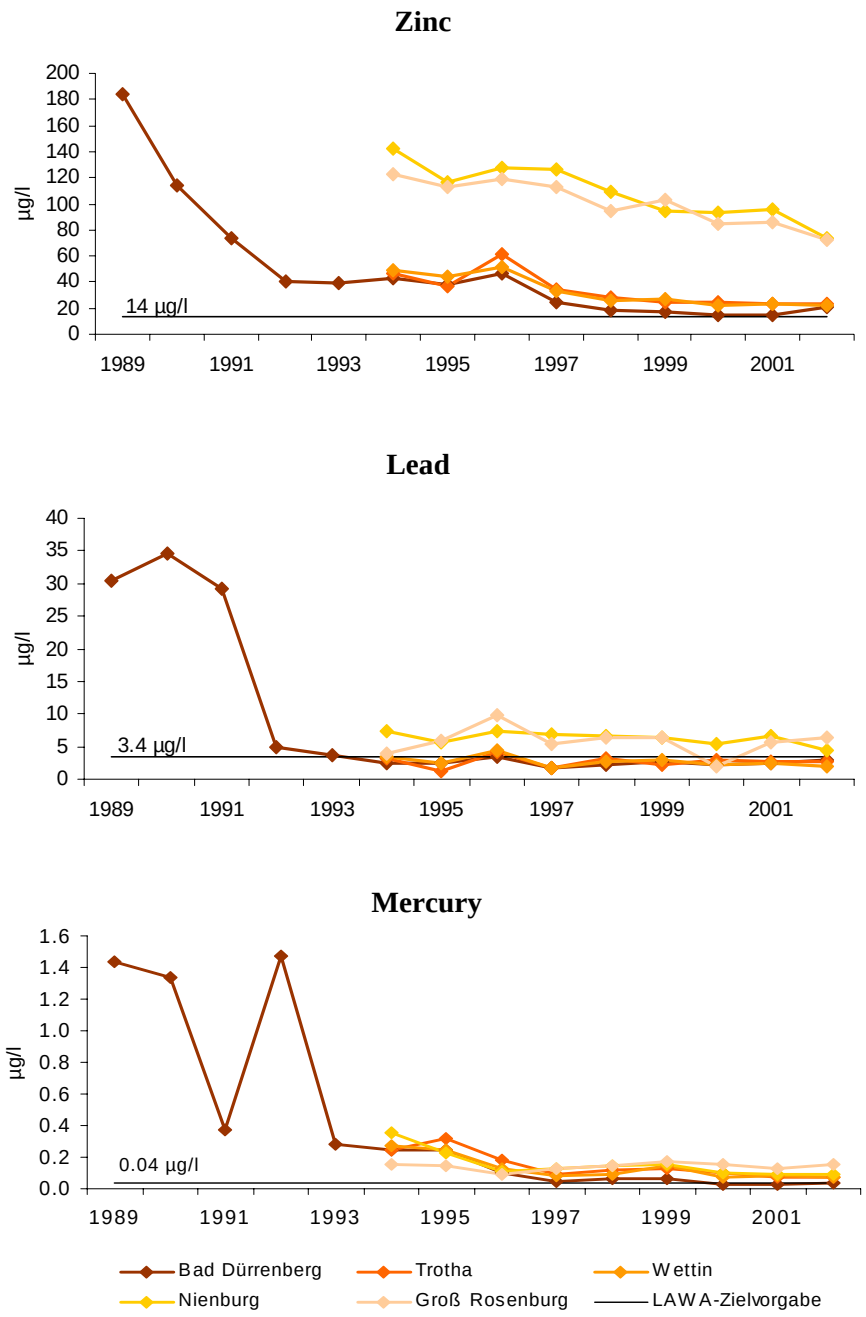
The concentrations of heavy metals in both the water and suspended sediment phases are higher in the Saale compared to other large rivers in Germany (see Figure 19). Especially lead, mercury and zinc

concentrations are high and are seldom exceeded by those in the Elbe. The geogenic loading, too, is relatively high but anthropogenic sources outweigh natural occurrence (Zerling, *et al*., 2003). Human-made sources include chemical industry, metal processing plants and mining. Communal wastewater treatment plants and storm runoff in urban areas are also potential sources of some metals (Winde and Frühauf, 2001). As indicated in Figure 20 reduction in heavy metal concentrations in the Saale occurred after German reunification due to the closing of many industries. Values are still higher than the recommended guidelines provided by the Federal States' Consortium for Water (LAWA, 1998). Both lead and zinc increase significantly at the two most downstream sampling stations, Nienbug and Groß Rosenburg, due to loadings from abandoned mine shafts via the Schlenze and Wipper tributaries.



(adapted from Hesse, 2004; data from LAWA under http://www.umweltbundesamt.de/hid/)

Figure 19: Heavy metal pollution in selected large rivers in Germany (annual means).



(adapted from Hesse, 2004; data from LAU Sachsen-Anhalt)

Figure 20: Annual mean concentrations of lead, mercury and zinc in Saale River water at selected sampling stations.

4.5 Limnological investigations between 1960 and 1991

In the early 1960s Meissner (1965) examined the changing relations between oxygen, nitrogen und carbon compounds in the Saale River. Dissolved oxygen concentrations were not disclosed; however mention is made of the evidently high denitrification activity occurring in the river course between Merseburg and Wettin. von Tümpling (1967) and von Tümpling and Ventz (1967) carried out many statistical investigations about the influence of the oxygen content in water (given as oxygen saturation index) on the saprobity of three river systems. Only the Elbe is explicitly mentioned but I suspect that

the Saale is one of the rivers investigated. They found strong negative correlations between oxygen content and saprobity which could be expressed quantitatively using linear statistical equation. von Tümpling (1974) also saw the importance of classifying rivers in categories of trophic status and lists typical physical, chemical and biological characteristics of oligotrophic, eutrophic, polytrophic and hypertrophic rivers in eastern German. Modelling exercises of the oxygen budget and the biological structure of nutrient-laden water bodies were also carried out (see for example Uhlmann, *et al*., 1978). This includes research in modelling the oxygen and phytoplankton dynamics in rivers (Gnauck, *et al*., 1987; Gnauck and Schramm, 1991) and reservoirs (Gnauck, 1975).

Heavy metal pollution was also a focus of research conducted on the Saale. A survey of precious metals in the Saale River and its basin is provided by Fischer (1966). Georgotas and Udluft (1973) show that during high-flow conditions the heavy metal content in the headwaters of the Saale increases, except for lead and chromium. They state that the lead loading stems primarily from groundwater in this area since its concentrations decrease along the river during floods. Heide, *et al*. (1978) refer to the high concentrations of lead and mercury in the river. A synopsis of tin in the river is given by Heide and Reichardt (1975). Geiss and Einax (1991) characterised loads along selected stretches of the Saale using factor analysis to evaluate sources of contamination. They concluded that the copper, chromium and zinc stem primarily from industry sources and the high cadmium load was emitted by wastewater treatment plants.

Sampling campaigns of the biological structure of the Saale were also carried out. Braune (1975) gives a detailed description of the dynamics of the algae populations in the Saale in the vicinity of the city of Jena between September 1963 and September 1965 and documented the change in microphyte community structure due to the waste loading of the city. For the Saale course between the multireservoir system and the Ilm confluence Ronneberger (1976) investigated the plankton, seston and phytoplankton oxygen production along the Saale in 1971 and 1972. He found that discharge conditions and loading of organic material were the main factors that controlled the oxygen production by phytoplankton. The influence from solar radiation played a secondary role in algae oxygen input. Parallel to this survey Schönborn (1976) measured biological oxygen demands after 5 days ($BOD_5 < 6$ mg O_2/L) and oxygen consumption rates and concludes that the increased waste loading into the Saale inhibited the self-purification capacity of the river. Schönborn (1976) and Schönborn and Proft (1976) additionally studied the periphyton and concluded that the periphyton only contributed 7% to the BOD_5.

The increasing demand by society and industry for potable water could not be covered solely by groundwater and bank infiltrated water (Giessler, 1957). Surface water from the Saale River needed to be extracted to cover the demand. The water treatment plant in Halle-Beesen provided the facilities to

purify the water. Attention to the treatment processes are given in the literature due to the high pollution load in the Saale (Meissner, *et al*., 1967).

4.6 Weirs (941 – present)

The first weir was constructed on the Saale near Alsleben in A.D. 941 for the operation of a water mill (Schubert, 2001). Water mills were used extensively for the production of flour and lumber. Thereafter weirs were also installed to regulate water discharge to secure a sufficient water supply for lumber rafting during times of low flow and to provide local flood protection at times of high flow.

Ship navigation also gained importance on the Saale. The first locks (earliest record from 1366 (Schubert, 2001)) were simple sluiceways, which are channel constrictions formed in the river when a weir does not fully extend across the width of the river. The stowing of the water by the weir and the channelling of the flow by the constriction provides a continuous and gradual water level change allowing a safe throughway for ships.

The first channel lock was constructed in Halle in 1694 and by 1822 17 lock-and-weir systems were installed on the lower Saale reach between the Unstrut confluence and the Saale mouth, making this total length of 157 km passable for ships. To ensure year-round navigation of shipping, one last lock-and-weir system needs to be constructed on the 20 km stretch between Calbe and the confluence. Since this may upset the naturally fluctuating groundwater levels in the floodplains in this area and adjacent floodplains along the Elbe river, which is designated as a biosphere reserve, the construction of a diversion channel from Calbe extending on the left side of the Saale River to the Elbe river has been proposed. The upper Saale was equipped only with weirs for the operation of mills (until the 19th century) and the production of electricity (19th and 20th centuries), but not for shipping.

Discharge regulation using locks and weirs have had detrimental effects on the aquatic ecosystem of the Saale:

- the continuum of the river passage is interrupted making migration of fish difficult
- the reduced current velocities have increased sedimentation on the river bed forming anoxic zones in the areas of stowed water
- the deepening of the water depths above the stowed areas have led to increased temperatures downstream from the control structures

4.7 Saale cascade: multireservoir system (1925 – present)

In the upper course of the Saale River a multireservoir system was constructed between 1925 and 1945 called the Saale cascade. The system consists of five reservoirs in series and extends over a 70km stretch between Blankenstein and Eichicht (see Figure 21). A longitudinal cross-section of the system

is given in Figure 22. The Bleiloch reservoir is the largest reservoir by volume in Germany with a storage capacity of 215 million m^3. Hohenwarte reservoir ranks third in Germany with a storage capacity of 182 million m^3.

There are several reasons why the multireservoir system was constructed. One was to ensure better flood protection after a catastrophic flood in November, 1890, which caused excessive damages between the upper Saale and Halle. The generation of hydroelectric power and a source of cooling and processing water were also important incentives during an era of rapidly growing industrialisation. An ample water supply also needed to be secured for water provision during dry spells and to allow year round rafting of timber, which continued on the Saale until the mid 1930s. The buffered water can also be released to supplement discharge in the Elbe river during low-flow conditions and allow year-round ship navigation on the Elbe. Later, important functions of the reservoirs included dilution of salt pollution in the lower Saale course and tourism. Much of this discourse has been drawn from Schubert (2002) and the reader is referred to that source for further details.

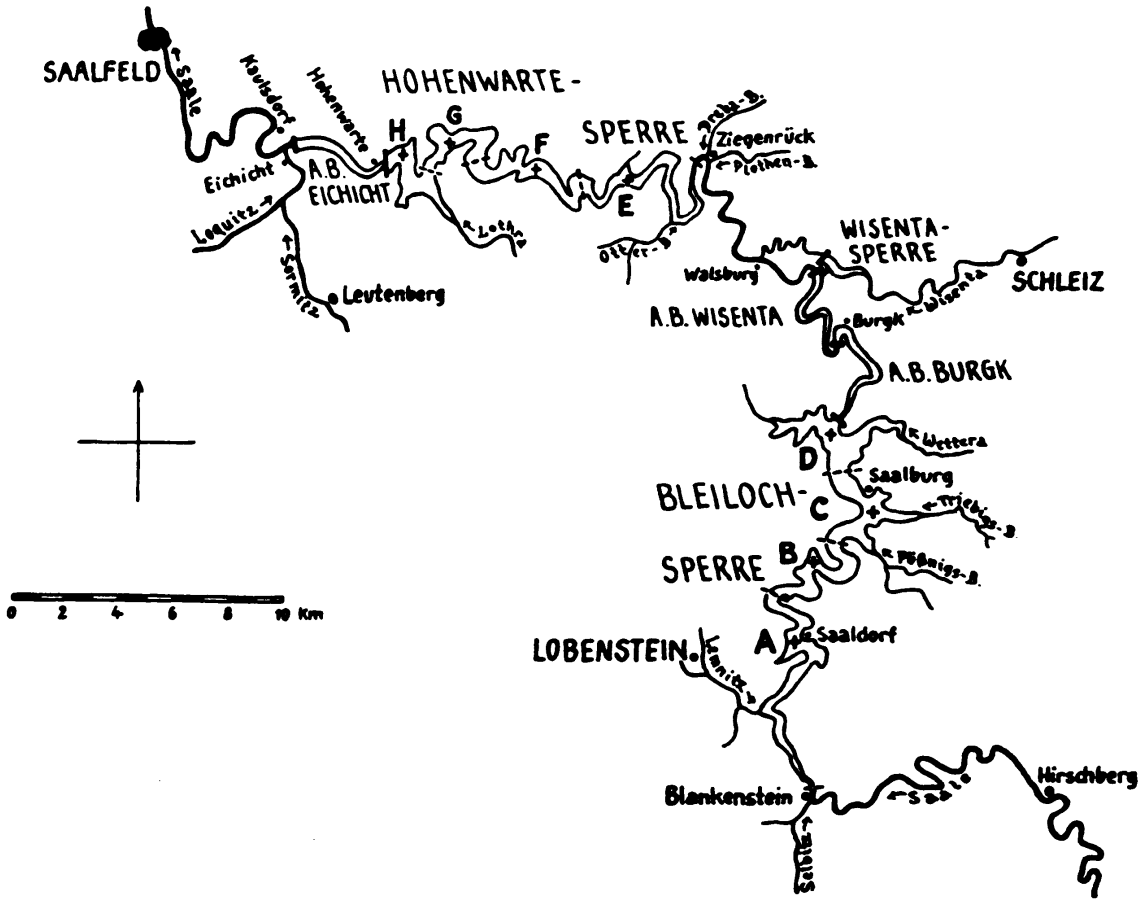


Figure 21: The multireservoir system in the upper Saale River called Saale cascade.
(from Schräder, 1958, cited in Schuber, 2001)

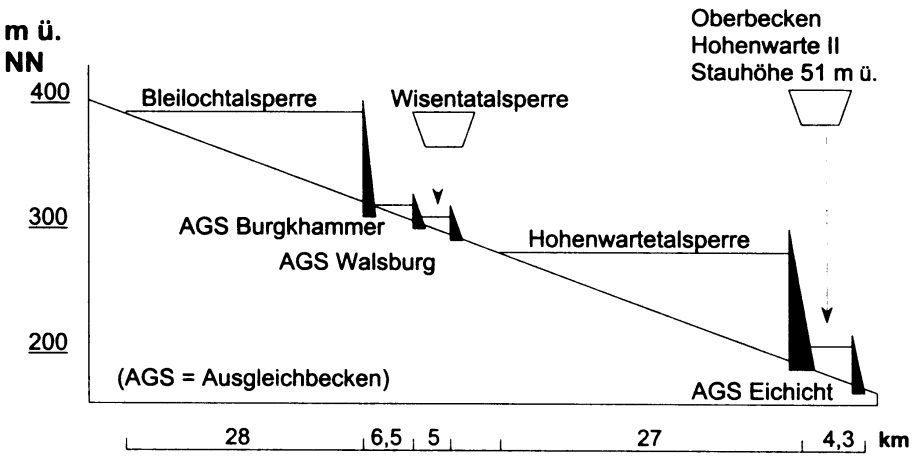


Figure 22: Longitudinal cross-section of the Saale cascade.
(adapted from Schuber, 2001)

4.8 Salt-load control system (1963 – 1994)

Potash mining has been carried out in the northern portion of the Unstrut subbasin (southern area of the Harz mountains) for almost a century. Only 20% of the raw material mined could be produced to fertilizer; the remaining 80% was waste material and heaped on large mounds (Schürer and Kulbe, 1997). These mounds consist of up to 90% salts (NaCl, $MgCl_2$ and $MgSO_4$) which easily dissolve and enter via surface runoff into receiving water bodies. This leads to exorbitant high concentrations of chloride and high values of hardness in the rivers preventing a species-rich flora and fauna to develop (Ziemann, 1967). This reduced the ecological and economical value of the river water and caused a general threat to the water supply for human use and consumption (Aurada, 1997).

A key user of the Saale water was the industrial complex between Leuna and Buna (see Figure 12). As its capacity and production increased, so did its demands on the river water to the point that at low flow conditions, this demand could not be fulfilled. In addition, the chloride concentrations and water hardness were so high, especially at low-flow conditions (concentrations are inversely proportional to discharge) that the water could not be utilised for production processes. Hence in 1963, a salt-load control system was developed in which salt loading from the mining areas and the discharge from the Saale reservoirs were regulated to ensure the chloride concentrations and water hardness at the Leuna gage never exceeded 470 mg/L and 40°dH, respectively. A schematic of the approach is given in Figure 23 (Theile, 1977). Water leached from the waste mounds are retained in storage basins and emitted into the Wipper und Unstrut during normal or higher discharge conditions. During low flows, the high salt content in the Saale was diluted by releasing water from the reservoirs.

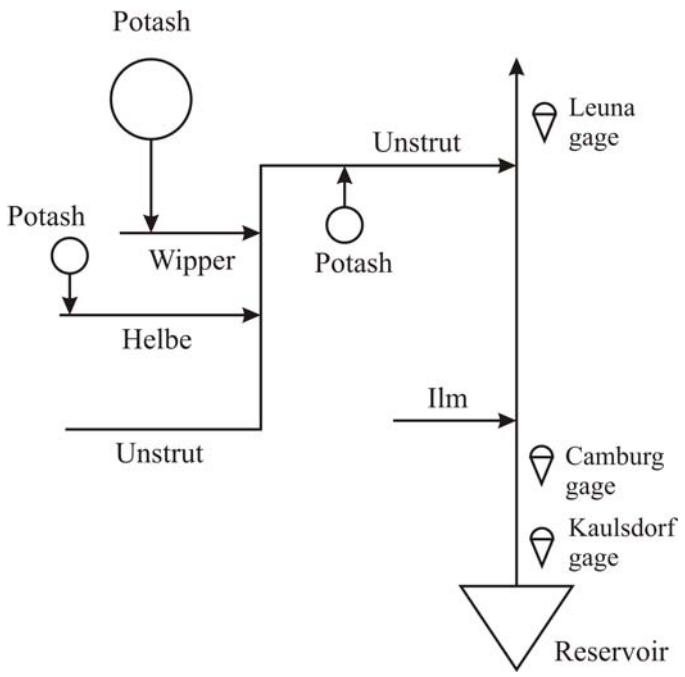


Figure 23: Schematic of the salt-load control system of the Saale River
(modified from Theile, 1977)

Since the distance between the Leuna gage and the upstream reservoirs is approximately 150 km, a forecast of discharge and water quality at least three days in advance needed to be made (Becker, *et al*., 1977). A forecast modelling system was developed which incorporated the following submodels:

- catchment model for precipitation-runoff simulations
- hydraulic model for discharge predictions
- substance transport model
- regression model

Between 1990 and 1994, all potash mines in this area were shut down which significantly reduced salt loadings into the river system and the salt-load control system was ceased.

4.9 Why the Saale River as pilot study?

There is a deficiency of knowledge pertaining to the Saale River. This is especially true for studies involving the Saale on the large scale. This deficiency is amplified due to the drastic change in the ecosystem of the Saale River since German reunification. The abrupt closure of most industries and the steady improvement in the treatment of wastewater has caused major effects in the ecological status and functioning of the river. An in-depth understanding of these changes is still required. The emissions of point sources have been drastically reduced since German reunification. However, the nutrient content in the river water is still very high (Behrendt, *et al*., 2001), particularly due to non-point inputs. Hence, an important question addressed in this study is: What impact would a reduction of non-point nutrient pollution (tributaries) have on the water quality? (see Section 6.13).

Presently, potash, salt, uranium, copper and lignite are the most important materials mined in the Saale River basin. There are also still many residual contaminated sites from past mining activities which act as perpetual sources of pollution for the river. These include tailings which are an important source of salts (e.g. near Bernburg) and heavy metals and abandoned mining shafts which still flush large amounts of the same substances into the surface waters (e.g. Schlüsselstollen in Mansfelderland (Schreck, 1998; Schreck, *et al*., 2005)). This study answers the question: What impact do these contaminants have on the water quality and how can their effect be reduced? (see Sections 6.1and 6.2).

The Saale is a unique river since it is dam regulated, has a high salt concentration, has a high nutrient content and has many contaminated sites. There is still a lack of understanding of the key ecological processes of the Saale, which is imperative to know before a successful management of the river, and its basin can be carried out. The questions to be addressed are: What are the key ecological processes in the Saale River and which are most sensitive for management measures? (see Section 5.6).

The Saale is also heavily modified. There are many lock-and-weir systems which can have an impact on the ecological functioning of the river:

- Dam regulation causes reduction of current velocities due to the increase in water levels and regulation of discharge. This may affect the ecosystem in several ways such as increase residence times favouring phytoplankton activity and increase tendency for deposition of suspended matter. The river is also less aerated due to reduced stream velocities. All these factors will increase the sediment oxygen demand. Question: What impact does regulation have on the water and ecosystem quality of the river? (see Section 6.12).
- Weirs also affect substance retention properties in the river. This issue is addressed in Section 6.2.
- Many morphological changes through dam regulation and straightening of the water course. Question: To what degree do morphological changes impact ecological status? (see Sections 6.7 and 6.11).
- Large-scale projects are planned to extend the Saale's capacity for shipping. Proposals include construction of an additional weir at Klein Rosenburg and construction of a lock-canal to divert shipping from the lower Saale reach between Calbe and confluence. Question: What impact do these projects have on the water quality of the Saale River? (see Section 6.12).

5 Model set-up

5.1 Sampling campaigns

For the calibration and validation of the models three data sets were available which were sampled along the Saale and its tributaries by UFZ - Centre for Environmental Research, Magdeburg, Germany (Baborowski *et al*., in preparation). The sampling periods are: i) 5. – 18. June 2001, ii) 19. – 21. June 2002 and iii) 8. – 10. September 2003 (see Table 7). The tributaries Luppe, Laucha, Weiße Elster, Salza, Schlenze, Wipper, Fuhne and Bode were sampled at their confluences. The sampling stations for the first sampling period include Halle-Trotha, Wettin, Bernburg, Calbe and Groß Rosenburg. Nienburg was included as a station in the second sampling campaign. The sampling resolution was increased to five additional stations for the third sampling campaign with the addition of Bad Dürrenberg, Meuschau, Planena, Halle (four additional stations), Brachwitz, Döblitz, Könnern, Alsleben, Gröna and the Saale confluence. An Eulerian sampling strategy was carried out for the first campaign in which each station was sampled once daily or every second day over the two week period. A Lagrangian approach was taken for the campaigns in 2002 and 2003 in which the sampled water parcel at the most upstream station was tracked and sampled along the course of the river.

Table 7: Sampling campaigns used for the calibration and validation of the models.

	# days	**Sampling strategy**	**Modelling procedure**		
			Middle Saale	Lower Saale	Calbe
High-frequency short-term					
5. - 18. June 2001	14	Eulerian	---	calibration	calibration
19. - 21. June 2002	3	Lagrangian	---	validation	validation
7. - 10. Sept. 2003	4	Lagrangian	calibration	validation	---
Low-frequency long-term					
7. June - 3. Aug. 1999	58	Eulerian	validation	---	---
19. June - 15. Aug. 2001	58	Eulerian	---	validation	validation
14. May – 30. July 2002	78	Eulerian	---	validation	validation

A 24-hour diel study at the Calbe lock-and-weir complemented the first two sampling campaigns on 10. – 11. June 2001 and 23. – 24. June 2002. Only the most upstream and downstream stations were sampled. Trends of the data at the other stations, lock entrance, upper weir, ferry and diversion, were interpolated from a weekly sampling program of all stations during the first half of 2002 (Eckert, 2002).

The substances sampled were:

- carbon (particulate and dissolved organic fractions)
- heavy metals (particulate and dissolved fractions of arsen, copper, chromium, iron, lead, manganese, nickel and zinc).
- nitrogen (total and dissolved bound fractions; particulate and organic fractions; inorganic components – ammonium, nitrite and nitrate)
- oxygen demand (total, carbonaceous and nitrogenous biological oxygen demand; total and dissolved fractions of chemical oxygen demand)
- phosphorus (total, particulate, dissolved and reactive fractions)
- phytoplankton (chlorophyll-a)
- salts (calcium, chloride, magnesium, potassium, sodium and sulfate)
- silicon (total and dissolved fractions)
- suspended solids, both organic and inorganic fractions (as dry weight and loss on ignition)

Oxygen, water temperature, pH, conductance and Secchi depths were also measured on site. For a detailed description of the analytical methods used, see Eckert (2002). Additional long-term validation periods were simulated using data from LAU – Saxony-Anhalt Bureau for Environmental Protection (Approval # LAU/3.3/01/2004) and BfG – Federal Bureau of Hydrology, Koblenz, Germany (unpublished data kindly provided by A. Schoel and V. Kirchesch).

5.2 Discretization

The investigated course of the Saale was discretized using 360 segments, each approximately 500 m in length. Cross-sectional profiles every 100 m along the river were available from which initial hydraulic radii and segment water volumes (calculated from mean water levels) of each segment were determined. Simulation results are output on a daily time step. The Calbe lock-and-weir system was discretized using 63 segments each approximately 100 m in length (see Figure 24). A detailed description of the river morphology was derived from sonar graphs kindly provided by the WSA – Water and Shipping Authority, ABZ Bernburg, Germany. Each segment is divided into a water column and a sediment compartment.

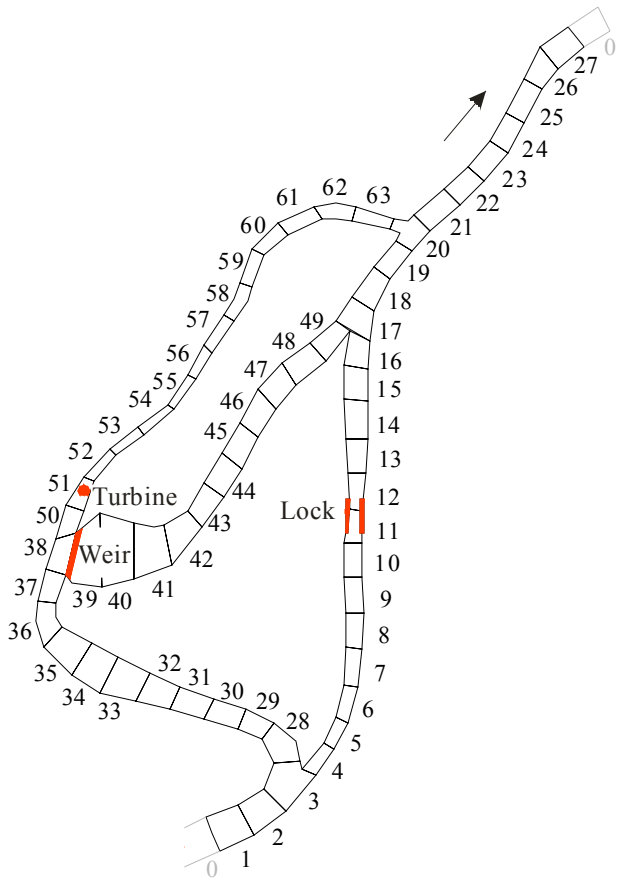


Figure 24: Segment numbering of the model discretization of the Calbe lock-and-weir system.
(adapted from Lindenschmidt, Eckhardt, et al., 2004)

5.3 Flows and exchanges

The mean discharge of this river course varies from 41.5 m^3/s at Saaleck to 99 m^3/s at Trotha and 115 m^3/s at Calbe and is regulated by lock-and-weir systems (see Figure 12) at Saaleck, Bad Kösen, Öblitz, three in Weißenfels (Beuditz, Brückenmühle and Herrenmühle), Bad Dürrenberg, Rischmühle, Meuschau, Planena, four in Halle (Böllberg, Halle-Stadt, Gimritz, Trotha), Wettin, Rothenburg, Alsleben, Bernburg and Calbe. Eleven tributaries, Unstrut, Wethau, Rippach, Luppe, Laucha, Weiße Elster, Salza, Schlenze, Wipper, Fuhne and Bode, drain into the middle and lower Saale of which the Unstrut, Weiße Elster and Bode are the most significant in regards to water volume (see Table 6 and Figure 25 for discharges). No additional inflows into the Saale occur in Calbe. In a previous study flows were simulated dynamically for the Saale (von Saleski, *et al.*, 2004) and the Calbe lock-and-weir system (Lindenschmidt, Eckhardt, *et al.*, 2004; Wodrich, Lindenschmidt, *et al.*, 2005) using DYNHYD.

Dispersion of substances is modelled as an exchange between adjacent water column compartments. Diffusion of dissolved substances occurs between each water column compartment and their underlying sediment compartments.

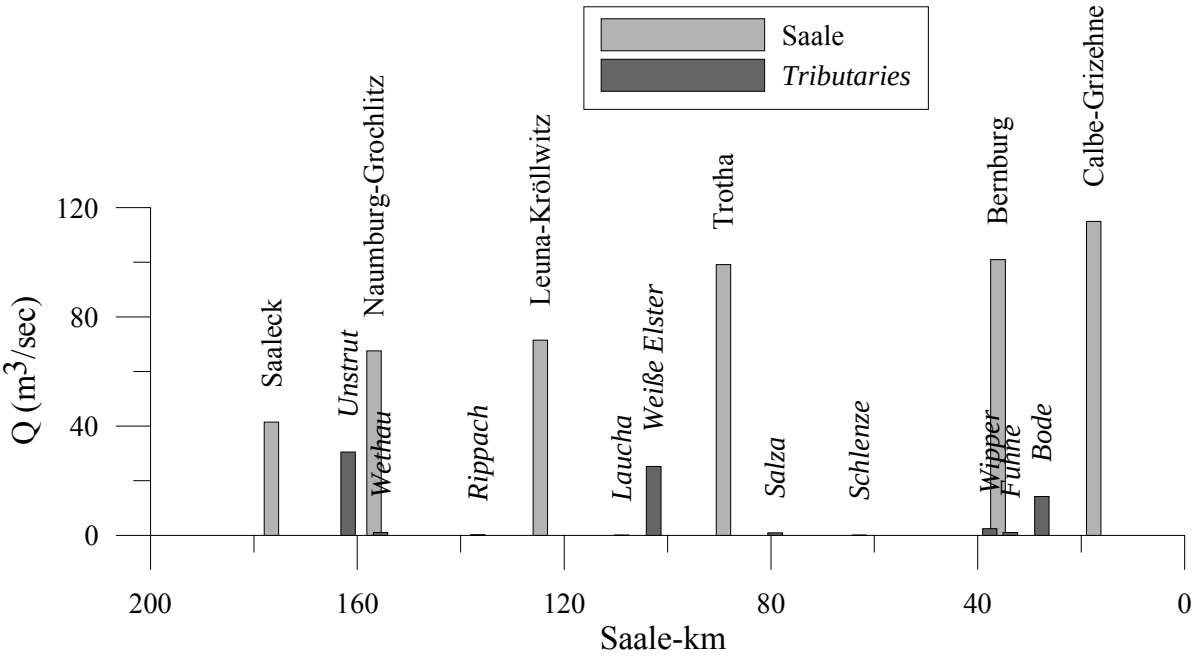


Figure 25: Mean discharges at selected stations along the Saale and its tributaries.

5.4 Loads

Many wastes from industrial plants and WWTPs (wastewater treatment plants) are loaded into the Saale. Only the data from 1997 to 1999 were available (IKSE, 2000, 2001), which were extrapolated for the simulated time periods in 2001 and 2002. Loads for all state variables are included shown exemplary in Figure 26 for total phosphorus and ammonium. The WWTPs have all been extended with facilities for secondary and tertiary treatment, reflected in the decreasing trend in nitrogen loading. The high loads from Bernburg industry are primarily from a soda production plant.

The most important industrial emitters of substances are at Leuna and Bernburg. The soda production plant at Bernburg in which soda ash (Na_2CO_3) is produced using salt (NaCl and $CaCO_3$) causes a large emission of chloride, calcium and sodium into the Saale. Data on the emissions were not available but could be derived from general emission values published by the German Environmental Agency (UBA, 2004) and from data produced by the Staßfurt soda plant located upon the Bode river (Sodawerk, 2002).

5.5 Boundary conditions

Boundaries, which include the eleven tributaries and the most upstream segment, are input as concentrations to the simulated system for all state variables. The yearly mean total phosphorus and ammonium concentrations for the years 1994 to 2002 are shown in Figure 27 for the most important tributaries, Unstrut, Weiße Elster and Bode. Since 2000 the nutrient concentrations in the Weiße Elster have progressively dropped to value comparable to those of the other two main tributaries. The water

quality of this river is significantly improving which is also evident in the increase in the oxygen concentrations (O_2 < 6.5 mg/L in 2000 to O_2 > 9 mg/L in 2002). Lindenschmidt (2006) shows that the loadings from these tributaries are in the same order of magnitude as the industrial and communal point loadings. Substances may have higher concentrations in the other tributaries, as is the case for ammonium (see Figure 28) but because of their significantly lower discharges, their loadings are relatively small.

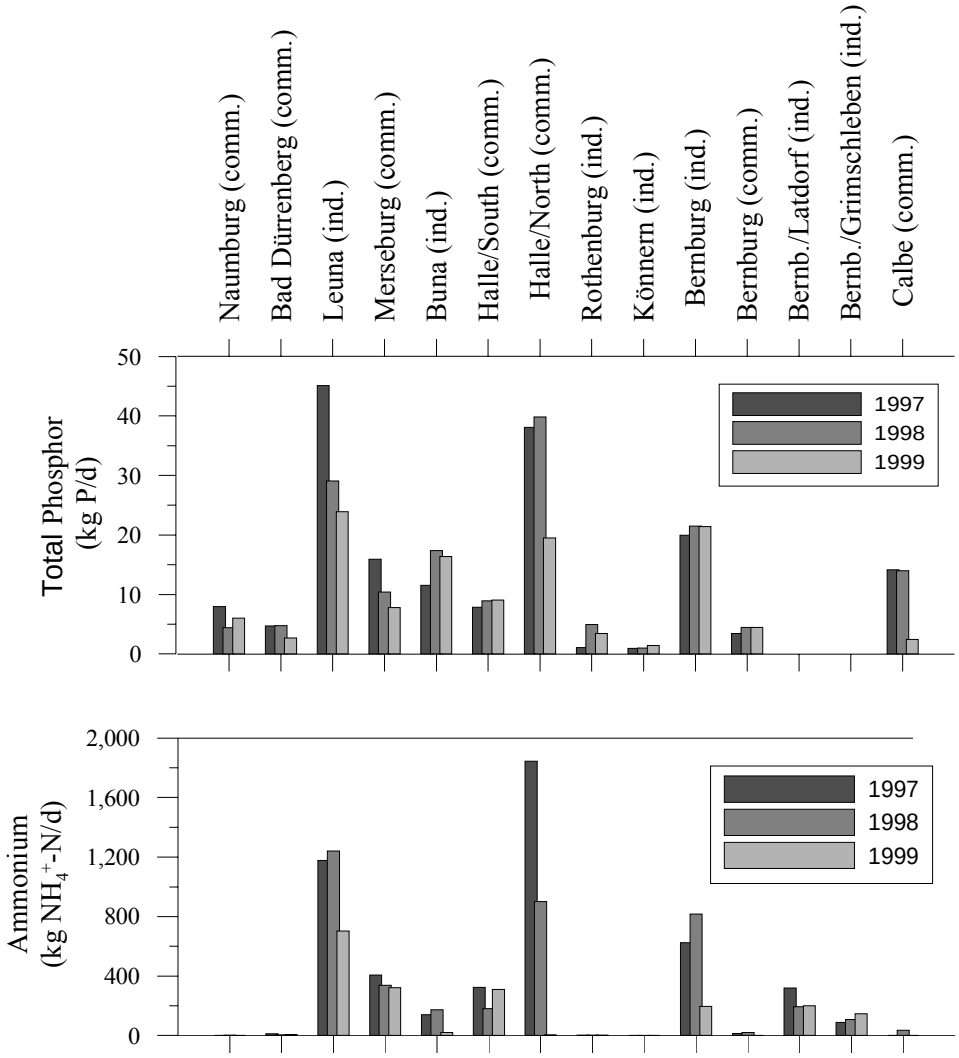


Figure 26: Point loadings along the middle and lower Saale courses for 1997, 1998 and 1999.

The main tributaries that emit heavy metals are Weiße Elster (iron, manganese, nickel), Wipper (cadmium) and Schlenze (arsenic, copper, lead, zinc) (LAU, 1999). Although the Schlenze has a very low discharge, it drains a large abandoned underground mine (called “Schlüsselstollen”) which has an exorbitant high concentration of metals.

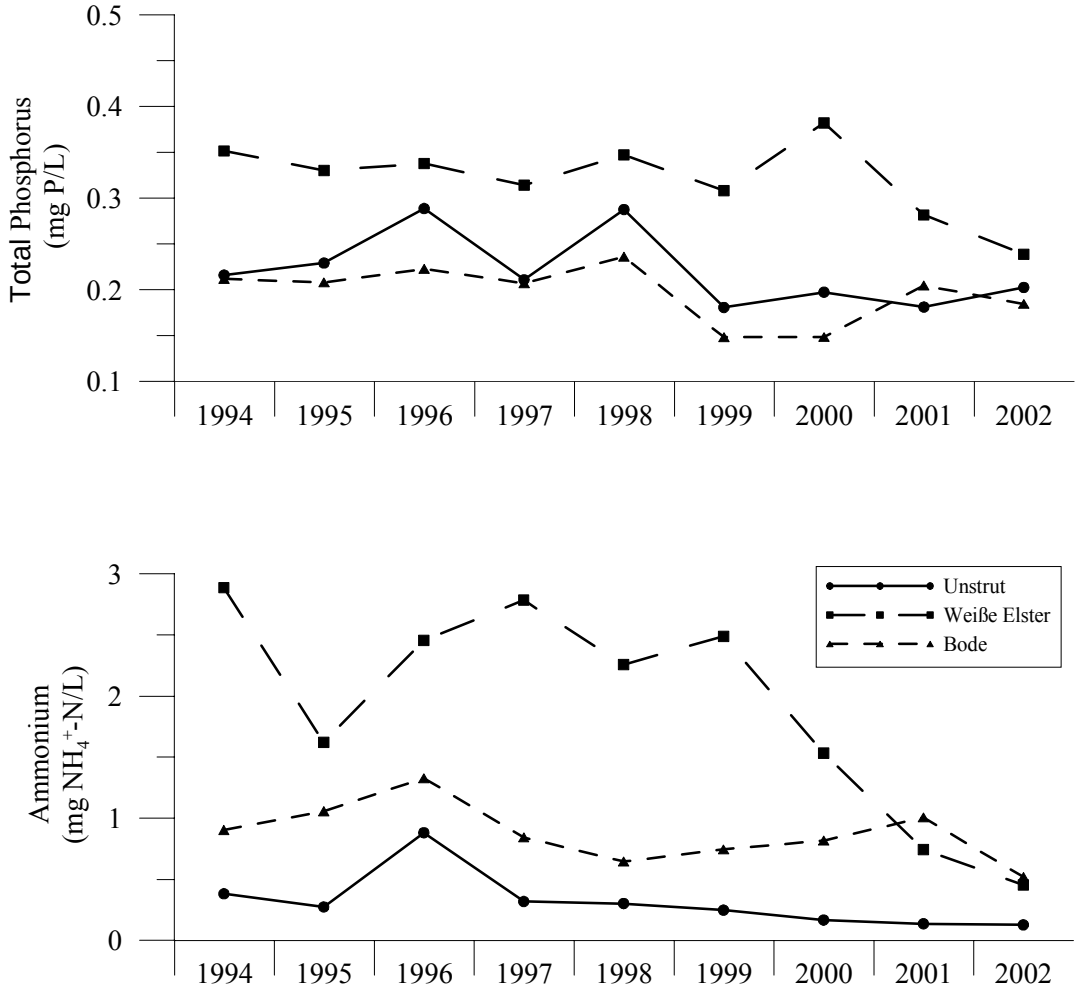


Figure 27: Total phosphorus and ammonium of main tributaries, Unstrut, Weiße Elster and Bode, as boundary conditions for the modelling of the middle and lower Saale course.

5.6 Parameters

The parameters values used for calibration in the most complex EUTRO model are given in Table 8 in the order of decreasing sensitivity for Complexity 5. In general, the values conform closely to those suggested in the WASP5 manual (Ambrose *et al*., 1993). Large discrepancies occur in the parameters governing the nitrogen dynamics of the system in particular the rates of mineralization, nitrification and denitrification (K_{71}, K_{12} and K_{NO3}) and the oxygen-limited half-saturation value for denitrification (K_{2D}).

Up to six parameters were used for TOXI:

- longitudinal dispersion D_x: can be calibrated alone by simulating the transport of a conservative substance such as chloride. This parameter plays an important role for model setups in which mean velocities vary substantially between discretized units, which is the case for the lock-and-weir system.

Table 8: Parameter descriptions and values of the most complex configuration used for calibrating EUTRO in order of decreasing sensitivity.
(adapted from Lindenschmidt, 2006)

Parameter	Calibrated	Recommend	Units	Description
K_{mP}	0.001	0.001	mg P/L	half-saturation constant for phytoplankton phosphorus uptake
K_{mN}	0.028	0.025	mg N/L	half-saturation constant for phytoplankton nitrogen uptake
K_{1D}	0.022	0.02	1/d	phytoplankton death rate
K_{71}	0.057	0.075	1/d	*ON*-mineralization rate at 20°C
K_{1R}	0.112	0.125	1/d	phytoplankton respiration rate
K_{12}	0.211	0.09 – 0.13	1/d	nitrification rate at 20°C
a_{NC}	0.293	0.25	mg N/mg C	nitrogen-to-carbon ratio
a_{PC}	0.030	0.025	mg P/mg C	phosphorus-to-carbon ratio
K_{1C}	1.886	2.0	1/d	maximum phytoplankton growth rate
f_{ON}	0.571	0.5	-	fraction of dead and respired phytoplankton recycled to *ON*
K_{PHY}	0.764	0.0 – 1.0	mg C/L	half-saturation constant of phytoplankton limitation on mineralization
K_{83}	0.196	0.22	1/d	*OP*-mineralization rate at 20°C
K_D	0.146	0.16 – 0.21	1/d	carbonaceous deoxygenation rate at 20°C
f_{OP}	0.505	0.5	-	fraction of dead and respired phytoplankton recycled to *OP*
K_{NIT}	1.339	2.0	mg O_2/L	half-saturation for nitrification O_2-limitation
a_{CCHL}	36.4	20 - 50	mg C/mg Chl-a	carbon-to-chlorophyll-a ratio
K_{NO3}	0.173	0.1	mg O_2/L	half-saturation for denitrification O_2-limitation
K_{2D}	0.137	0.09	1/d	denitrification rate at 20°C
K_{BOD}	0.249	0.5	mg O_2/L	half-saturation for carbonaceous deoxygenation O_2-limitation
I_S	239.5	200 - 500	langleys/d	saturation light intensity for phytoplankton
a_{OC}	2.605	2.76	mg O_2/mg C	oxygen-to-carbon ratio

- vertical diffusion D_y: describes the movement of substances between the bottom sediments and the water column. This parameter is important for the transport of inorganic substances which for the case of heavy metals tend to have higher concentrations in the bottom sediments than in the overlying water.
- sedimentation rate v_{sed}: serves as a sink of suspended, particulate matter through vertical transport from the water column to the sediments. Its rate is assumed to increase immediately upstream from weirs.
- resuspension rate v_{res}: describes the transport of particulate matter from the bottom sediments into the water column. Its rate can increase locally immediately downstream from weirs.
- substance concentration in the bottom sediment c_{sed}: is particularly important for substances with strong concentration gradients between bottom sediments and water, which is the case for heavy metal transport.
- partition coefficient for sorption of dissolved substances onto suspended matter K_D.: has different descriptions depend on the model complexity used (described above).

5.7 Initial conditions

A longitudinal profile of all the state variables is required at the commencement of each model simulation. Initial concentrations for all the discretized segments were linearly interpolated between the sampling stations (see Figure 28 as an example for ammonium).

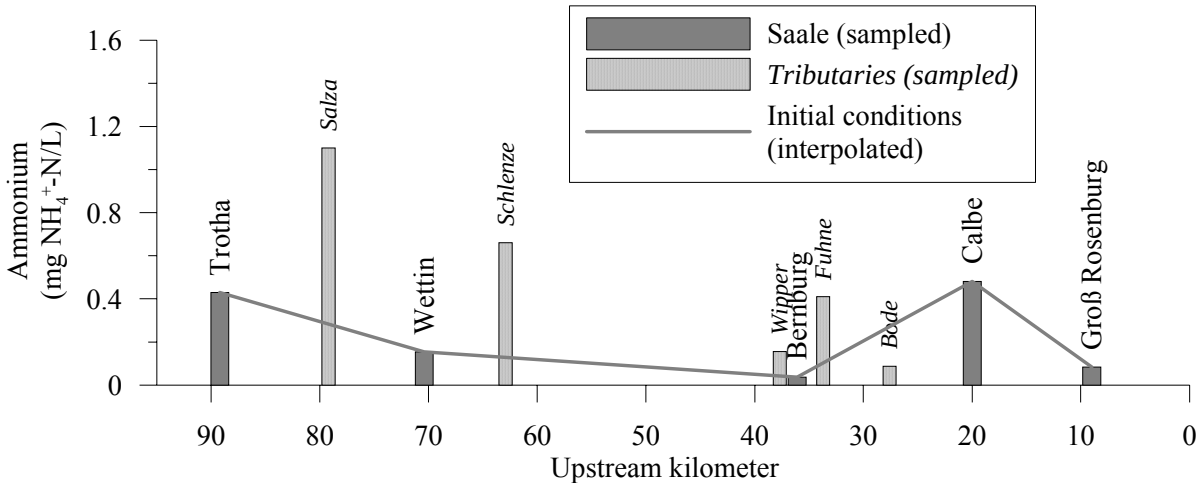


Figure 28: Example of initial conditions used for the simulation of ammonium along the lower Saale reach.

6 Results and Discussion

6.1 Calibration

Hydrodynamics

Calibration was carried out separately for low, medium and high flow conditions of the Saale using 7, 8 and 4 time frames of varying lengths of days, respectively, from a three year series (1997 - 1999). The parameters calibrated were Manning roughness coefficient *n* and the weir discharge coefficient α. *n* varied between 0.022 and 0.030 sec/m$^{1/3}$ and falls within the expected range of values given by Lange and Lecher (1993). Conspicuous is the higher value of n for the most downstream reach between Calbe and the confluence, although a lower value was initially expected. α was calibrated to a value of 1.8 which is much lower than the value given in the original version for small weirs in irrigation ditches (Warwick, 1999). This value complies with the range of values suggested by Lange and Lecher (1993).

For Calbe, too, actual flow measurements were not available and calibration could only be carried out using stage measurements. Care was taken to ensure a constant discharge of 22 m^3/sec through the diversion, which is required for the operation of an electrical generating turbine in the upper portion of the diversion reach. The discharge was regulated by incorporating a weir at the inlet to the diversion. Figure 29 shows the simulated water levels for compared with gage readings the river discharge of 55.5 m^3/sec (most frequent discharge = 60 m^3/sec) during the sampling period. There is good agreement between the two showing the model's capability to simulate the hydrodynamics within branched and dammed systems.

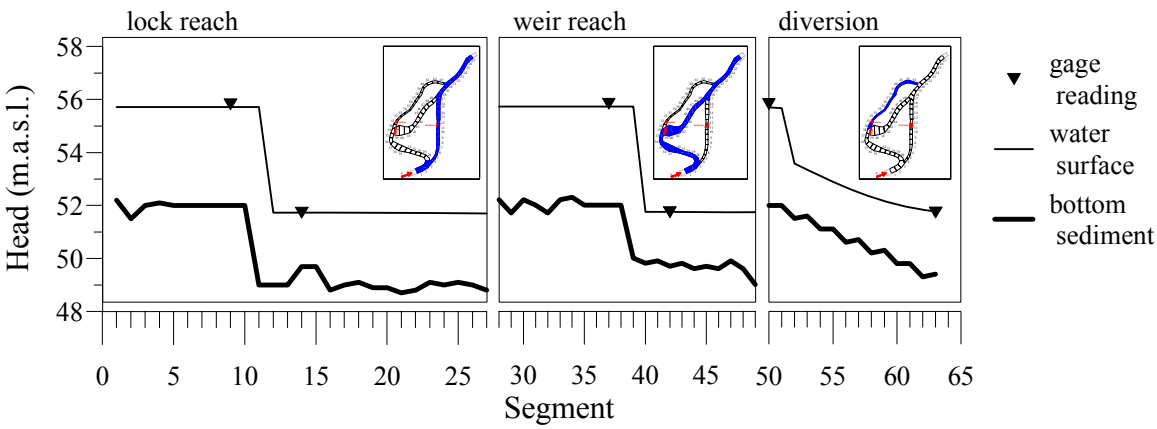


Figure 29: Calibrated water levels for the lock, weir and diverting reaches in the Calbe lock-and-weir system at a river discharge of 55.7 m^3/sec.
(adapted from Wodrich, 2004)

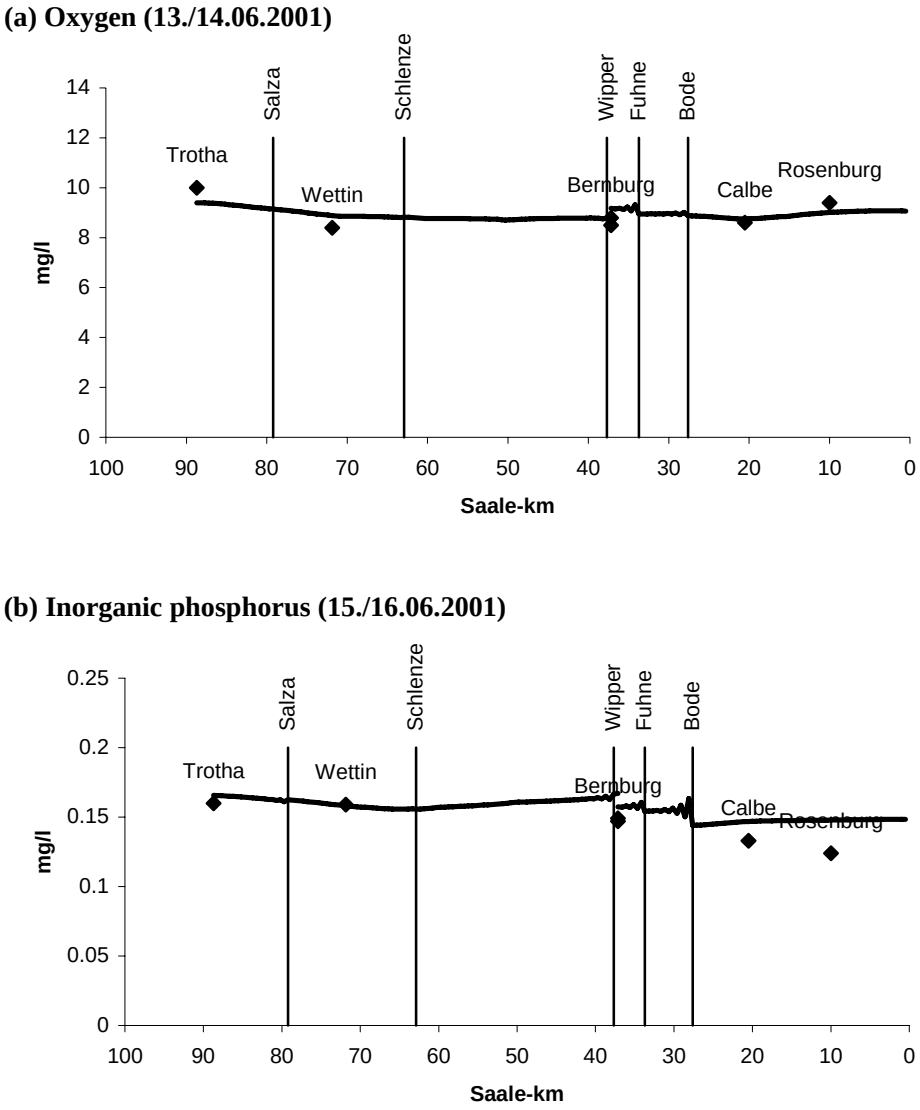


Figure 30: Longitudinal profiles of dissolved oxygen and inorganic phosphorus simulations calibrated for the lower course of the Saale River.

Lower Saale

Comparisons between simulated and sampled values for *DO* and *IP* are given in Figure 30. *DO* simulations generally fitted well to measurements. Likewise nutrients, however *IP* tended to be overestimated downstream from the Bode tributary. Figure 31 shows time series for *Chl-a* and NH_4^+-*N* at the sampling stations Bernburg, Calbe and Groß Rosenburg. There is reasonably good agreement between simulated and sampled values. *Chl-a* was difficult to fit to samples due to the high variability and uncertainty in the measurements. Notice, for example, the large differences in *Chl-a* measurements between Days 12 and 14 at both Calbe and Groß Rosenburg. These discrepancies are partially attributed to sampling error and also to insufficient knowledge of specific processes. Pertaining to NH_4^+-*N*, an ammonium surge from the city of Halle at the upstream boundary due to a storm event just prior to the sampling and simulation time span was difficult to reproduce. Exact fitting of the surge concentration was compromised in order to insure a good fit of the simulation to

the data sampled during the second half of the calibration time period. A significant degree of uncertainty is present in the data as seen, for example, in the sampled ammonium value of Day 8 at Groß Rosenburg.

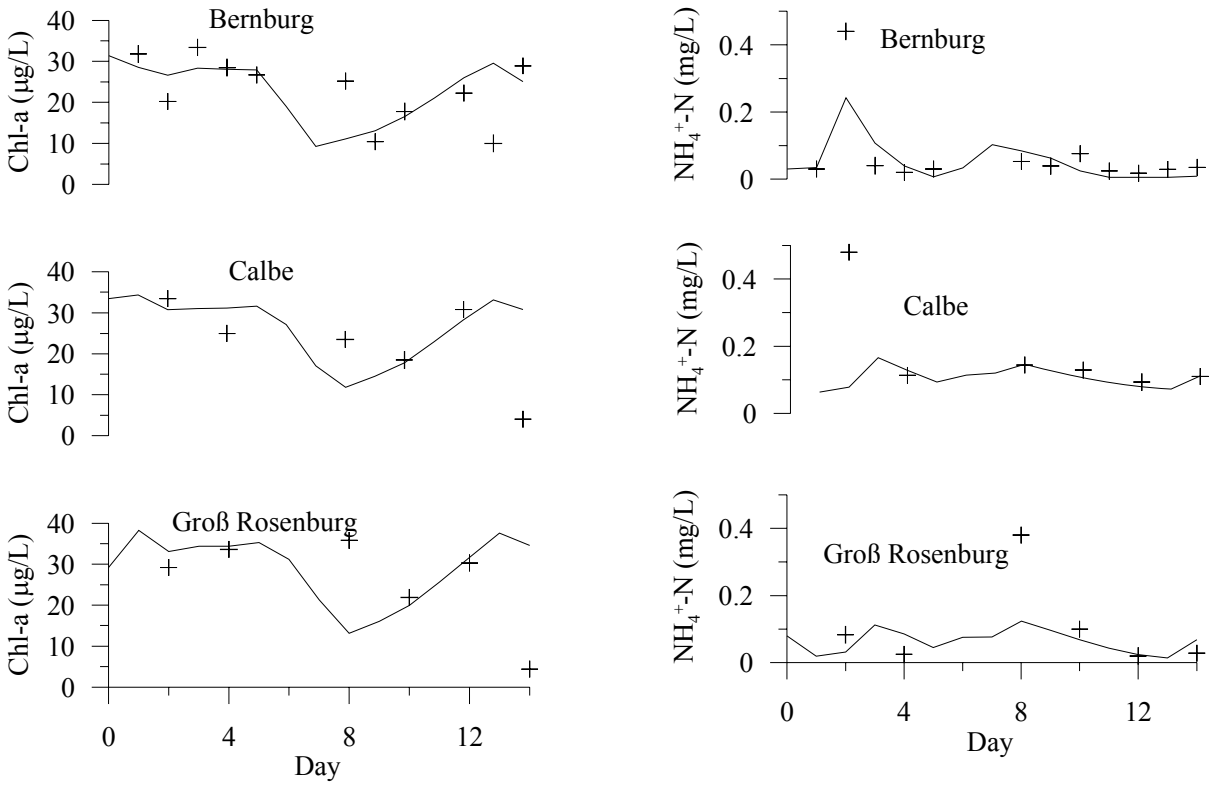


Figure 31: Time series of chlorophyll-a and ammonium simulations calibrated for the lower course of the Saale River.

There is good agreement between the simulation and measured values of suspended solid concentrations, which remained fairly steady along the course of the lower Saale River (see Figure 32(a)). There is higher uncertainty in the sampled values at Wettin due to unavoidable excessive resuspension of bottom sediments during sampling at the shore and at Nienburg due to mixing effects by the Bode inflow. Increased sedimentation at the lock-and-weir systems is not evident. A good fit of the simulation to the data was also obtained for the chloride concentrations (see Figure 32(b)). The industrial emission at Bernburg proved to be an important point load for the overall substance balance downstream from Bernburg. Emission values were not available but were derived roughly from production figures. Hence, the simulations downstream from Bernburg are sometimes over- or underestimated, as seen by the discrepancies between the simulations and the samples from Calbe and Groß Rosenburg. The Schlenze tributary is an important source of heavy metals to the Saale, evident in the drastic increase of total zinc concentrations immediately downstream from the Schlenze confluence. The simulations of the total zinc concentrations were initially overestimated and could only be corrected by assuming increased sedimentation of zinc at the lock-and-weirs (see Figure 32(c)).

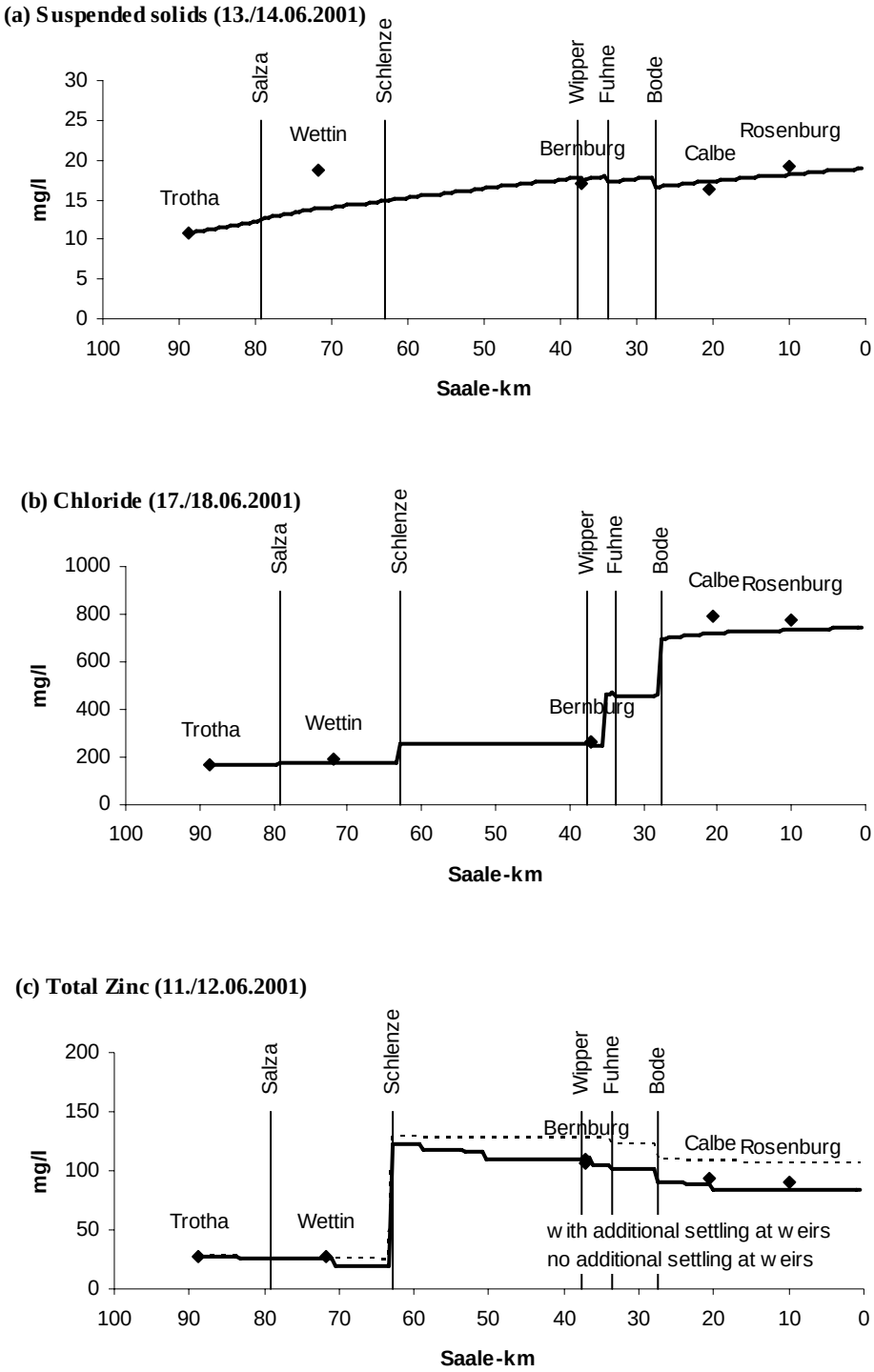


Figure 32: Longitudinal profiles of suspended solids, chloride and total zinc simulations calibrated for the lower course of the Saale River.
(adapted from Lindenschmidt, Hesse, et al., 2005)

Middle Saale

A sampling campaign was carried out in September 2003 between Bad Dürrenberg and Trotha which served as a basis for calibration of the middle Saale. The water quality of the Saale in the flow direction along this stretch is or has been heavily impacted by the industrial areas of Leuna,

Lützkendorf and Buna (outfalls at Saale-km 121.7, 116.9 and 109.4, see Figure 12), the tributary Weiße Elster (inlet at Saale-km 102.7) and the city of Halle (between Saale-km 98 and 89). It was evident that the emissions from the industrial areas have drastically reduced since the 1990s to loads that remain unnoticed after mixing in the Saale River. High concentrations of some metals and salts were measured in the Laucha, which drains the Buna site but the discharges and hence the emitted loads are minute (see Figure 33 for chloride). The Luppe tributary drains an agricultural catchment and exhibits high concentrations of nutrients and sediments. However, its discharges and loadings, too, are very small compared to the mass of the substances present in the Saale at that vicinity. The Weiße Elster, whose mean discharge is approximately one-third of that of the Saale immediately upstream of the Weiße Elster inflow, has a large impact on the Saale's water quality. The Weiße Elster i) concentrates the heavy metals such as chromium, copper and iron, which stem from the mining areas in the upper catchment area of the Weiße Elster and ii) dilutes chloride, suspended solids and chlorophyll-a.

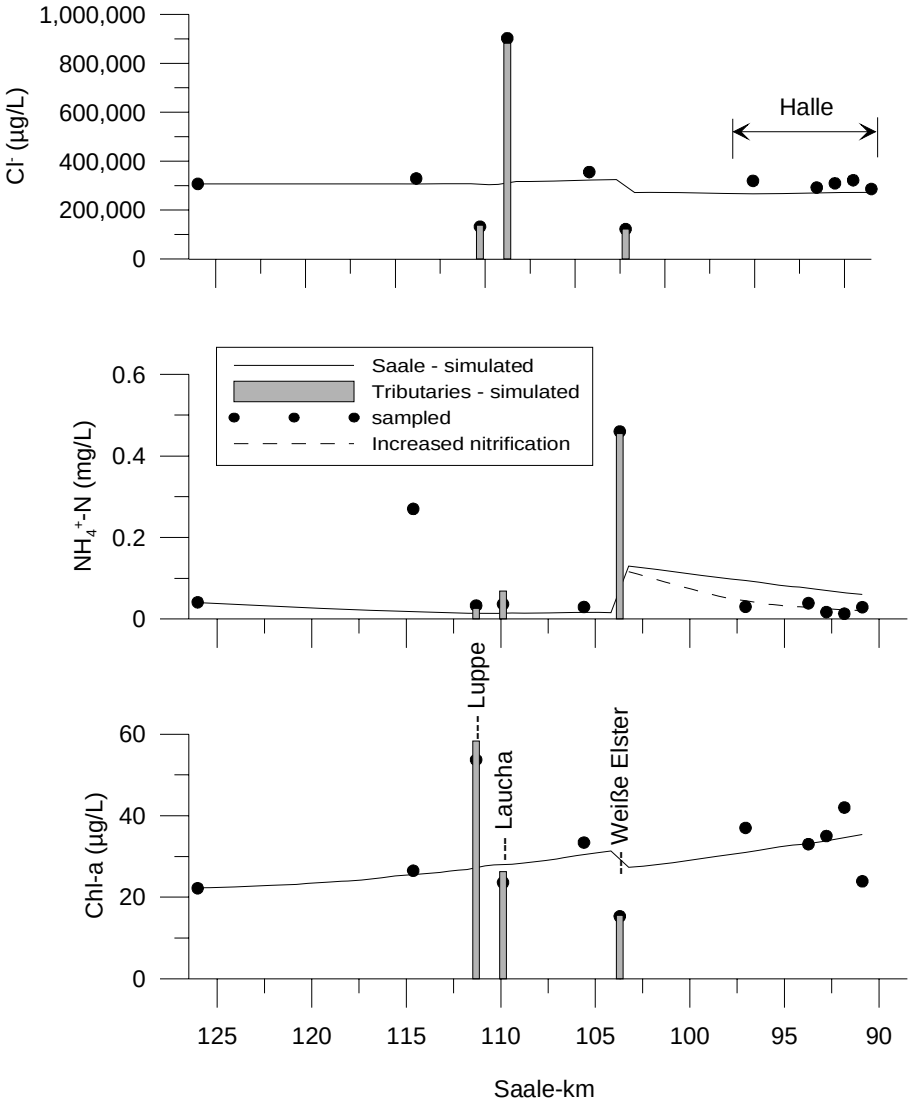


Figure 33: Longitudinal profiles of chloride, ammonium and chlorophyll-a simulations calibrated for the Saale River between Bad Dürrenberg and Halle-Trotha
(modified from Eckhardt, 2004)

The chlorophyll-a values are not as high as in the Saale since the travel distance is not long enough for the ecological state to have reached is maximum productive capacity. Large amounts of ammonium are emitted by the Weiße Elster (see Figure 33) which undergoes a rapid turnover immediately downstream from the tributary. This process is replicated in the modelling by locally increasing the nitrification rate. This rate is known to increase in areas of high ammonium concentration due to the abundance of nitrifying bacteria in such areas and is common in many rivers in Germany (A. Schöl, BfG, pers. comm.). Significant emissions of substances were not detected from the city of Halle. Evident is the high variability between the many sampling stations in Halle, especially *Chl-a* (see Figure 33) which may be partly due to the variability of the flow regime within the highly branched section of the river flowing through the city.

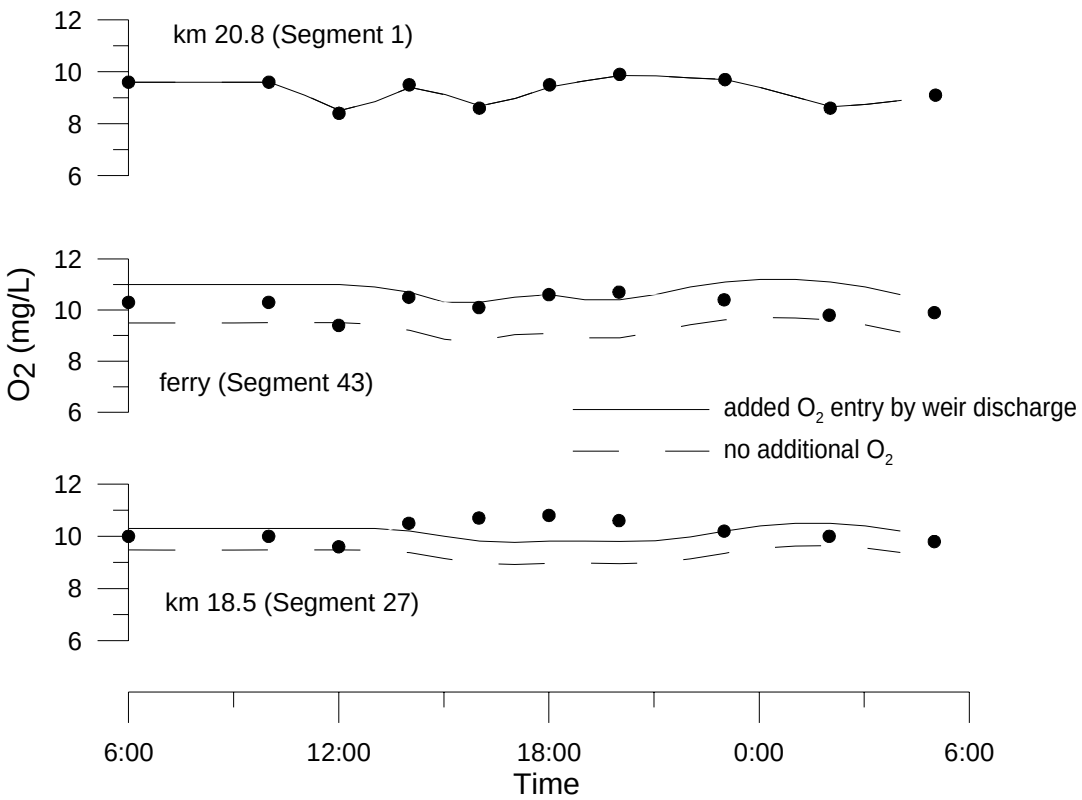


Figure 34: Dissolved oxygen at stations along the weir reach in sequence with flow direction.
(from Lindenschmidt, Eckhardt,et al., 2004)

Calbe

Figure 34 and Figure 35 show *DO* and NH_4^+*-N* for the 24-hour sampling campaign for selected sampling stations at the lock-and-weir system at Calbe. For better *DO* simulation fits to the data additional entry of oxygen was simulated at the weir according to the formula from Avery and Novak (1978) (cited in Haag (2003)). The gap between simulations with and without oxygen entry closes with further downstream distance from the weir (compare stations *ferry* and *km 18.5*), indicative of rapid consumption of the additional oxygen. The decrease in NH_4^+*-N* between the most upstream and

downstream stations indicates the weir's potential role for denitrification. Both processes, oxygen entry and denitrification at weirs, were observed only locally, not in the large scale modelling of the Saale River course.

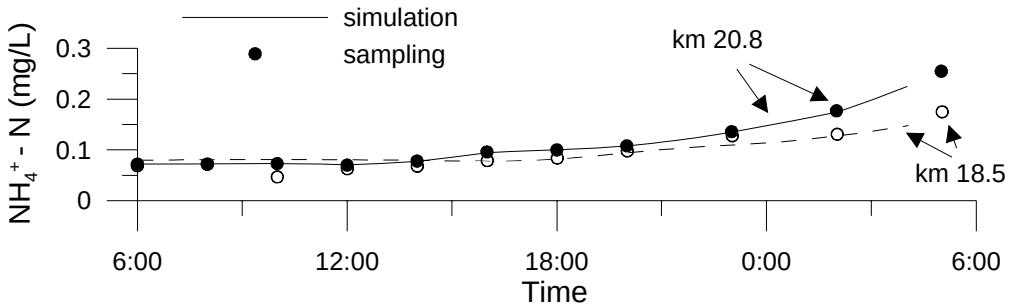


Figure 35: Simulated and sampled ammonium concentrations at the most upstream (km 20.8) and downstream (18.5) stations of the lock-and-weir system.
(from Lindenschmidt, Eckhardt,et al., 2004)

Figure 36 gives a snapshot at 6:00 pm of the concentrations of suspended solids and the total and dissolved fractions of zinc in all areas of the lock-and-weir system. The concentrations in the lock reach are less due to the low flow through the lock and the longer residence times within this reach, allowing more solids to settle out. The sedimentation rate above the weir was increased (more settling) and the resuspension rate below the weir was increased (more erosion) in order to better fit the simulations to the sampled data. This trend occurred for all heavy metals; not arsenic.

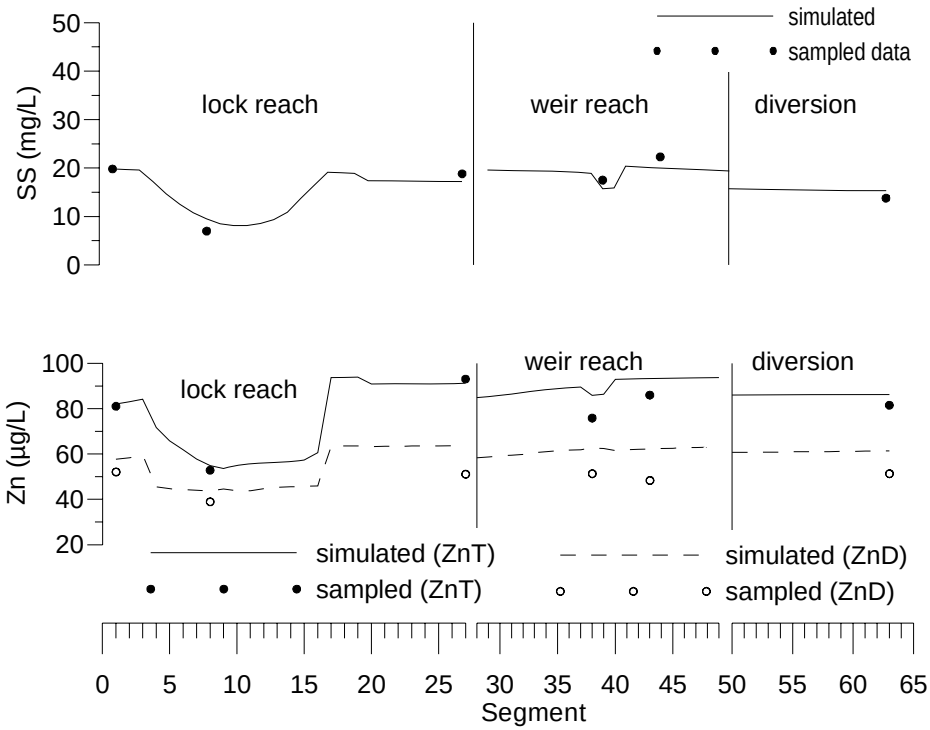


Figure 36: Longitudinal profiles at 6:00 pm along the lock, weir and diverting reaches for suspended solids *SS* and zinc: total *ZnT* and dissolved *ZnD* fractions.
(compiled from Wodrich, Lindenschmidt, et al., 2004 and Wodrich, 2004)

6.2 Validation

Hydrodynamics

Figure 37 shows validation results for the reach between the weirs Trotha and Wettin, corresponding to the downstream gage at Trotha and the upstream gage at Wettin. The simulation is three years in length, from 1 January 1997 to 31 December 1999. The model gives particularly good validated results for low flow situations; the validation becomes less accurate for extreme floods since flow becomes overbanked and different effective roughness coefficients are to be expected. At Trotha, there is good agreement between the gage readings and the model predictions. Some extreme deviations exist for single days with extreme flooding, such as 27. February 1997 but such large errors do not persist for more than one day. It is apparent that the simulation is slightly overestimated for most days of the simulation. Perhaps a simulation with a slightly lower value for n would give a better fit. The deviations between the model results and gage readings are somewhat larger for Wettin but still within an acceptable range. At this gage the water level simulations are overestimated for high flows and underestimated for low flows. This weir-upstream gage is more affected by the weir discharge. The simulation may have been more accurate if the data on the operation of the weir cap, which can slightly extend the crest height, had been available. The error in the input data (up to ± 10%) also contributes to the overall uncertainty in the results (Pelletier, 1988).

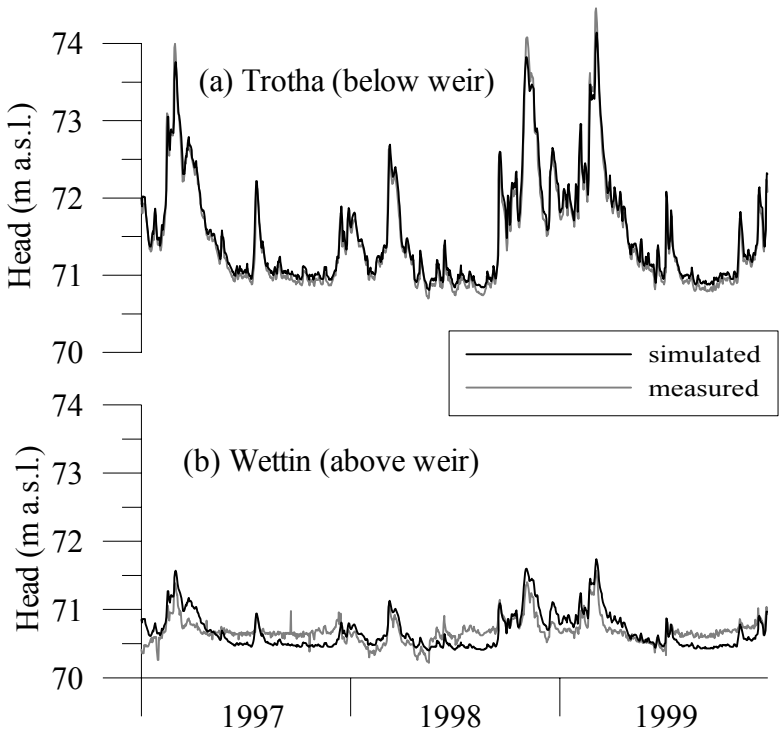


Figure 37: Hydrodynamic validation using water levels for a reach flowing from the (a) gage below the weir at Trotha to the (b) gage above the weir at Wettin.
(adapted from von Saleski, et al., 2004 and von Saleski, 2003)

In Table 9, the average velocities simulated for MQ (mean discharge) and MNQ (mean lowest discharge) are compared with field measurements made from a government authority (STAU, Halle) for the flow reaches along the lower Saale. Overall good agreement was obtained between measurements and simulations when considering the high uncertainty in the field measurements (up to ± 10%, see Pelletier, 1988).

Table 9: Comparison of flow velocities measured in the field and simulated results.

	Velocities at MQ (m/s)		Velocities at MNQ (m/s)	
	field	simulated	field	simulated
Trotha				
	0.6	0.51	0.35	0.26
Wettin				
	0.6	0.59	0.4	0.29
Bernburg				
	0.45	0.53	0.3	0.26
Calbe				
	0.8	0.91	0.5	0.51
Confluence				

field data from STAU, Halle

The validation of the hydrodynamics for the Calbe lock-and-weir system was successful and the errors between simulated and measured water levels were minimal, comparable to the calibration.

Lower Saale

There is good agreement between simulations and sampling points shown exemplary in Figure 38 for *DO* and NH_4^+-*N* at Groß Rosenburg in for the long-term sampling period of 14. May – 30. July 2002. Large uncertainties in the sampling exist for ammonium as seen in the discrepancies between the sampled values from different institutions (e.g. Days 1 and 72 for LAU and BfG), which is due to different sampling strategies. The validation was successful for the chosen time frame due to the relatively high temporal resolution of the samples taken at the stations Trotha, Wettin, Nienburg and Groß Rosenburg (≤ 14 days) and due to the relatively higher than normal discharges in the river. Ammonium is a very sensitive variable with peaks and valleys coinciding inversely with those of global radiation and phytoplankton growth (not shown).

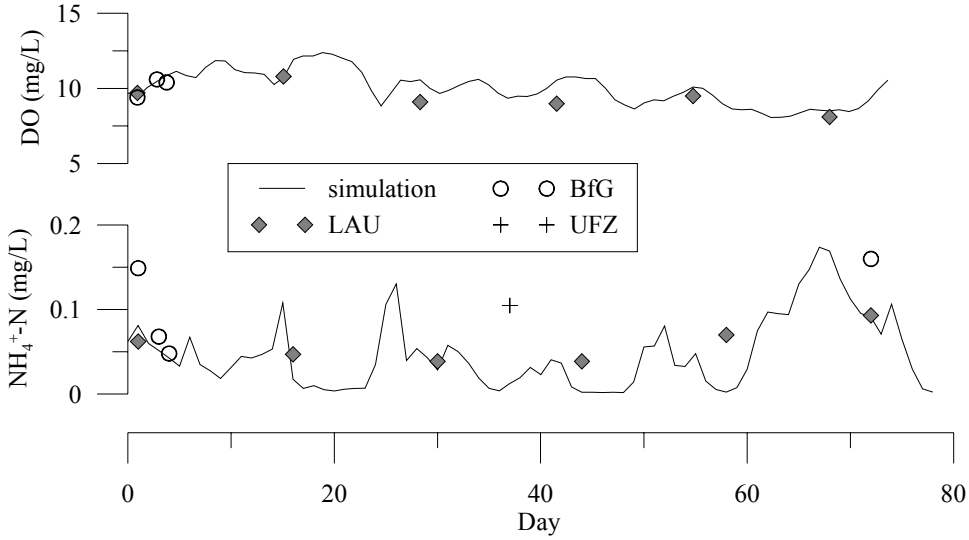


Figure 38: Dissolved oxygen and ammonium at Groß Rosenburg for the validation period 14. May – 30. June 2002.
(modified from Lindenschmidt, Schlehf, et al., 2005)

There is good agreement between the simulation and measured values of suspended solid concentrations, which remained fairly steady along the lower course of the Saale River (see Figure 39). There is higher uncertainty in some sampled values: at Döblitz and Wettin due to unavoidable excessive resuspension of bottom sediments during sampling at the shore and at Nienburg due to mixing effects by the Bode inflow. Increased sedimentation at the lock-and-weir systems is not evident.

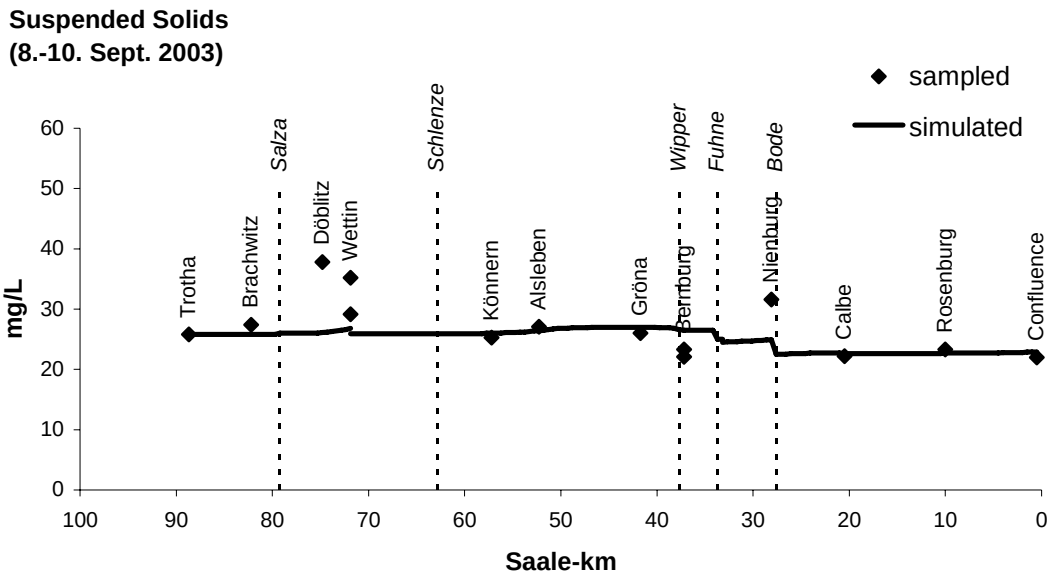


Figure 39: Longitudinal profiles of suspended solids along the lower course of the Saale River for the short-term validation time frame.
(from Lindenschmidt, Wodrich and Hesse, 2006)

A good fit of the simulation to the data was also obtained for the chloride concentrations (see Figure 40). The industrial emission at Bernburg proved to be an important point load for the overall substance balance downstream from Bernburg.

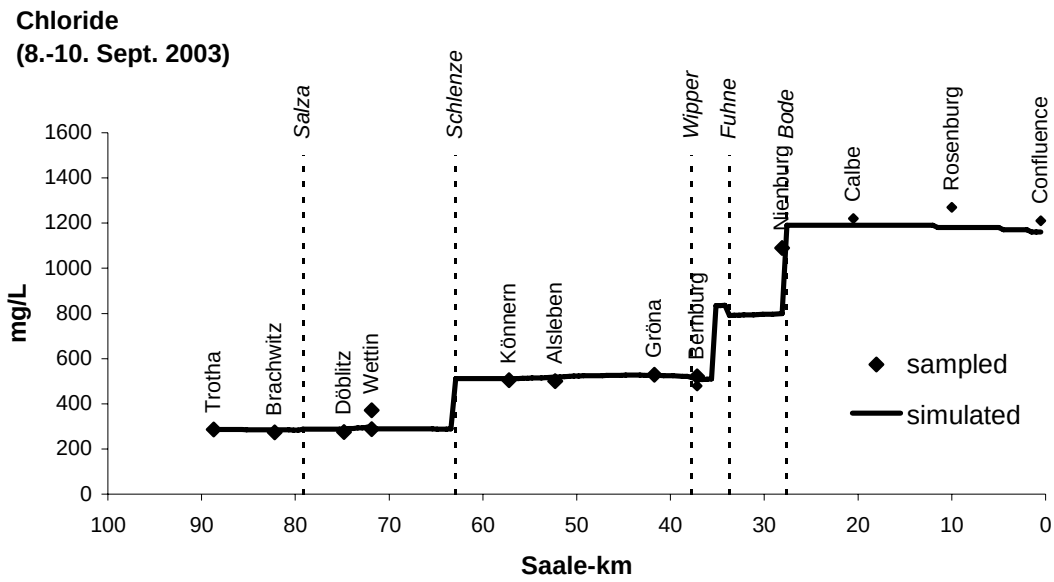


Figure 40: Longitudinal profiles of chloride along the lower course of the Saale River for the short-term validation time frame.
(from Lindenschmidt, Wodrich and Hesse, 2006)

The Schlenze tributary is an important source of heavy metals to the Saale, evident in the drastic increase of total zinc concentrations immediately downstream from the Schlenze confluence (see Figure 41). The simulations of the total zinc concentrations were initially overestimated and could only be corrected by assuming increased sedimentation of zinc at the lock-and-weir systems. Zinc in the Schlenze is predominately present in dissolved form and requires approximately 30 hours for the dissolved and particulate fractions to reach an equilibrium sorption state (in this simulation the time corresponds to a flow distance between the Schlenze confluence and Bernburg). By implementing a more complex sorption process in the modelling to allow K_D to increase linearly from 10000 L/kg at the Schlenze confluence to 40000 L/kg at Bernburg, this dynamic sorption process was accurately simulated.

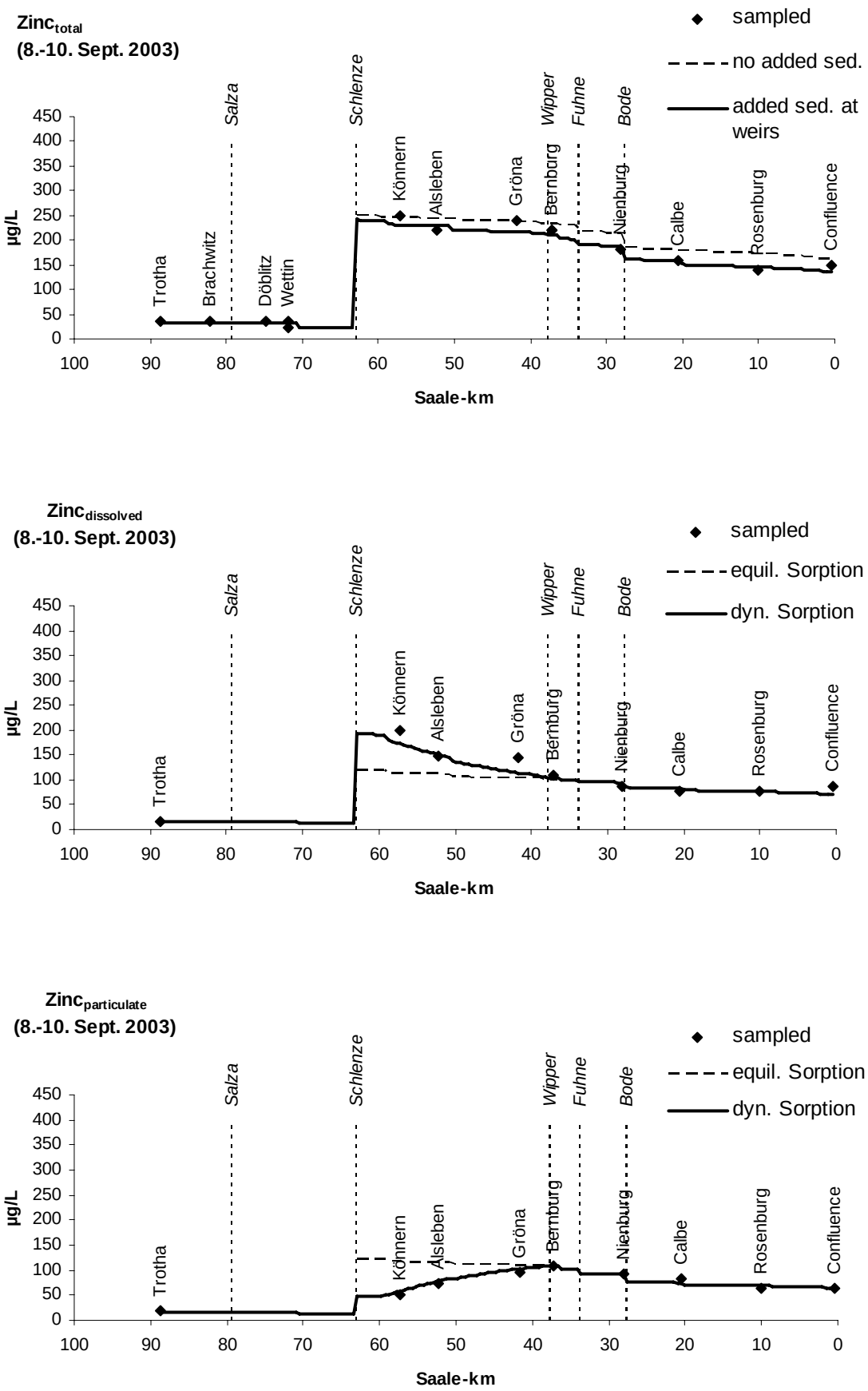


Figure 41: Longitudinal profiles of total zinc and its particulate and dissolved fractions along the lower course of the Saale River for the short-term validation time frame.
(compiled from Lindenschmidt, Wodrich and Hesse, 2006 and Lindenschmidt, Hesse, et al., 2005)

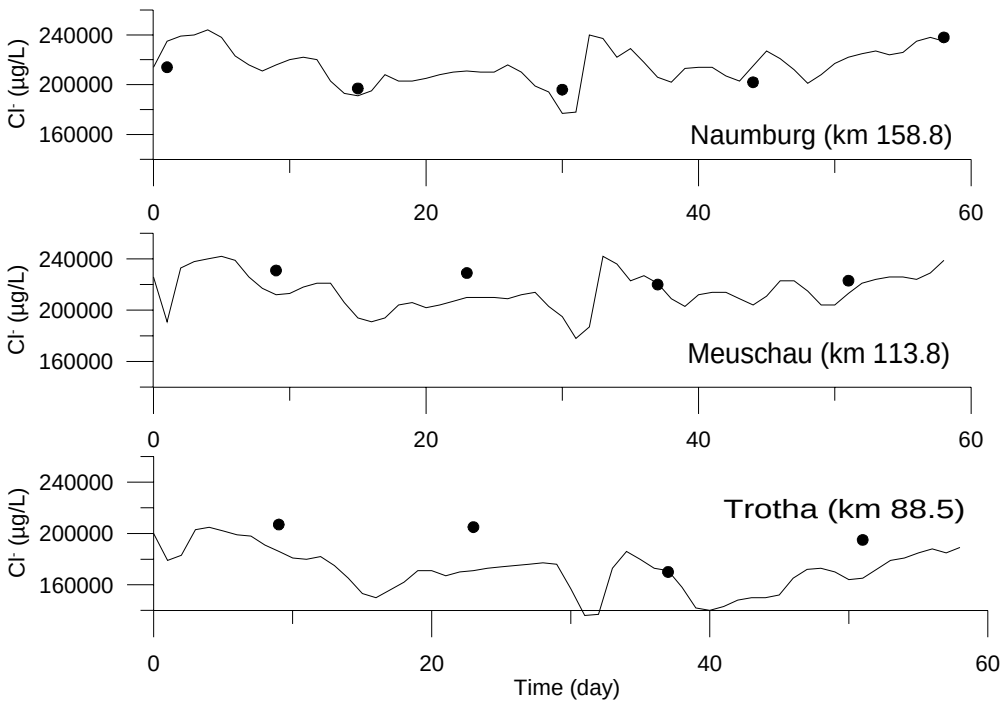


Figure 42: Simulations of chloride concentrations for the middle course of the Saale River.
(compiled from Lindenschmidt, Eckhart, et al., 2005 and Eckhardt, 2004)

Middle Saale

Despite the low frequency data available for the model validation of the middle Saale (7. June – 15. August 1999), the simulations fit reasonably well to the measured data. The substances present and transformed in the river water are in balance with the substances entering (tributaries and pollution outfalls) and exiting (most downstream segment) the system, shown exemplary for chloride in Figure 42. A high nitrification rate downstream from the Weiße Elster tributary (km 102.7) is also required in order to match simulated values to measurements at Trotha (see Figure 43).

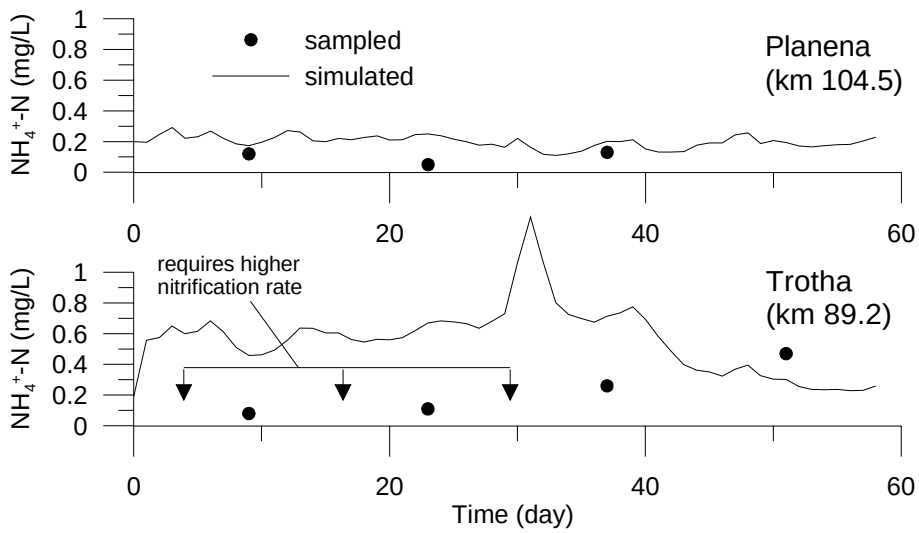


Figure 43: Ammonium concentrations simulated along the middle Saale; a higher nitrification rate is required between the Weiße Elster tributary (km 102.7) and Trotha.
(compiled from Lindenschmidt, Eckhart, et al., 2005 and Eckhardt, 2004)

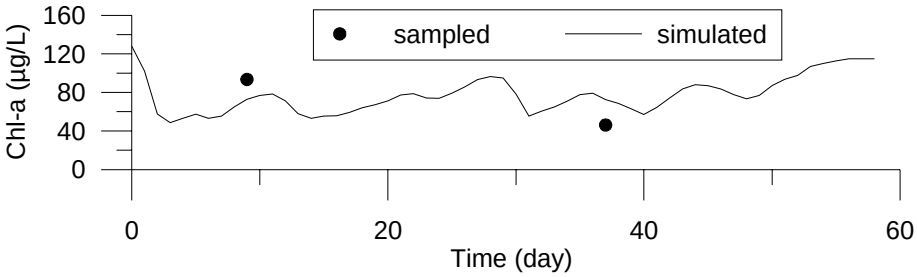


Figure 44: Chlorophyll-a concentrations at Halle-Trotha (km 89.2).
(from Lindenschmidt, Eckhart, et al., 2005)

Chl-a was also well modelled but it was sampled only every four weeks making its validation assessment more uncertain (see Figure 44). The suspended solid concentrations were underestimated for Day 23 for the lower stretch of the middle Saale between Meuschau and Trotha (see Figure 45 for Trotha). This high concentration is not a result of rains or a discharge surge, as evident from the graphs in Figure 45. Unfortunately, chlorophyll-a was not sampled on this day (see Figure 44), however, the organic fractions of the nutrient, *ON* and *OP* were also underestimated and the nutrients *NH4+-N* and *IP* were overestimated so that exuberant phytoplankton growth just prior to this sampling date is suspected to have caused the high suspended sediment load. In order to test this hypothesis, the phytoplankton growth rate was doubled. Figure 46 and Figure 47 show simulations for growth rates of 2 d^{-1} (solid line) and 4 d^{-1} (dashed line) for the time frame Day 19 – 25 for the stations Bad Dürrenberg, Meuschau, Planena and Trotha. Increasing the growth rate improved the fit of all simulated state variables to the sample from Day 23. A better fit is attained for ammonium at Trotha when the nitrification rate is increased.

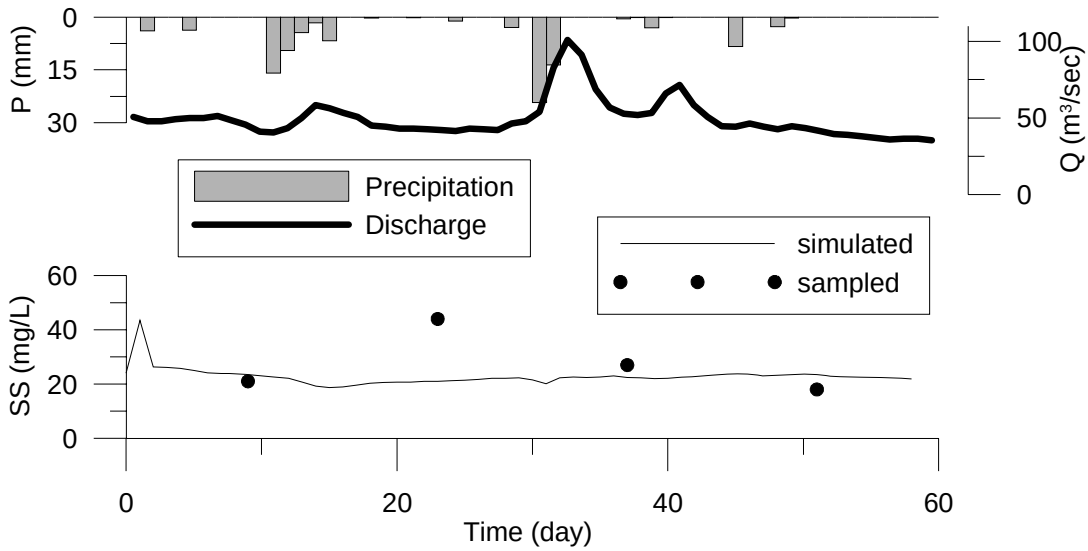


Figure 45: Suspended solids *SS*, precipitation *P* and discharge *Q*; the *SS* sample on Day 23, which is attributed to exuberant phytoplankton growth, is missed by the simulations.

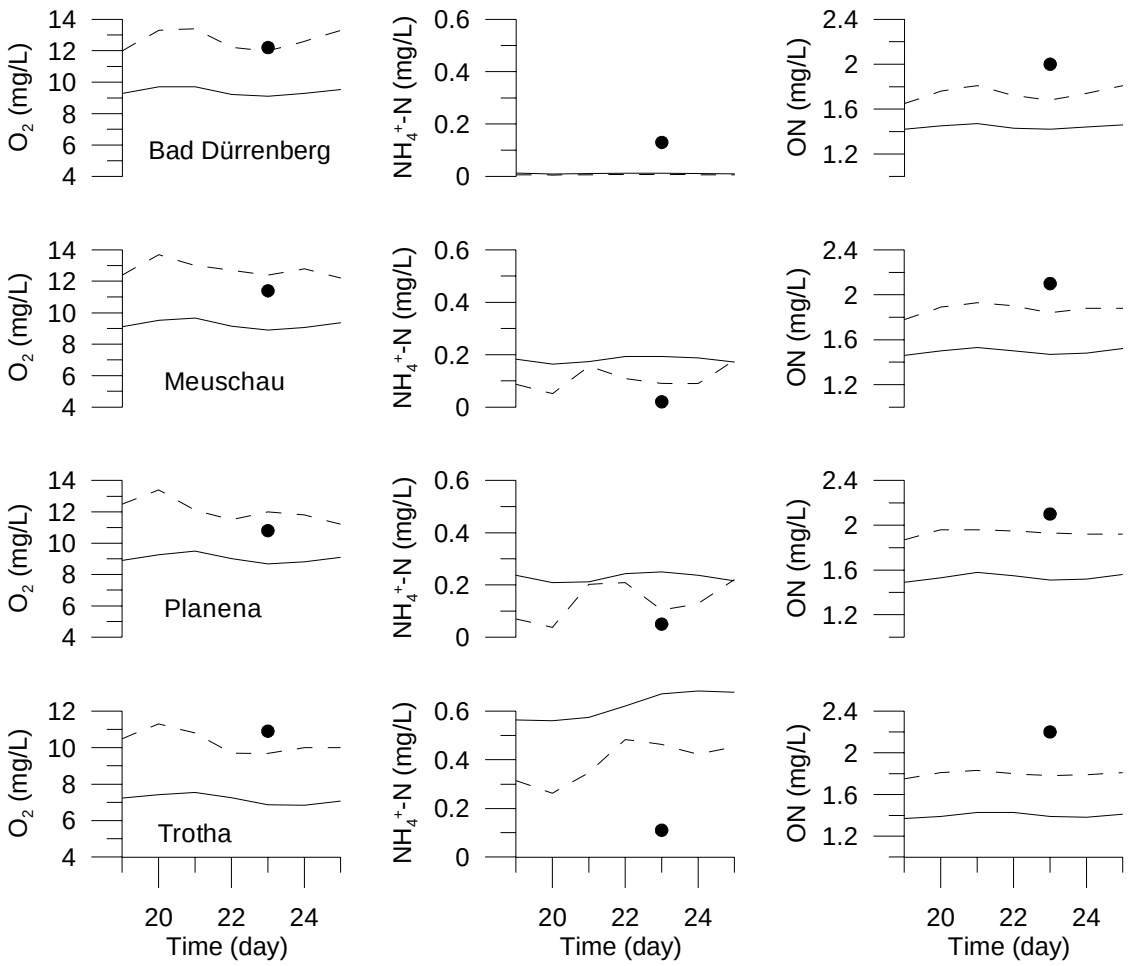


Figure 46: Simulations of dissolved oxygen O_2, ammonium NH_4^+-N and organic nitrogen ON using phytoplankton growth rates of 2 d^{-1} (solid line) and 4 d^{-1} (dashed line).

Calbe

Large differences in the systems behaviour did not occur between the calibration and validation of the eutrophication variables, which is indicative of the model's predictive power at this scale. Discrepancies did occur, however, for the heavy metals (Figure 48), as indicated by the likelihoods of the simulated variables for both calibration and validation. This is due to the high sensitivity of the metal concentration in the sediments on the model results. For the validation the concentrations are not known *a priori* and only the calibrated values were used. However, this is a source of high uncertainty due to the high temporal and spatial variability of substance concentrations in the sediments. It is very probable that more heavy metals were present in the sediments during the 2001 sampling campaign compared to the campaign one year later, since the discharges prior to the first campaign were lower for a much more extended period of time.

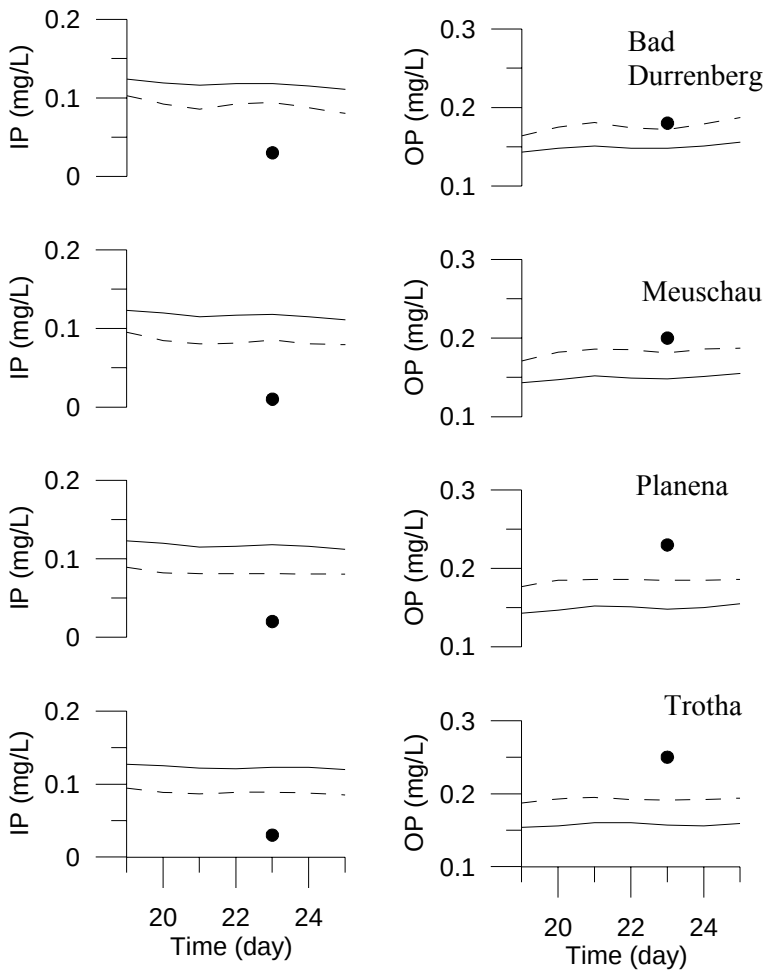


Figure 47: Simulations of inorganic and organic phosphorus (*IP* and *OP*, respectively) using phytoplankton growth rates of 2 d^{-1} (solid line) and 4 d^{-1} (dashed line).

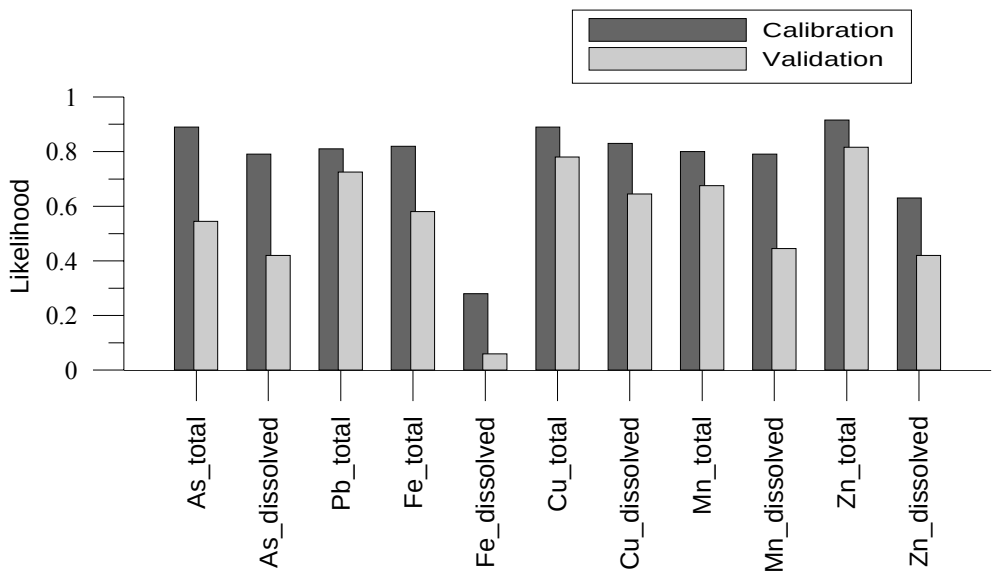


Figure 48: Agreement between measured and simulated values for the calibration and validation given as likelihood values (1 = perfect fit; 0 = no fit) for total and dissolved fractions of arsenic *As*, lead *Pb*, iron *Fe*, copper *Cu*, manganese *Mn* and zinc *Zn*.
(adapted from Wodrich, 2004)

6.3 Uncertainty vs. Complexity

The steps taken to superimpose model uncertainty variables, sensitivity and error, with model complexity will be given in greater detail here for the eutrophication model. A high degree of detail for the micro-pollutant transport modelling will be given in the next subsection with a focus on the effect scaling has on the uncertainty-complexity relationship.

Table 10: Global sensitivities of calibrated EUTRO parameters for each model complexity listed in descending order for Complexity 5.
(from Lindenschmidt, 2006)

Parameter	Complexity					
	1	2	3	4 (P-limited)	4 (N-limited)	5
K_{mP}				28.12		34.33
K_{mN}					44.19	29.53
K_{1D}				8.80	9.74	9.74
K_{71}			44.05	0.00	17.69	5.91
K_{1R}			0.45	5.13	5.47	5.44
K_{12}		19.58	6.39	0.00	4.96	4.19
a_{NC}				0.41	5.76	3.34
a_{PC}				6.17	5.55	2.52
K_{1C}			0.14	1.23	1.90	1.39
f_{ON}						0.95
K_{PHY}						0.65
K_{83}				2.45	0.00	0.63
K_{D}	1.17	0.94	1.14			0.49
f_{OP}						0.24
K_{NIT}						0.17
a_{CCHL}				0.02	0.11	0.08
K_{NO3}						0.04
K_{2D}						0.03
K_{BOD}						0.03
I_{S}				0.01	0.02	0.01
a_{OC}			0.01	0.00	0.00	0.01
Normalized total	*1.00*	*1.05*	*1.18*	*1.86*	*2.16*	*2.90*

Sensitivity

The global sensitivities of each EUTRO parameter for all calibrated complexities are given in Table 10. The names of the parameters are found in the Appendix. The parameters are ranked in decreasing order of sensitivities for the most complex model. In general, the parameters that have the largest

impact on the state variables are the half-saturation constants for phytoplankton nutrient uptake (K_{mP} and K_{mN}), the phytoplankton loss rates, death and respiration (K_{1D} and K_{1R}) and the rates governing the reduction of nitrogen components, mineralization and nitrification (K_{71} and K_{12}).

Stoichiometric nutrient ratios in phytoplankton (a_{NC} and a_{PC}) have a greater impact in Complexity 4, when the oxygen dynamics are not included in the phytoplankton-nutrient dynamics. This is also portrayed in the minor impact the parameters, which control the deoxygenation of organic matter (K_{1C} and K_{BOD}), have on the simulations in the most complex model. The DO-BOD cycle is only loosely coupled to the phytoplankton-nutrient cycle which is substantiated by i) the high POC:DOC ratio (ratio between the particulate and dissolved fractions of organic carbon, ii) the increasing shift from primary to secondary loading due to the improvements in wastewater treatment, iii) the correlation of chlorophyll-a concentrations with *POC*, iv) the very eutrophic nature of the Saale with a high nutrient availability and v) the light-limited conditions in the lower Saale (Karrasch *et al*., 2001).

Table 11: Error between simulated and sampled data for each state variable and complexity.
(complied from Lindenschmidt, Schlehf, et al., 2005 and Lindenschmidt, 2006)

Variable	Complexity					
	1	2	3	4 (P-limited)	4 (N-limited)	5
DO	0.287	0.278	1.278			0.344
CBOD *	0.441	0.423	0.556			0.595
PHYT				1.552	1.556	1.559
NH_4^+-*N* **		1.922	0.908		0.369	0.314
NO_3^--*N*			0.214		0.250	0.244
ON			0.386		0.429	0.386
OP				0.116		0.088
IP				0.071		0.071
Normalized total	*0.83*	*0.45*	*0.52*	*0.37*	*0.42*	*0.29*

* *TBOD* for Complexity 1
** *NBOD* for Complexity 2

Error

The error for each variable and for each model complexity is given in Table 11. A large error is present between the simulations and samples for *NBOD* in Complexity 2. Modelling nitrogen as a bulk parameter leads to many shortcomings such as the inaccuracy in lag times, the impossibility of modelling inhibition of nitrification at low *DO* concentrations and the possibility of unrealistically simulating negative values for *DO* (Chapra, 1997). There are also shortcomings due to the model's internal conversion of *NBOD* to Kjeldahl nitrogen which is considered to be the component of the total

nitrogen that can be oxidised. Modelling the nitrogen cycle using NH_4^+-*N*, NO_3^--*N* and *ON* in the higher complexities gives less erroneous results.

The error for *DO* in Complexity 3 was relatively large due to an overestimate of the simulation results. Phytoplankton is not a dynamic state variable in this model but is input as a function with time in which chlorophyll-a concentrations are averaged over the spatial domain for each time step. Hence, nutrient uptake is also not required. These restrictions on the phytoplankton-nutrient dynamics results in an imbalance in the *DO* concentrations.

Modelling phytoplankton dynamically with its associated nutrient turnover processes in Complexity 4 reduces model error, even through the DO-CBOD interactions are not considered. Large errors resulted in *PHYT* due in part to the high uncertainty in the sampled data. There is a high variability in chlorophyll-a concentrations both temporally (diel variations) and spatially (near-shore or mid-river). Unfortunately, limited resources did not allow higher resolution phytoplankton data to be sampled with which an averaging and a better representation of the chlorophyll-a concentrations at the corresponding sampling stations could be attained. These problems carry through to the most complex model in which *PHYT*, too, is the variable with the largest error.

Utility

The normalized total errors and sensitivities for each model complexity are plotted in superposition in Figure 49. It is distinct that error decreases and sensitivity increases as the model becomes increasingly complex. The P- and N-limitation models of Complexity 4 are plotted on the same abscissa value since both have the same variables and the same number of parameters (equal complexity). Both the sensitivity and the error values are higher for the N-limitation model.

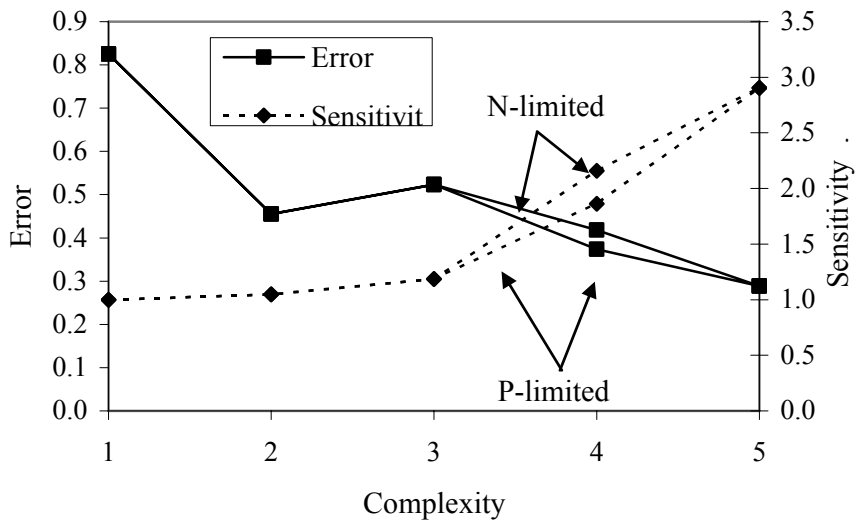


Figure 49: Total model error and sensitivity versus model complexity.
(from Lindenschmidt, 2006)

The index of utility for each model is shown in Figure 50, for which error was given a higher weighting than sensitivity. The least complex model in which only DO-BOD dynamics are represented has the lowest utility. Increasing model complexity by differentiating *BOD* into its carbonaceous and nitrogenous components (Complexity 2) substantially benefits the model simulations. The next higher complexity has a lower utility due to the non-dynamic structure of phytoplankton, whose state is not simulated but input as a function. The model of Complexity 4 in which only the phytoplankton-nutrient dynamics are considered has a high utility if phosphorus serves as the limiting nutrient. Since nitrogen is less limiting to the phytoplankton in this river, modelling its dynamics reduces model usefulness. Increasing the complexity of the model to include both the DO-BOD and phytoplankton-nutrient cycles (Complexity 5) increases the model's usefulness, but not very substantially when compared to the model complexity in which only the phytoplankton-nutrient dynamics are considered (P-limited Complexity 4).

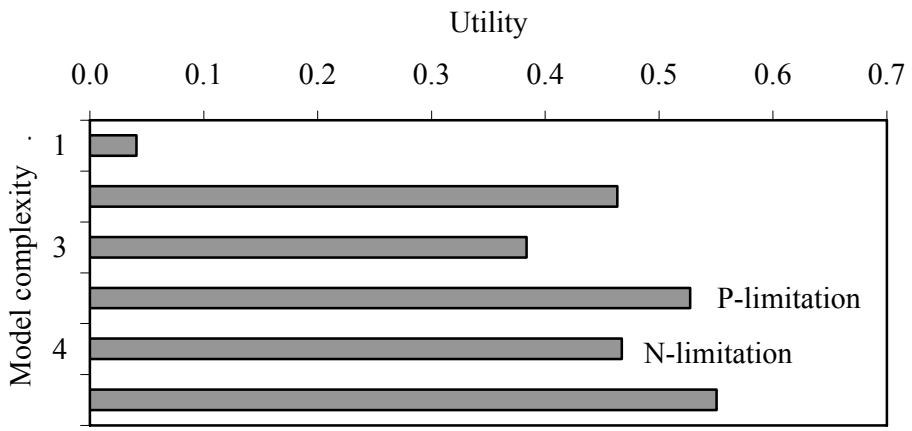


Figure 50: Utility of each model complexity by minimising both sensitivity and error.
(from Lindenschmidt, 2006)

6.4 Scale

The uncertainty analysis with sensitivity and error calculations can be found in Lindenschmidt, Wodrich and Hesse (2006). The complexities versus error and sensitivity curves are shown in Figure 51 for total zinc *ZnT* and its particulate *ZnP* and dissolved *ZnD* fractions. The curves are shown for both scales. In general, the trends for error decrease and for sensitivity increase with increasing complexity. An exception is the error for *ZnD* at the small scale where no particular trend is noticeable.

The errors are generally higher for the model complexities of Calbe than for the Saale River. It appears as if complexity must be increased more for an extrapolated error curve to reach values comparable to values attained by the large scale. The sensitivities are also larger for the model applied on the small scale compared to that of the large scale. However, there is a levelling off of the sensitivities at higher complexities suggesting that there is an upper bound of model sensitivity. Both error and sensitivity

are generally lower for *ZnT* than for the particulate and dissolved fractions. This difference is more pronounced at the larger scale. The modelling exercises confirm the hypothesis by Snowling and Kramer (2001) for both scales. The error and sensitivities tend to shift in relation to complexity at different scales.

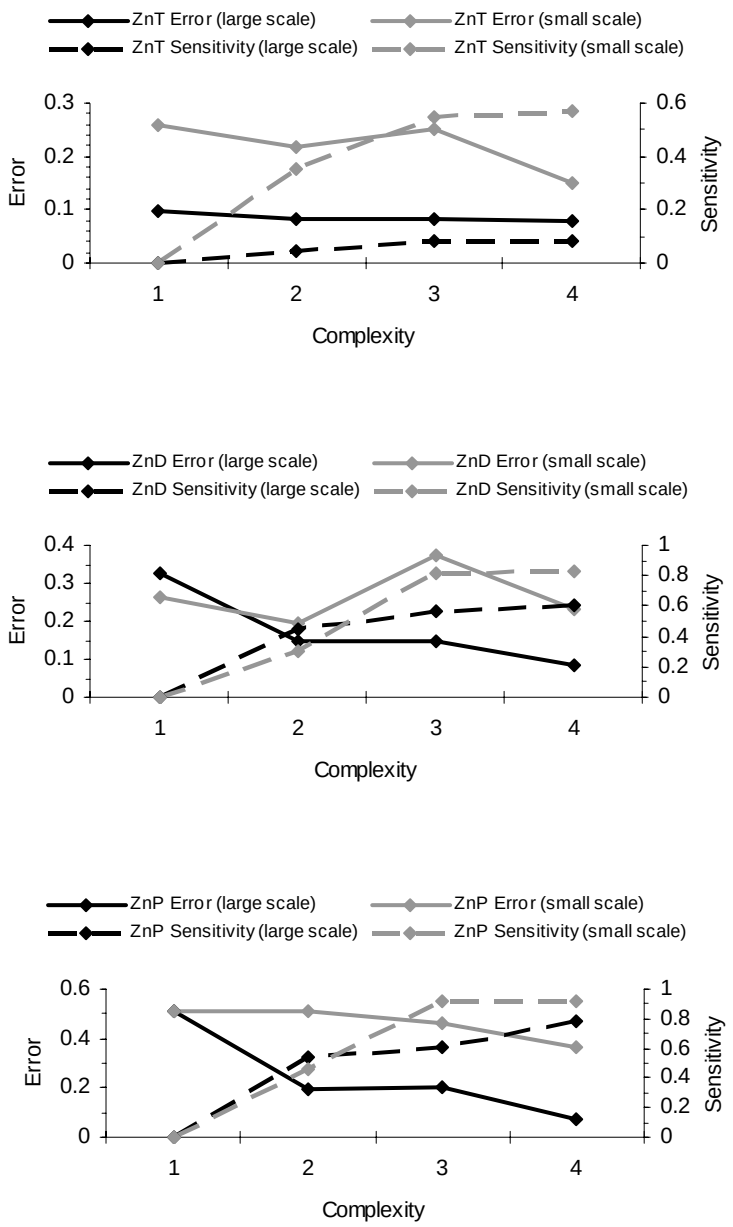


Figure 51: Scale differences: complexity versus error and sensitivity for zinc derived from the Saale (large scale) and Calbe lock-and-weir system (small scale) modelling exercises.
(from Lindenschmidt, Wodrich and Hesse, 2006)

The utility of each complexity is shown in Figure 52 exemplary for the simulation of the total concentration of zinc. The trend of the error with complexity curve was taken for the utility calculation and both error and sensitivity have equal weighting. For both scales, Complexity 2 is the "best" model, for which sorption is a function of the fraction of particulate matter consisting of organic carbon.

Although the more complex models have a larger reduction in simulation errors, predictive ability is diminished. The utility of Complexities 3 and 4 decrease more for the small-scale model and overall, the utility for the large-scale model is higher than for the small scale. Hence, TOXI is best implemented for modelling exercises of large river reaches.

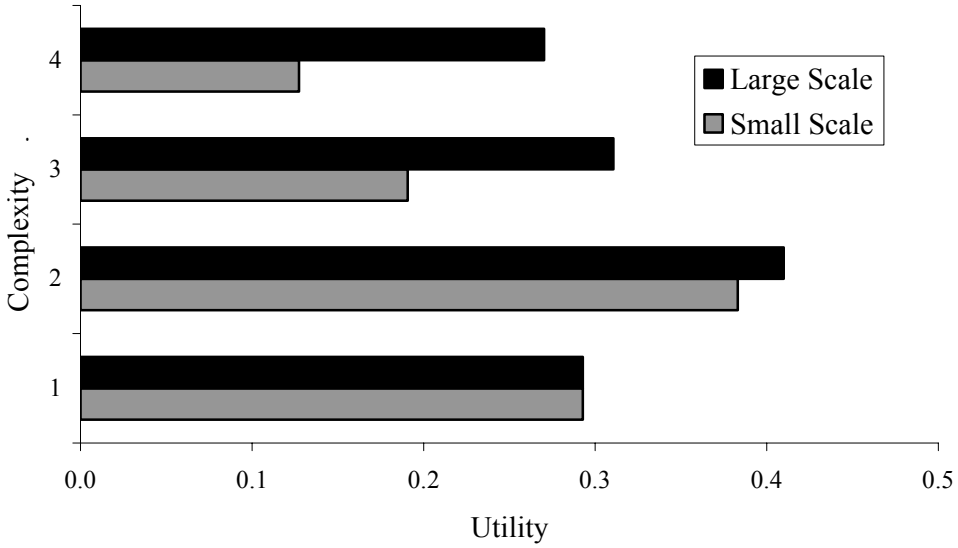


Figure 52: Utility of each model complexity at the two different scales.
(from Lindenschmidt, Wodrich and Hesse, 2006)

6.5 Uncertainty, complexity and scale

The modelling exercises confirm the hypothesis by Snowling and Kramer (2001) for various scales. Greater complexity increased model sensitivity and decreased the error in the output simulations. In a more theoretical framework Cox (1999) also shows that for models used in risk assessment, greater complexity leads to more certainty in risk estimates. He does state, though, that the additional complexity included in the model must allow additional relevant observations to be incorporated. This is the case in our models in which added process complexity is accompanied by substance concentrations that also act as state variables in the model (e.g. the addition of suspended solids and metals concentration for a more complex sorption process).

The error and sensitivities tend to shift in relation to complexity at different scales. Models of smaller scale require a more detailed description of the processes to accurately simulate the state of the modelled area for a given time frame. Sivapalan (2003) mentions that increased complexity is required to capture the hydrological response at the hill slope scale compared to the catchment scale. For example, Butts *et al*. (2004) and Perrin *et al*. (2001) found that hydrological variables modelled for large river basins were more accurately simulated using simpler process descriptions. van der Linden and Woo (2003), who applied models with increasing complexity to simulate hydrological conditions

in subarctic catchments, also found that with decreasing temporal and spatial scale, process representation needs to be more complex.

For the utility calculations, TOXI is more suitable for applications at larger scales (long river reaches) such as developing computer-aided decision support systems for river basin management. On the smaller scale, more processes need to be implemented to acquire the accuracy attained on the larger scale. Moreover, on the small scale, the bottom sediments play a crucial role in the transport of inorganic substances. Hence, more dynamics in substance turnover should be included in the sediment layers differentiating between aerobic and anaerobic zones. For future work on small-scale applications it may be worthwhile to incorporate a geochemical model such as PHREEQC (http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/) into TOXI, which would enable a more differentiated and detailed simulation of the bottom sediment. TOXI could still provide the advective transport of the substances in the overlying water.

6.6 Transferability

The parameter sets for the eutrophication model were almost identical for the lower and middle Saale reaches. There is a high degree of transferability between the two models. A significant exception occurred in modelling a phytoplankton bloom in the middle Saale, which had become dampened once it reached the lower portion of the river. In order to capture the bloom in the simulation very high growth rates needed to be implemented, which are unrealistically high compared to laboratory growth studies but is not uncommon practice by many modellers (Veronique Vandenberghe, pers. comm.). I suspect that the model structure has to be extended to include both the main channel flow and storage zones alongside the main channel. There are many river appendages along the middle Saale in which the water current is very slow compared to the advective current of the main channel. Examples of such areas are shown in Figure 53 for the areas of Planena and Meuschau. These storage zones can be havens for accelerated phytoplankton growth (Reynolds, 1996). A change in the flow conditions, for example a storm event after a period of prolonged low flow, can flush the phytoplankton from these zones and “inoculate” the main channel with a surge of algae biomass (Reynolds, 1995). Nijboer and Verdonschot (2004) also suggest including parameters describing stream geomorphological characteristics into water quality models to capture certain phytoplankton-nutrient dynamics.

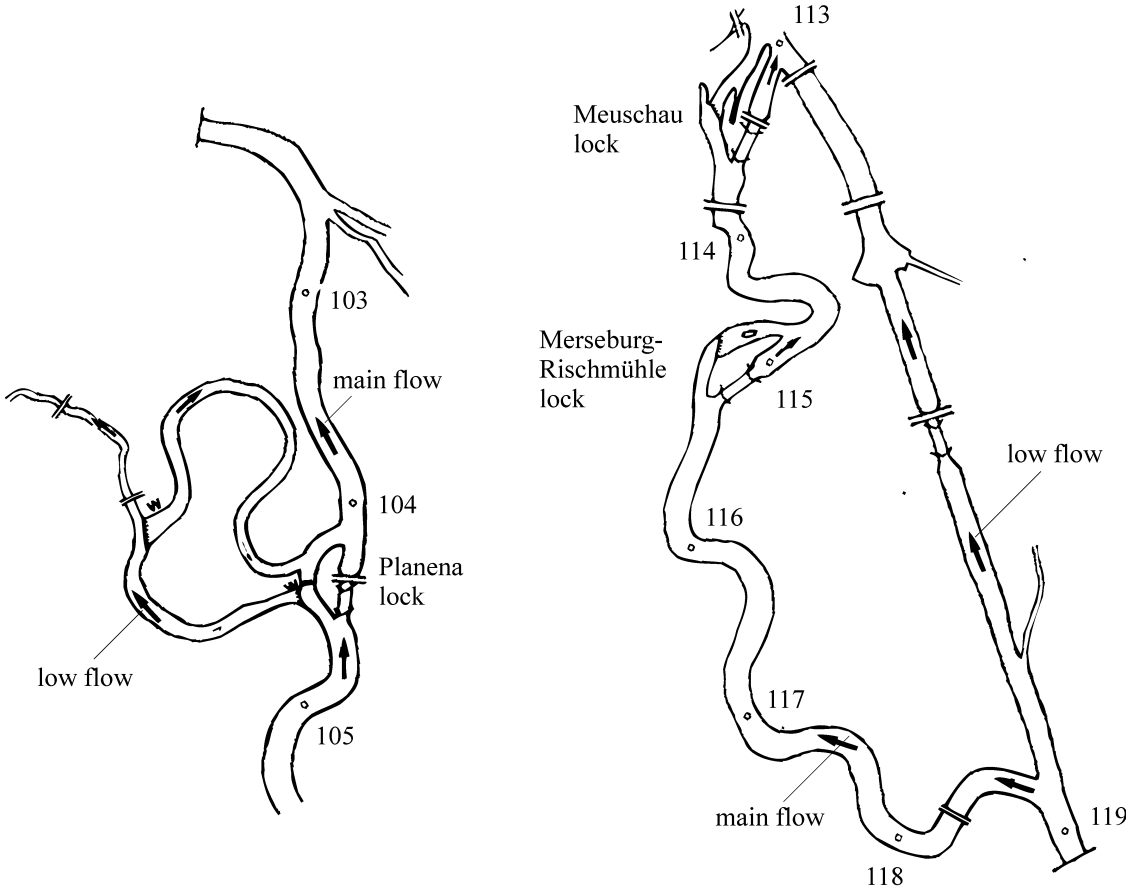


Figure 53: Areas of low and higher (main) flow at the locks at Planena and Merseburg; low flow areas can be havens for exuberant phytoplankton growth.

Table 12 on Page 89 shows the TOXI parameters sets used for simulating suspended solid, arsenic and selected heavy metals, copper, iron and manganese, for the middle and lower Saale reaches. Due to the more advective nature of the middle Saale, its dispersion coefficient D_x is higher than in the lower Saale for suspended solids. The sedimentation rate v_{sed} is higher for the middle Saale due to the higher inorganic to organic ratio in the upstream river sections (Lindenschmidt, Wodrich and Hesse, 2006). The density of inorganic material is larger than organic matter and, hence, sinks more rapidly (Chapra, 1997). The ratio decreases in the flow direction as phytoplankton biomass (organic matter) increases. Substantially more arsenic and less iron is simulated in the bottom sediments of the lower Saale in order to model these substances accurately. The partition coefficient is also more for arsenic and less for manganese in this river section complying with the respective decrease and increase in the dissolved fractions of these metals with flow direction. Copper remained relatively unchanged.

The extension of the Snowling and Kramer (2001) hypothesis (see Figure 3) to test model transferability was applied for copper. Figure 54 shows the error and sensitivity versus model complexity curves for simulations of both the middle and lower courses of the Saale River. The curves for total copper *CuT* and its dissolved *CuD* and particulate *CuP* fractions overlap relatively well. The

accuracy of the middle Saale simulations for *CuD* are improved somewhat, for *CuP* slightly lessened, compared to the lower Saale simulations. However, the curves superpose enough to conclude that TOXI is transferable between the two river courses.

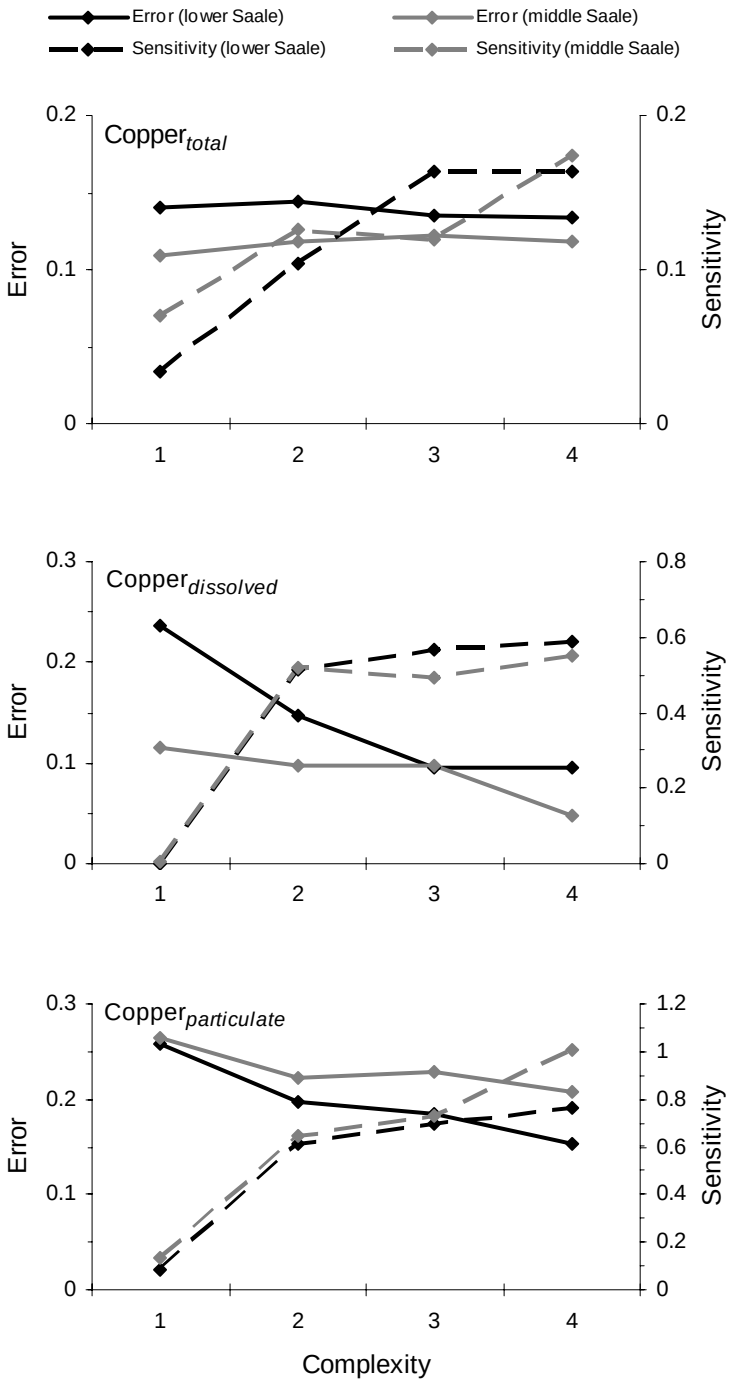


Figure 54: Transferability: complexity versus error and sensitivity for copper derived from the middle and lower Saale modelling exercises.

Table 12: Calibrated TOXI parameters for the middle and lower courses of the Saale River.

Parameter	Units	*Middle Saale*					*Lower Saale*				
		SS	As	Cu	Fe	Mn	SS	As	Cu	Fe	Mn
dissolved	%	0	95	54	4	**29**	0	87	65	10	**62**
D_x	m^2/sec	**10**	0.2	0.2	0.2	0.2	**0.2**	0.2	0.2	0.2	0.2
D_y	m^2/sec	$\mathbf{10^{-5}}$	10^{-4}	10^{-4}	$\mathbf{10^{-4}}$	10^{-4}	10^{-4}	10^{-4}	10^{-4}	10^{-5}	10^{-4}
v_{sed}	m/d	**0.5**	0.2	0.2	0.2	0.2	**0.2**	0.2	0.2	0.2	0.2
v_{res}	m/d	10^{-5}	10^{-6}	10^{-5}	10^{-5}	10^{-5}	10^{-5}	10^{-5}	10^{-5}	10^{-5}	10^{-5}
c_{sed}	mg/L	1.2×10^6	**0.0018**	50	**20000**	50	10^6	**50**	50	**50**	50
K_D	L/mg		**2000**	31275	10^6	**70000**		$\mathbf{10^4}$	40000	10^6	**50000**

6.7 Morphological parameter effects on hydrodynamic and water quality variables

The DYNHYD → EUTRO/TOXI coupling using HLA was required for this investigation. Figure 55 shows the variations in the mean daily water stages at the lower gages of the weirs in Halle and Calbe for the 14 day calibration time span. The 5% and 95% percentiles stem from a Monte Carlo analysis (MOCA) of 2000 simulations extracting α (weir discharge coefficient) and *n* (roughness coefficient) randomly from a normal probability distribution for each 14-day simulation. The largest variation is obtained at the lower gages of each weir, which is primarily due to the variation in *n* (von Saleski, *et al.*, 2004). The upper gage water stages are most sensitive to the parameter α but the range of possible α values used in the Monte Carlo analysis was too narrow to have caused a large uncertainty in these water levels.

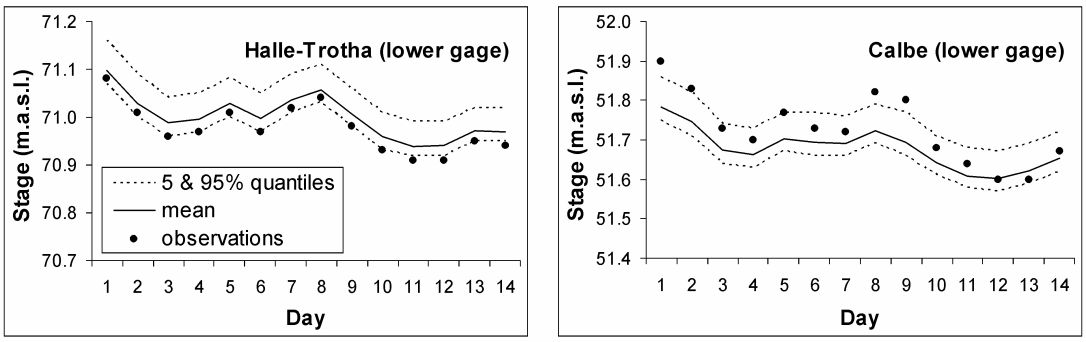


Figure 55: Water levels of gages downstream from the weirs at Halle-Trotha and Calbe.
(from Lindenschmidt, Poser and Rode, 2005)

Figure 56 shows the results of the MOCA analysis for three eutrophication variables, *Chl-a*, *DO* and NH_4^+-*N* based on the uncertainty of the hydrodynamic parameters α and *n*. The variation in the output

distributions increased with distance along the flow direction of the river course. An exception was the backwater immediately upstream from weirs where little variation occurred. Uncertainty in the observed data is larger than the hydrodynamic data. This is due to the larger analytic error and to the error in sampling. The latter is particularly sensitive to the time of day when the sample was taken and the location in the river where sampling occurred.

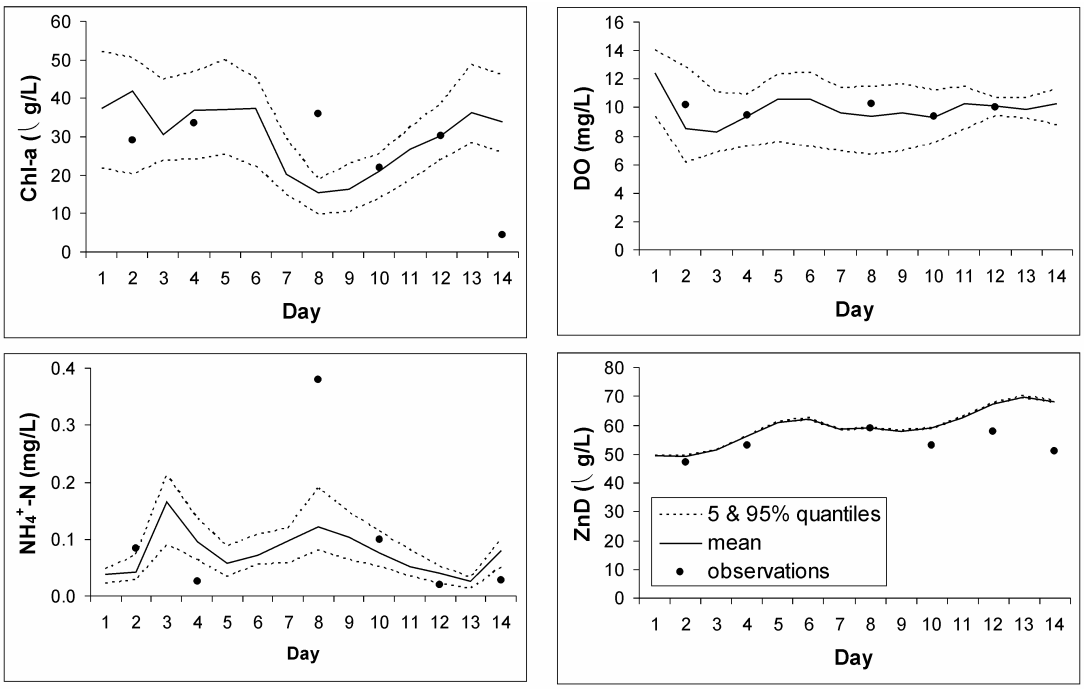


Figure 56: Selected water quality constituents at Groß Rosenburg.
(from Lindenschmidt, Poser and Rode, 2005)

The best fit between simulations and observations was obtained for *DO*. Oxygen reaeration is calculated from the hydrodynamic variables (flow velocity and water depth) and the oxygen deficiency from its saturated concentration in water. Since the water was well saturated with oxygen during the time of sampling, little effect will be observed in the *DO* concentrations due to varying α and *n*. The variation observed here is due to the variation in chlorophyll-a concentrations, evident in the high oxygen values (> 10.5 mg O_2/L) within the 90% probability bounds. The effect of hydrodynamic parameters on *DO* becomes more pronounced as the oxygen deficit in the water becomes larger and the phytoplankton growth diminishes.

MOCA enabled a marked improvement in the calibration for NH_4^+-*N* to be made. The first peak at Day 3 is due to a surge load at Day 1 into the most upstream portion of the reach at Halle. Sampling was carried out at most every two days and, unfortunately, an observation of the surge at Groß Rosenburg was missed. The surge is, however, verified at other upstream sampling points along the river. The second peak on Day 8 is due to the mineralization of particulate organic nitrogen *ON* produced by the strong algal growth prior to this day. The growth of phytoplankton is also reduced so

that fewer nutrients are being taken up by the algae. Ammonium analyses are also prone to large uncertainties (max. ± 3%), hence the numerous observations that lie outside of the 90% bounds of the simulation distributions. This peak could only be captured after the MOCA analysis was carried out.

The hydrodynamic parameters had little effect on the TOXI variables, as shown exemplary for dissolved zinc *ZnD* in Figure 56. This is primarily due to the fairly steady discharge conditions between mean flow and mean low flow. It is suspected that the variations will increase during floods, which is a focus of future work.

6.8 Boundary discharge effects on hydrodynamic and water quality variables

The MOCA with the normal distributed parameter settings was repeated and extended with a normal distribution setting of the variation in the flow discharges at the boundaries. Flows are calculated from current velocity profiles along the cross-section of the river and the main sources of error in the calculations are (Herschy 1995, p. 453ff):

i) current meter reading (up to ±4%; personal communication of the Waterways and Navigation Bureau, Magdeburg, Germany),
ii) mean flow calculations using a velocity-area method (up to ±4%) and
iii) stage-discharge relationship (up to ±2%).

Assuming the co-variance between the errors is negligible, a maximum error range of up to ±10% can occur in the discharge input data. This error range is justified when comparing the flows calculated from the Calbe gage which those calculated from the gage at Calbe-Grizehne, which is three kilometers downstream from Calbe (see Lindenschmidt, Rauberg, *et al*., 2005). There are no significant water withdrawals or emissions between the two locations, but deviations between the two gages fluctuate between −10% and +10%. For each MOCA run, every discharge value was incremented or decremented with a deviation selected from a normal distribution (mean = 0.0; range from −0.1 to +0.1; standard deviation = 0.05, which corresponds to the distribution have approximately 90% of the values lying within the range). An example of the variations around the input data is shown for the flow boundary at the confluence in Figure 57. Each box-whisker bar represents the 1500 data values used for the Monte Carlo runs.

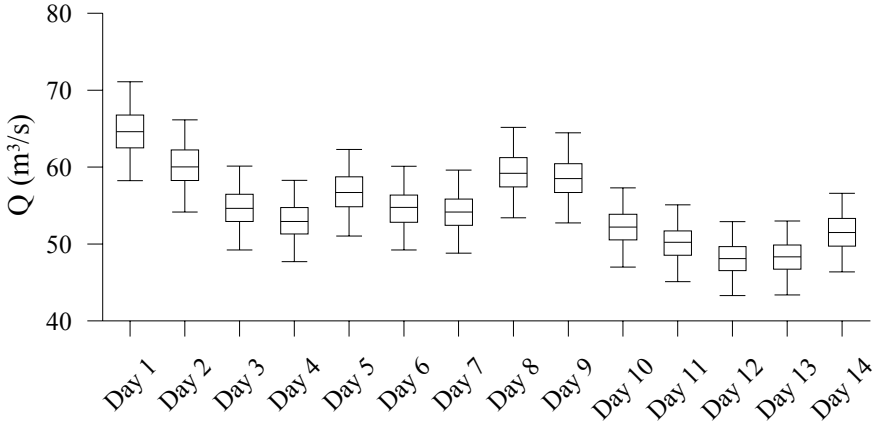


Figure 57: Up to ±10% variation in the boundary discharges (exemplary for the confluence).
(from Lindenschmidt, Rauberg, et al., 2005)

The means of the distributions of the hydrodynamic output variables discharge *Q*, velocity *U* and depth *d* remained approximately the same, when compared to the parameter-only MOCA (see Figure 58). The standard deviations, and hence the coefficient of variations, approximately doubled for all these variables of the upper gage at Calbe, which is to be expected since more factors are now being varied in the model to cause a large range in the output variables. For the lower gage, only the CV for *Q* doubled with the CVs of *U* and *d* remaining unchanged. This indicates the buffering potential the weirs have on the flow variation of the boundaries on current velocity and water stages as water flows through the system.

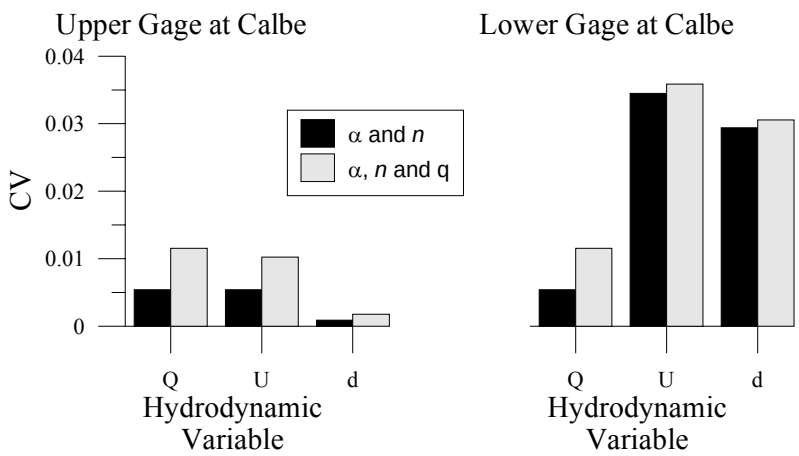


Figure 58: Coefficient of variation *CV* of hydrodynamic variables (discharge *Q*, velocity *U*, depth *d*) for parameter-only (α & *n*) MOCA and MOCA with parameter and boundary discharge variation *q*.

The means of the distributions for all the EUTRO variables also remain approximately the same for both gages at Calbe. An exception is the reaeration coefficient k_2 with a slight decrease of 7% for the upper gage. Surprisingly, all CVs decrease at both gages by as much as a factor of two for all the variables with the exception of NH_4^+-*N*, whose CV increased by a factor of ten (see Figure 59). This is primarily due to the input of the Bode river, the largest and most immediate upstream tributary from the Calbe weir, has a diluting effect of the river water, since its concentrations of most of the sampled

substances are lower than in the Saale River. The exception is ammonium, which has concentrations up to five times of those found in the Saale. Hence, dilution of substances will decrease the deviation of the simulated output distributions; concentrating will increase the deviation.

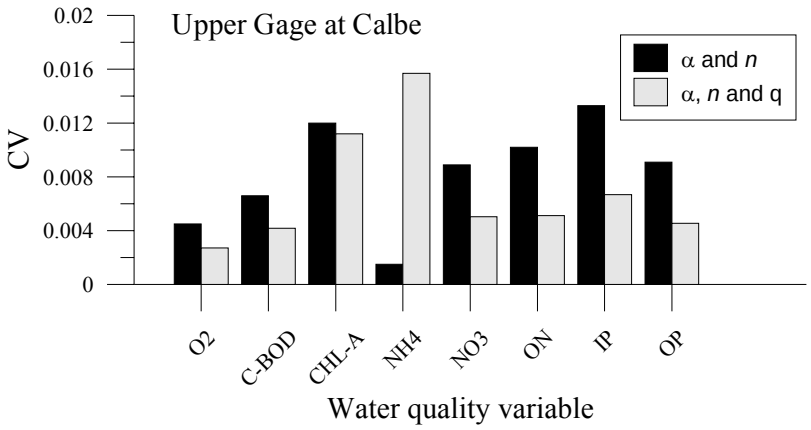


Figure 59: Coefficient of variation *CV* of water quality variables for parameter-only (α & *n*) MOCA and MOCA with parameter and boundary discharge variation *q*.

6.9 Interactive model coupling and uncertainty

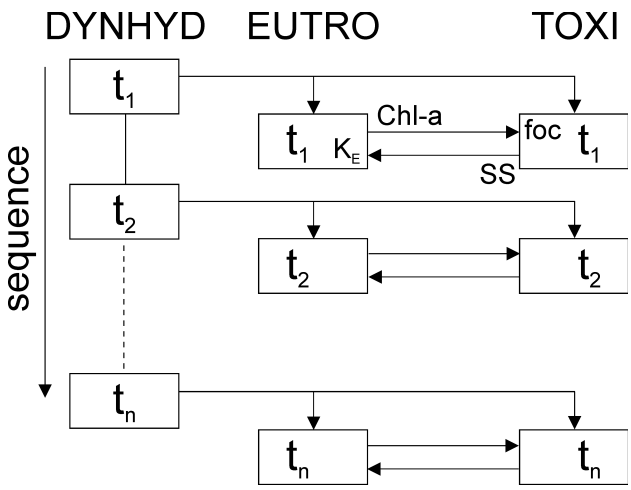


Figure 60: Interactive coupling between EUTRO and TOXI in the HLA environment; hydrodynamic data is still received by the two models from DYNHYD after each time step.
(from Lindenschmidt, Hesser, et al., 2005)

Coupling EUTRO and TOXI together in the HLA environment allows ease of interactive communication between the two models (Figure 60). Chlorophyll-a concentrations *Chl-a* correlate well with particulate organic carbon *POC* content in the water (Figure 61) and brings forth the structure for the EUTRO → TOXI coupling using the equation:

$$POC = 0.04 \cdot Chla + 1.4$$

By dividing *POC* with the concentration of suspended sediment *SS* simulated in TOXI, the weight fraction of organic carbon in suspended matter (*foc*) is obtained [Ambrose *et al*., 1993, Chapra, 1997]:

$$foc = \frac{POC}{SS}$$

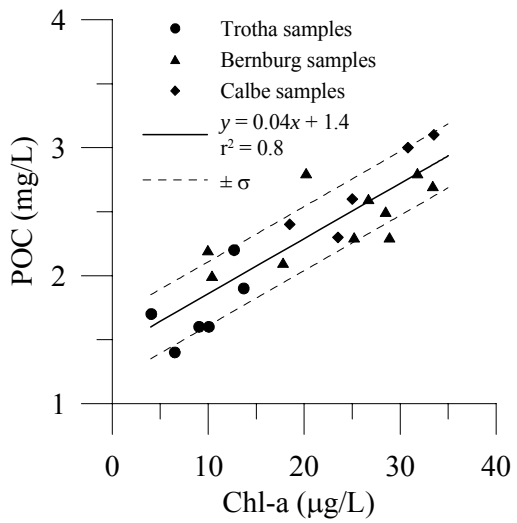


Figure 61: Correlation between chlorophyll-a *Chla* and particulate organic carbon *POC*.

The partitioning of heavy metals *M* in the water can now occur between the dissolved phase M_{DIS} and the organic carbon of the particulate phase M_{OC} using the partition coefficient K_{OC}

$$K_{OC} = \frac{K_D}{foc}$$

This is an extension of the simplified partitioning of heavy metals between the dissolved and total particulate fractions of heavy metals (M_{DIS} and M_{PART}) using the partition coefficient K_D:

$$M_{DIS} = \frac{1}{1 + K_D \cdot SS} \qquad M_{PART} = \frac{K_D \cdot SS}{1 + K_D \cdot SS}$$

Information is also transferred from TOXI to EUTRO. In the original WASP5 version, the extinction coefficient K_E of light passing through the water column is a constant parameter implemented for each discretized unit of the modelled river. With the communication between TOXI and EUTRO, K_E can now vary depending on *Chl-a* (µg/l) and phytoplankton biomass *Phyto* (mg/l) computed in EUTRO and *SS* (mg/l) calculated in TOXI [equation modified from Schöl, *et al*., 2002]:

$$K_E = 0.052 \cdot (SS - Phyto) + 0.013 \cdot Chla + 1.06$$

The coupling was tested using EUTRO Complexity 5 and TOXI Complexity 2 with zinc as the micro-pollutant. The simulations were supported by the data from the 5. – 18. June 2001 sampling campaign

of the lower Saale River. Through the coupling an improvement in model results was gained, especially for dissolved fractions of zinc at Calbe (see Figure 62). The decrease in dissolved zinc concentrations corresponds to an increase in the particulate concentrations. Overall the coupling allowed a more accurate balance between dissolved and particulate fractions in the sorption process. The effect of the coupling becomes more significant with increasing downstream distance, hence the deviations in the metal fraction concentrations between uncoupled and coupled simulations are more pronounced at Calbe than at Bernburg.

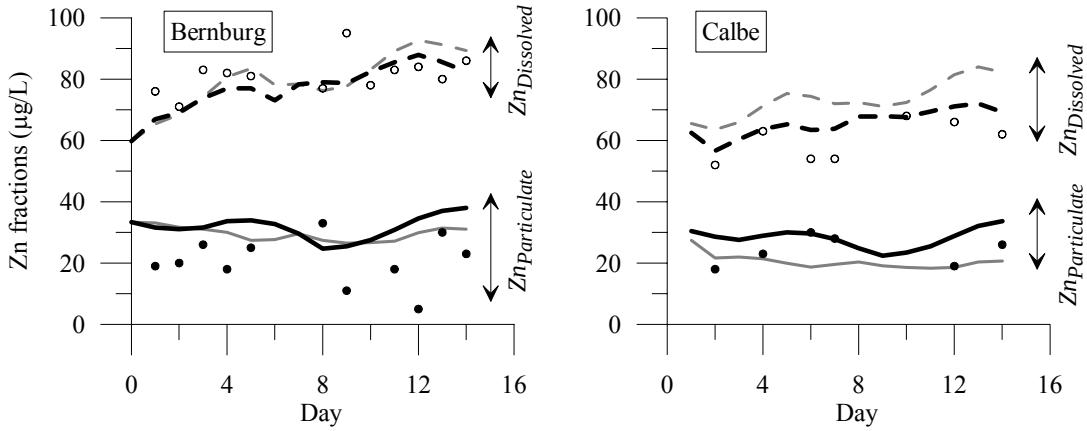


Figure 62: Comparison for dissolved and particulate zinc concentrations between uncoupled (grey lines) and coupled (black lines) simulations at sampling stations Bernburg and Calbe. Points are sampled values (unfilled – dissolved zinc; filled – particulate zinc fraction).

A Monte Carlo Analysis (MOCA) was also carried out for both the uncoupled and coupled model system configurations by varying the hydrodynamic coefficients α (weir discharge) and *n* (river bottom roughness)Each MOCA consisted of 500 runs in with α and *n* were randomly selected from uniform distributions each varying ±18% from their respective mean values. The ranges for the simulated variable values increased through the coupling by as much as 7% for dissolved oxygen and 13% for chlorophyll-a (see Figure 63). The range also increased also for dissolved zinc concentrations (+10%) but decreased for the particulate concentrations (-13%) (see (a) in Figure 64). Uncertainties propagating through a system of coupled models are affected by the uncertainties in the process reactions, in this case sorption of dissolved substances along the river coarse and increased sedimentation of particulate substances at the locks and weirs.

The equation which couples EUTRO to TOXI gives opportunity to investigate structural uncertainty in modelling systems. Figure 61 shows the uncertainty in the *POC* versus *Chl-a* correlation and can be implemented in regression equation as:

$$POC = 0.04 \cdot Chla + 1.4 \cdot (1 \pm \sigma)$$

where σ is the standard deviation. Signorino (2003) labels the additional term the uncertainty due to regressor error.

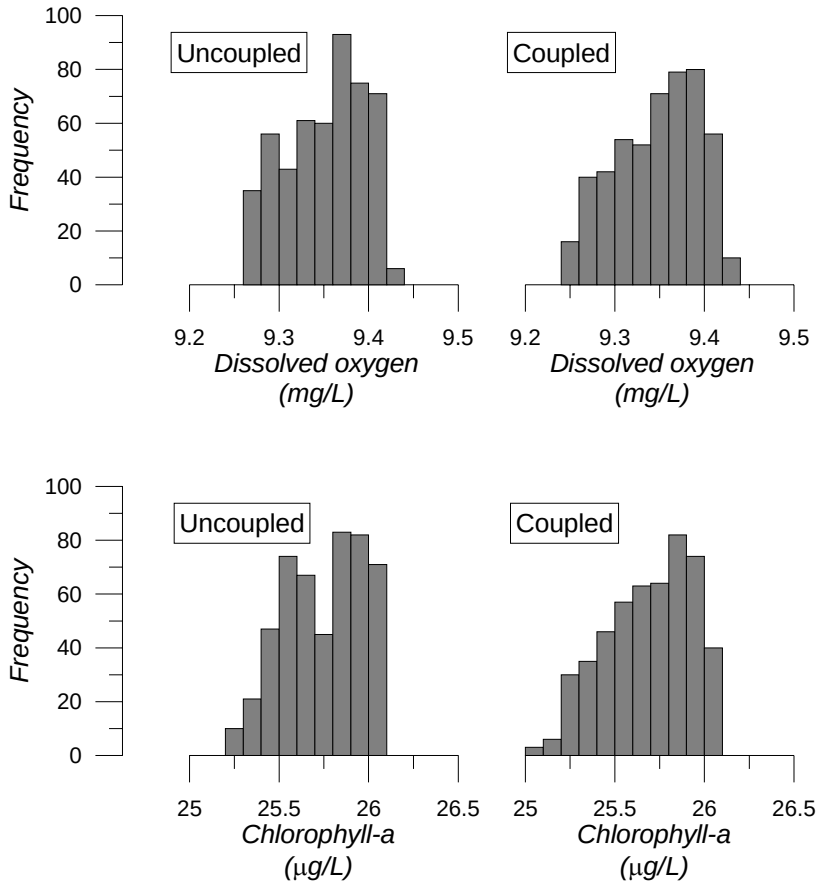


Figure 63: Distributions of dissolved oxygen and chlorophyll-a from MOCA considering only parameter uncertainty for both uncoupled and coupled model system configurations.

A MOCA was carried out for zinc using three configurations of the source of uncertainty: i) parameters only, ii) parameters and boundaries and iii) parameters, boundaries and model structure. As previously in Section 6.8, the boundary discharge varies within the range ±10%. For the *POC* vs. *Chl-a* regression curve ±σ corresponds to a range variation of ±18%. TOXI results are summarized in Figure 64 for the Calbe station which shows that the most significant uncertainties for the dissolved and particulate zinc fractions are found in the model system structure, followed by parametric uncertainty and for a minimal extent, uncertainty stemming from boundary conditions. The uncertainty for total zinc stems solely from the parameter sources and is not influenced by boundary or structural uncertainty.

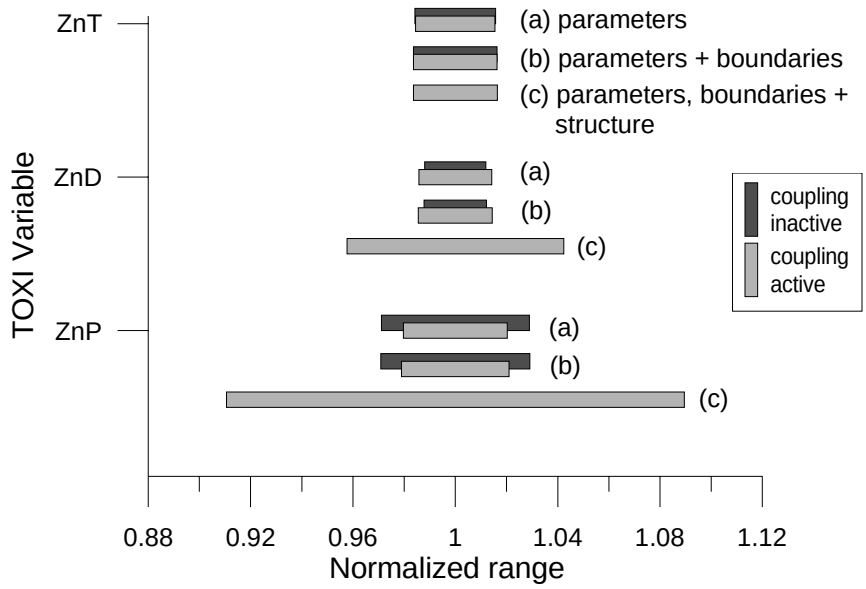


Figure 64: Ranges from MOCA normalized to the mean for selected TOXI variables; uncertainties stem from (a) parameters only, (b) parameters and boundaries and (c) parameters, boundaries and model structure.

Structural uncertainty was also introduced in the equation for the TOXI → EUTRO coupling by introducing a regression error term in the coupling equation:

$$K_E = 0.052 \cdot (SS - Phyto) + 0.013 \cdot Chla + 1.06 \cdot (1 \pm \sigma)$$

however with little effect, due to the equation's low sensitivity on EUTRO variables. ?? shows the uncertainty range for dissolved oxygen, chlorophyll-a and ammonium using the same MOCA configuration as for zinc and shows that the source of uncertainty is in the following order of decreasing significance: parameter, boundary and structure. Comparison of the uncertainty ranges in Figures ?? and ?? indicates that parameters and boundary conditions are a more important source of uncertainty for EUTRO variables whereas model system structure is the most significant source of uncertainty for TOXI variables.

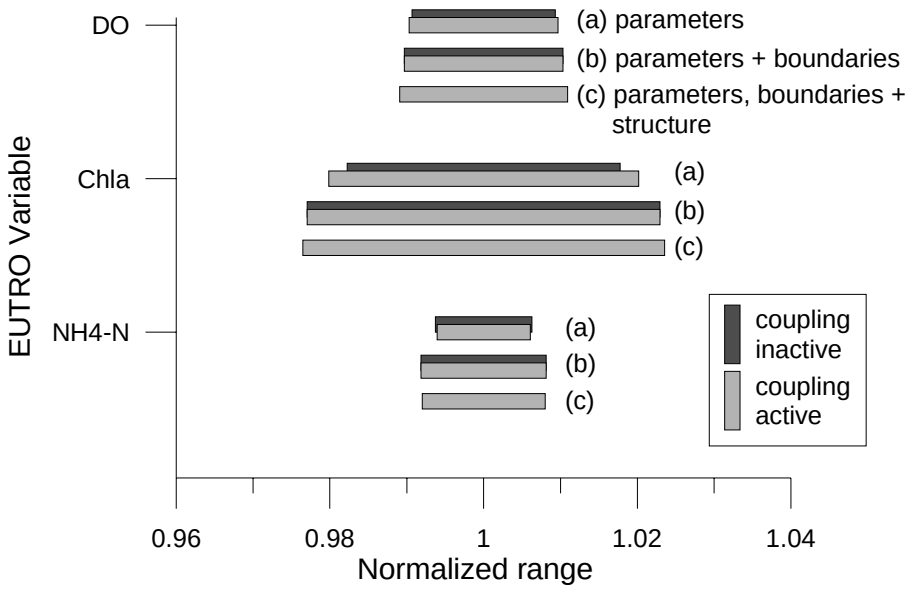


Figure 65: Ranges from MOCA normalized to the mean for selected EUTRO variables; uncertainties stem from (a) parameters only, (b) parameters and boundaries and (c) parameters, boundaries and model structure.

Models may act as filters and reduce uncertainty, which has been confirmed by Refsgaard, *et al*. (1998). They found that the uncertainties of their integrated model are less than those of the individual models due to two reasons: "i) in the integrated model the internal boundaries are simulated by neighbouring model components and not just assessed through qualified but subjective estimates by the modeller and ii) the integrated model makes it possible to explicitly include more sources of data in validation tests that can not all be utilised in the individual models" (Refsgaard, *et al*., 1998, p. 462). I found that uncertainty propagated through a chain of coupled models can either accentuate or diminish depending if the substances are respectively being concentrated or diluted and their process description.

6.10 Influence of locks and weirs

Lindenschmidt, Eckhardt, *et al*. (2004) found that locally on the small scale locks and weirs influence the transport of both suspended solids and the total concentrations of most heavy metals substantially. This is particularly due to the large differences in the mean velocities between the various areas in the lock-and-weir system. Increased sedimentations immediately upstream from the weir and higher resuspension rates downstream from the weir were modelled. Also, for this particular lock the low flow conditions led to more sedimentation of solids than elsewhere in the system. On the larger scale for the lower Saale River and for similar low-flow conditions the lock-and-weir systems have little effect on the suspended solid concentration. The simulations agree well with the measurements without having to include higher sedimentation rates in the upstream areas of the weirs. This is contrary to the total zinc concentration for which higher sedimentation rates need to be included for

the simulations to coincide with sampled values. Hence, two processes exist which counteract each other:

i) large particulate zinc fraction (mostly inorganic) that is formed immediately downstream from the large emission of dissolved zinc from the Schlenze tributary settles out and causes a lose of suspended solids and

ii) inorganic solids that are settled out reducing the water's turbidity allowing an increase in phytoplankton growth which replaces the settled inorganic fraction of the suspended solids.

The chlorophyll-a and particulate organic carbon (*POC*) both increase in the flow direction in the Saale. The increase of the ratio of organic to inorganic material along the river's course is also confirmed in Lindenschmidt, Wodrich and Hesse (2006), in which both the weight fraction of the total carbon in the solid material (f_{OC}) and the loss-on-ignition increase in the flow direction along the Saale from Wettin to the Saale confluence.

6.11 Influence of morphology

A comparison is made in Figure 66 between the effects:

i) the two hydrodynamic parameters have on water quality variables,

ii) the four most identifiable water quality parameters have on these variables (see Schlehf and Lindenschmidt, 2005) (the most identifiable parameters are the parameter combination which is most sensitive to the system as a whole and has the least dependency and co-linearity between them (Reichert and Vanrolleghem 2001)); and

iii) all 21 water quality calibration parameters have on these variables (see Schlehf and Lindenschmidt, 2005).

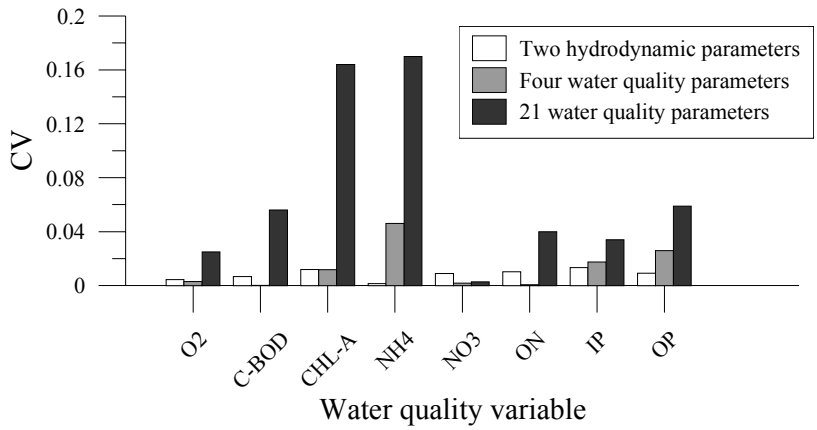


Figure 66: Coefficient of variation *CV* of the water quality variables for three Monte Carlo analyses by varying only the: i) two hydrodanamic parameters, ii) four of the most identifiable water quality parameters and iii) all 21 water quality parameters used for calibration
(modified from Lindenschmidt, Rauberg, et al., 2005)

For most variables, there is an increasing trend in the coefficient of variation (CV) when more parameters are implemented in the Monte Carlo analysis (MOCA). This is due to the increase in the number of varying parameters in the model which leads to an increased spread in the distributions of the simulated results. An exception is nitrate due to the very high NO_3^-N concentrations (> 4 mg/l) found in the water. Hence, this substance reacts more to the water transport than to biological factors. Little reaction was found in the *C-BOD* and *ON* variables when using only the four most identifiable parameters for the MOCA. The parameters influence *C-BOD* and *ON* are only sensitive to these variables and are not very identifiable to the system in its entirety.

The variability in O_2 and *Chla* is approximately the same for the MOCA using the four identifiable water quality parameters and the MOCA using the two hydrodynamic parameters. Hence, uncertainty in the hydrodynamic parameters can contribute a significant amount of uncertainty in the water quality modelling. This implies that the parameters characterising the morphology of the river can contribute almost as much variability in the water quality constituents as the biological factors. This shows the significant impact morphological effects may have on the water quality of a river this size.

Figure 67 shows a comparison between the Saale (5th Strahler stream order) and Weiße Elster (4th Strahler stream order) of the ranges in the variable distributions resulting from MOCAs in which only the roughness coefficient n was varied (Saale: $0.022 < n < 0.030$ s/m$^{1/3}$; Weiße Elster: $0.025 < n < 0.035$ s/m$^{1/3}$). The ranges have been normalised to the mean value. The variation of chlorophyll-a *Chla* is larger for the Weiße Elster than for the Saale. Hence, morphological effects pertaining to bed roughness has a larger impact on the smaller river (lower order) than on the larger. This is largely due to the larger variation in flow velocity although the discharges remained fairly steady in both cases (Saale: $56.5 < Q < 58.5$ m^3/s; Weiße Elster: $5.0 < Q < 5.1$ m^3/s). Phytoplankton gives preference to ammonium for their nitrogen source causing the largest effect on this substance in comparison to other nutrients.

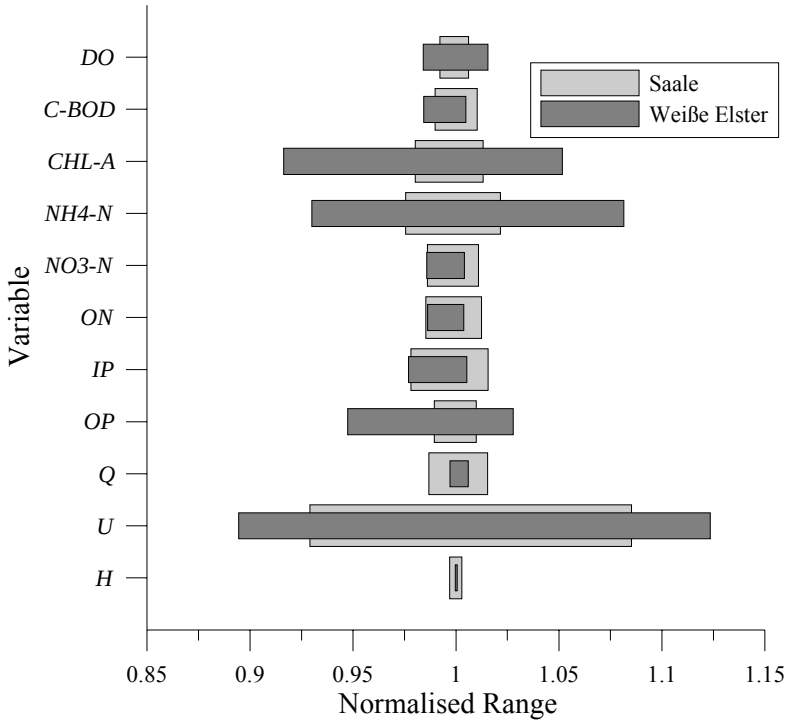


Figure 67: Normalised ranges of the simulated hydrodynamic and water quality variables for the two rivers Saale and its tributary Weiße Elster.
(modified from Wagenschein, Lindenschmidt, et al., 2005)

6.12 Effects of weirs in the Saale on water quality (two scenarios)

Locks and weirs are often required in rivers to make them navigable for shipping. Backwater increases the volume of water in the river and decreases the longitudinal slope of the river bed, two important aspects to enhance ship travel. There are, however, many implications on the ecological status of the river and its riparian areas. Water velocity is reduced which reduces aeration at the water surface. Sedimentation is augmented due to the slower currents. The clearer water allows deeper impingement of solar radiation through the water column and an increase in water temperature, which in turn accelerates biological activity. Hence, backwaters can become havens for phytoplankton. The sediment load also finer grainer causing backwater areas to silt up. The corresponding bottom sediments become more susceptible to anoxia promoting nutrient redissolution. This accelerates phytoplankton growth, which can become exuberant. The flow regulation also has detrimental effects for flood plains but this was not investigated in this study.

Two scenarios are presented to investigate the effects locks and weirs have on the water quality of the Saale River (for details see Sonnenschmidt *et al*., 2003):

i) insertion of a lock-and-weir system at Klein Rosenburg (Saale-km 5). The slope of the reach between the most downstream lock-and-weir system at Calbe and the confluence is still too steep to guarantee year-round navigation for 1000 tonne ships. This hindrance would be alleviated with this additional regulating structure but the damming may deteriorate the river's water quality

ii) removal of the three weirs in Weißenfels (between Saale-km 142 and 148). This has been proposed in order to improve flood defence in this region (DDC, 1996). The simulations are to check if the negative effects of weirs on the river's water quality are amended.

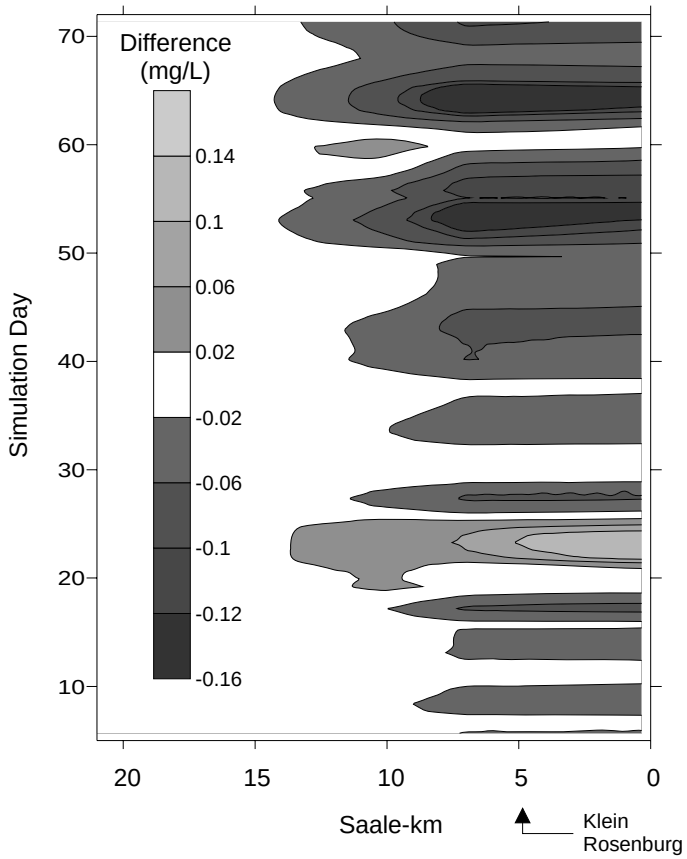


Figure 68: Differences in dissolved oxygen concentrations (with weir – current state) through additional flow regulation at Klein Rosenburg.

The simulations for the first scenario were carried out using the Lower Saale model for the time frame 14. May – 30. July 2002. Figure 68 shows the differences in the dissolved oxygen results between simulations with and without the lock-and-weir system at Klein Rosenburg. Positive(negative) values correspond to an increase(decrease) in oxygen concentrations due to the additional flow regulation. The largest differences occurred for oxygen (maximum ±1.5%) and chlorophyll.a (maximum ±4%) which may be due to the very advective nature of this simulated year. Sonnenschmidt *et al*. (2002) also show that for very low flow conditions the oxygen content decreased by 7% (see Figure 69).

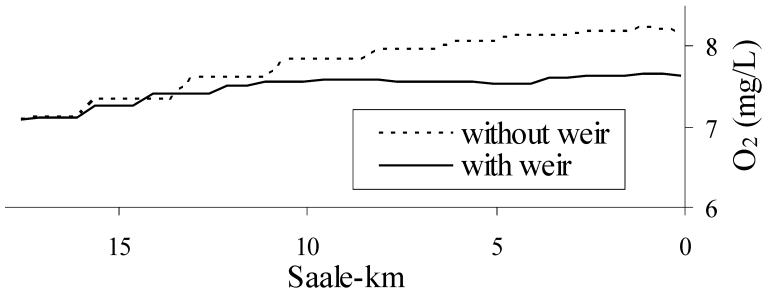


Figure 69: Reduction in dissolved oxygen at low flow conditions due to addition insertion of a lock-and-weir system at Klein Rosenburg (Saale-km = 5) using the model QSIM.
(modified from Sonnenschmidt et al., 2002)

The second scenario indicates that removal of the three weirs at Weißenfels has only a minute effect on the dissolved oxygen, phytoplankton and nutrient content in the river. Figure 70 shows for the 1999 simulation time frame (refer to Table 7) a total decrease of 2 % in inorganic phosphorus concentrations when the weirs are removed. A decrease in oxygen content no more than 1% was found by Sonnenschmidt *et al*. (2002) for a simulation with high discharge.

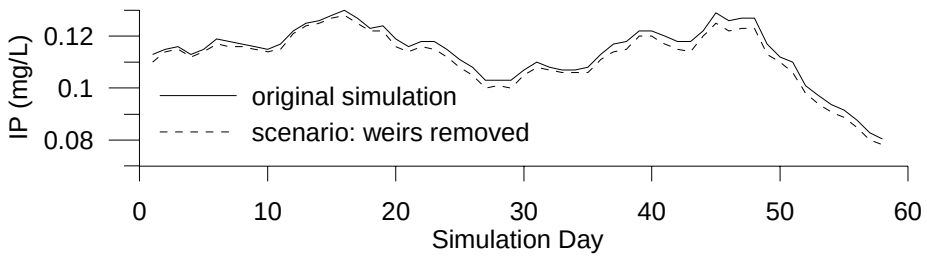


Figure 70: Reduction in inorganic phosphorus at Bad Dürrenberg due to the removal of the three weirs at Weißenfels.

6.13 Reduction of nutrient loading (scenario)

Much effort has been carried out in the past ten years to reduce the point loading along the Saale River. As shown in Figure 26 most wastewater from communal wastewater treatment plants undergoes secondary and tertiary treatment (reduction in nitrogen and phosphorus). However, the nutrient concentrations in the Saale are still high, stemming primarily from non-point sources (Behrendt *et al*., 2001) and to a lesser degree some persistent point loading from industries (e.g. phosphorus from Bernburg in Figure 26), and not limiting to phytoplankton growth. Hence, a scenario is simulated in which the nutrient concentrations at the boundaries (non-point source) are reduced by half which is perceived as a best-case scenario. Such a reduction is reasonable and coincides with scenario calculations found in the literature. Vache *et al*. (2002) could potentially reduce nutrient loads by 54 to 75% through substantial changes in agricultural practices (e.g. conversion to conservation tillage, strip intercropping, rotational grazing and setting aside conservation areas) and use of best management practices (e.g. implementing riparian buffers, engineered wetlands, filter strips and field borders). By

improving sewage treatment, setting aside 20% of arable land and rehabilitating certain river reaches Kronvang *et al*. (1999) deemed a 53% reduction in nitrogen and 46% reduction in phosphorus as reasonable for scenario simulations. Additional options include increasing organic farming, extensivation of grassland production and re-wetting riverside areas are considerations made by Kersebaum *et al*. (2003) for the Elbe river catchment.

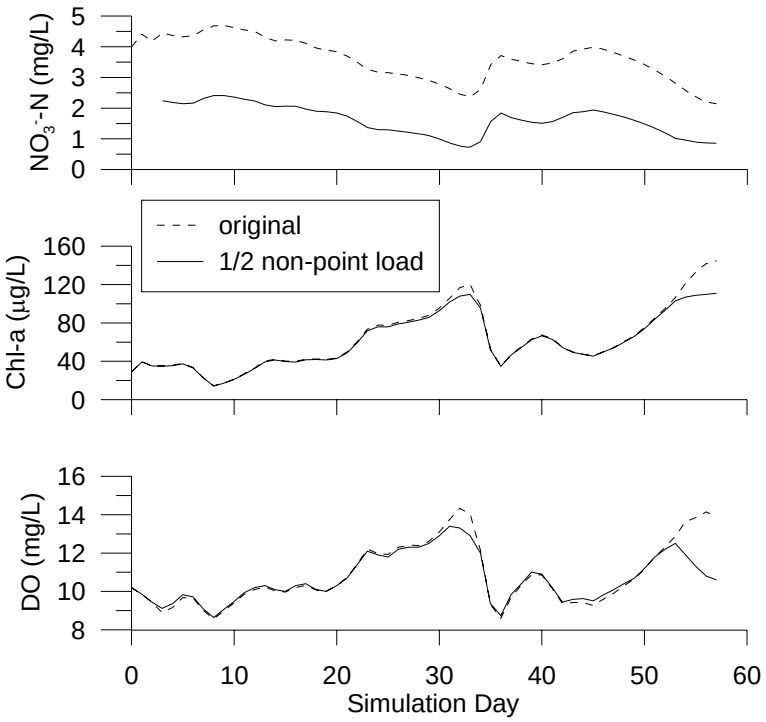


Figure 71: Scenario 2001: the effect of a 50% reduction in non-point nutrient loading on nitrate NO_3^--*N*, chlorophyll-a *Chl-a* and dissolved oxygen *DO* at Groß Rosenburg.

The scenario was carried out using both the 2001 and 2002 validation simulations of the Lower Saale River (see Table 7). In both cases the nitrate, ammonium and inorganic phosphorus concentrations at the boundaries were halved. The results for nitrate, chlorophyll-a and dissolved oxygen for the 2001 simulation are shown in Figure 71. A significant decrease in the latter two is attained only between the 30th and 34th simulation days and the last five days of the time period. In general, the aquatic environment of the Saale is light limited but on these days, the nutrient concentrations are low enough to induce nutrient limitation of phytoplankton growth (see Figure 72).

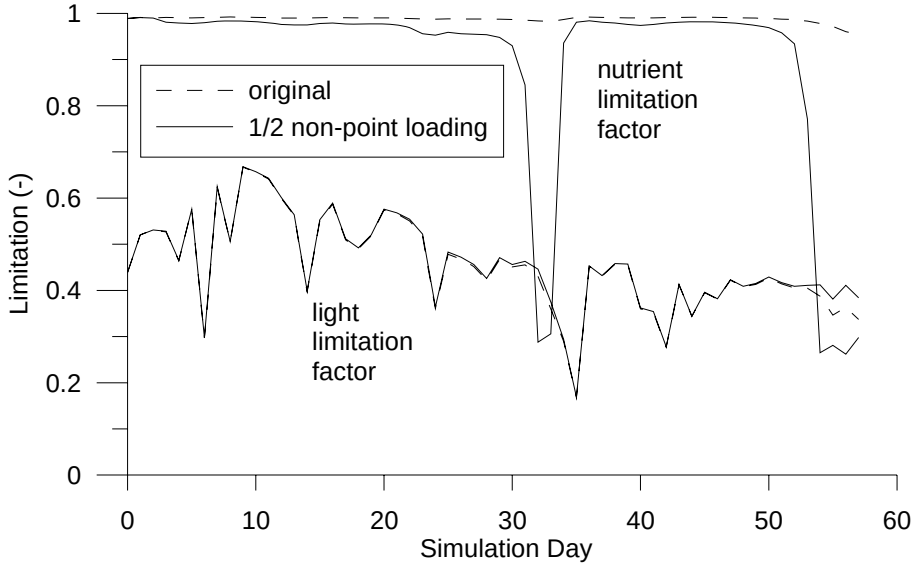


Figure 72: Nutrient and light limitation at Groß Rosenburg during the 2001 simulation time period for the original state and for a 50% reduction in non-point nutrient loading.

Nutrient limitation also occurs between the 18th and 25th simulation days of the 2002 scenario, results of which are shown for inorganic phosphorus *IP*, chlorophyll-a *Chl-a* and dissolved oxygen *DO* in Figure 73. The value *IP* concentrations reduce the *Chl-a* and *DO* concentrations by a maximum of approximately 25% on these days. After the 25th simulation day *IP* remains low by even more than half of the original simulation due to the stronger limitation of this nutrient than by the inorganic nitrogen components. However, the system falls back into an overall light-limited state and no large reduction in algae growth occurs between the 25th and 80th simulation days.

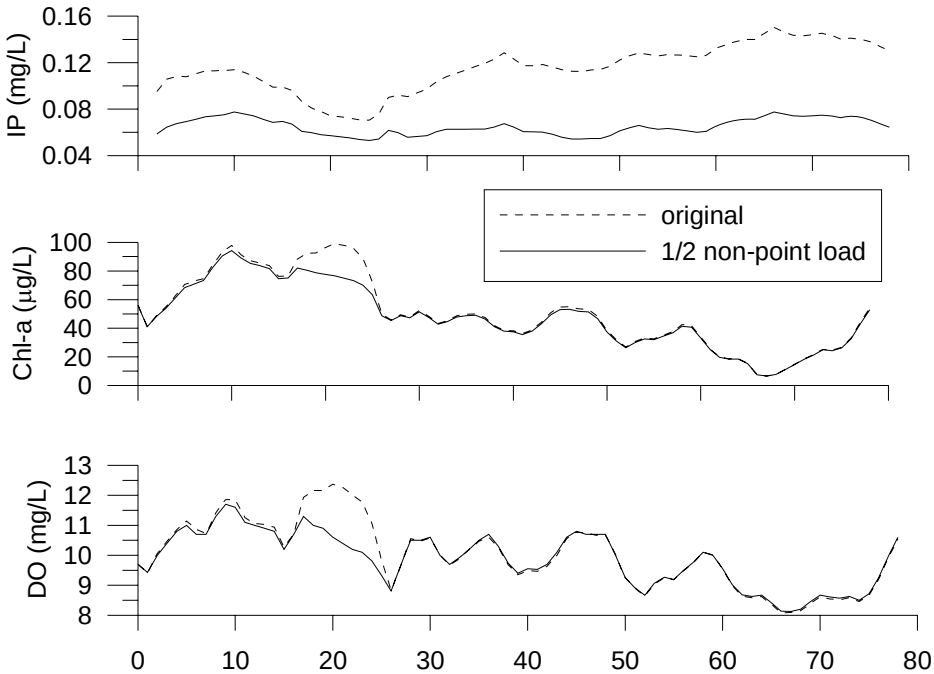


Figure 73: Scenario 2002: the effect of a 50% reduction in non-point nutrient loading on inorganic phosphorus *IP*, chlorophyll-a *Chl-a* and dissolved oxygen *DO* at Groß Rosenburg.

The non-point nutrient loading was also reduced further by 60, 70, 80 and 90% and a summary of the results is depicted in Figure 74. The graph shows the percentage of the total simulated time the aquatic environment is nutrient limited versus the percentage reduction in non-point loading. The two years may be viewed as extremes in which 2001 has an overall lower discharge and 2002 is a very advective year. Nutrient limitation may occur up to 60% more often than light limitation if a nutrient input of 90% is attained.

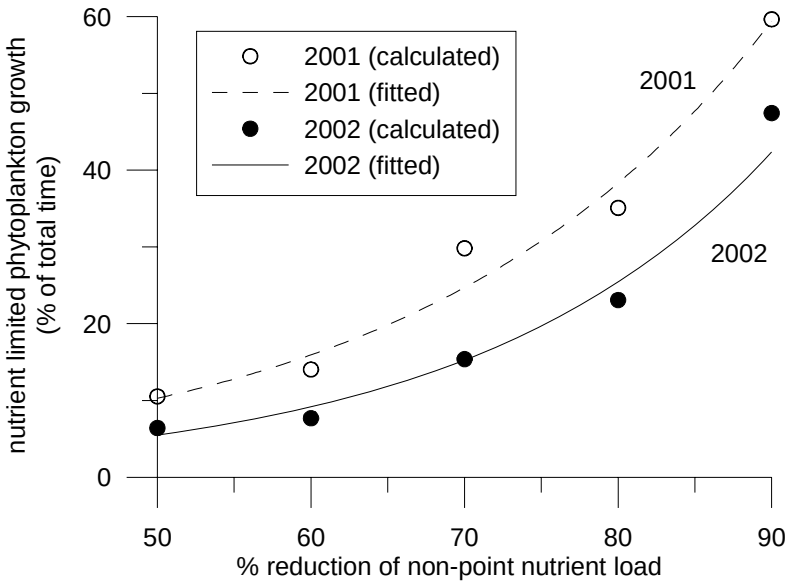


Figure 74: Percentage time phytoplankton is nutrient limited versus the percentage reduction in non-point nutrient loading.

7 Conclusions

Complexity vs. Uncertainty

- The hypothesis proposed by Snowling and Kramer (2001) could be confirmed for river water quality modelling exercises at both large and small scales.
- The hypothesis proposed by the authors that the relation of model error and sensitivity with complexity, as suggested by Snowling and Kramer (2001), shifts for different scales was confirmed.

Scale and transferability

- An extension of the Snowling and Kramer hypothesis allows easy testing of model transferability to other sites. The model calibrated and validated for the lower Saale could be transferred to the middle course of the river. Some modification in the model structure is required in order to capture phytoplankton blooms in the simulations.
- There are processes on the local scale (lock-and-weir system) that become dampened on the global scale (Saale River): oxygen input by weir discharge, denitrification and increased settling/resuspension immediately upstream/downstream from the weir.
- The retention of heavy metals in the lock-and-weir systems is significant globally due to suspended solids becoming more organic in the flow direction to which dissolved metals have a greater affinity. These particles coagulate and settle out more rapidly.

Eutrophication

- The DO-BOD and the phytoplankton-nutrient dynamics are only loosely coupled to one another. The latter plays or more significant role in the oxygen balance of the Saale than the degradation of organic material
- Secondary pollution more of a problem than primary pollution. Phytoplankton-nutrient dynamics is more important than oxygen-BOD dynamics
- Increased sedimentation rates occurred on the small scale in the lock reach and immediately upstream from the weir. Resuspension was enhanced immediately downstream from the weir. For suspended solids these effects occurred only locally and were averaged out in the large scale modelling exercise.
- Denitrification plays a minor role for the lower Saale during this time frame, as evident in the low sensitivities of its parameters describing the process, K_{2D} and K_{NO3}.
- Nutrient content in the river can be reduced by throttling non-point nutrient inputs from the catchment area. However, a substantial reduction is required (up to 90%) for the phytoplankton growth to be nutrient limited for half of the vegetative period.

Micro-pollutant transport

- Physical processes are more dominant on the large scale whereas chemical processes become more important on the smaller scale.
- TOXI is a model suited for the transport of inorganic substances on the large scale. For small-scale applications additional processes must be incorporated which describe the complexity of the transport and transformation dynamic of these substances in the bottom sediments.

Morphological effects on water quality

- Weirs have little effect on the water quality of the Saale, due to the river's advective nature. Both weir removal and the addition of a lock-and-weir system have minute effects on the oxygen, phytoplankton and nutrient contents.
- The roughness coefficient has an effect on the water quality of the Saale. This signifies the potential re-naturalization measures (e.g. reconnection of oxbow lakes and dyke shifting) have on the natural recovery of the river.
- The smaller the river order the more influence morphology has on river water quality.

8 Outlook and future research perspectives

Continued modelling research of the Saale River

Sampling and modeling a flood event in the river is imperative for a complete understanding of the ecological and retentive functioning of the river. The substances retain by weirs can be released as surge pulses during floods and affect the ecology in the water after the flood. This will also increase our understanding of how dyke shifting and re-connection of oxbow lake can improve the ecological and water quality of the river. The river's retentive capacity of water and substances will also change through such measures. Rode (2001) also states that although the Saale is heavily modified, there are still many close-to-nature reaches along the river's course providing much potential for natural recovery.

Habitat modeling is suggested. River channelling has ecological effects: ecotones are removed, habitats are homogenised and biodiversity decreases. Also retentive capacity of pollutants by the ecosystem is decreased. Channel straightening also removes important refugees for many species since pools of lower current are le numerous. Dam regulation also interrupts ecological continuum simplifying ecosystem structure and reducing ecological diversity.

More impetus should be given to the sediment dynamics, especially in lock-and-weir systems. Modeling of these dynamics needs to be supported by an extensive sampling program and additional laboratory experiments to determine parameter rates.

It is imperative to take sediment core samples for heavy metal modelling.

An extension of the WASP5 model by Shanahan (2001) includes the variable macrophytes. This allows interacting feedback constructs from EUTRO and TOXI to DYNHYD, shown in Figure 75, allowing investigations with an ecohydrology perspective to be carried out. Water bodies laden with many submerged plants may alter the hydrodynamics of the water course. High concentrations of particular micro-pollutants may inhibit the growth of phytoplankton and macrophytes. Alternatively, areas of greater or less sediment deposition may also influence the water flows and velocities, especially for shallow water bodies.

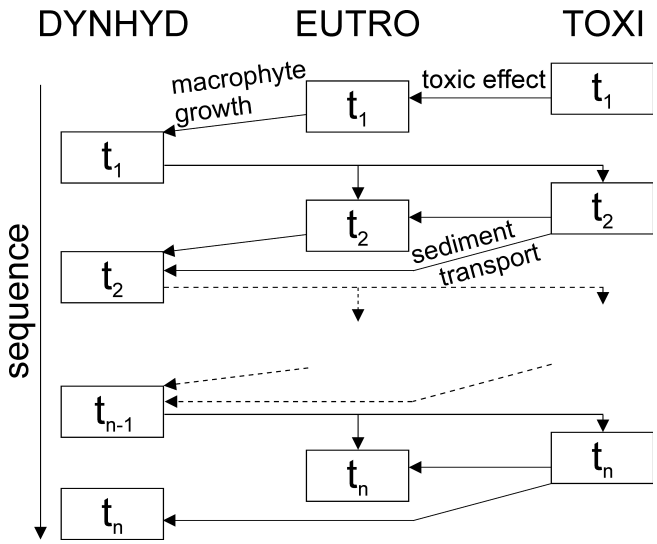


Figure 75: For an ecohydrology approach feedback from EUTRO and TOXI to DYNHYD is required. *(from Lindenschmidt, Hesser, et al., 2005)*

Computer modelling and the Water Framework Directive

One of the first steps in the implementation of the EU water framework directive (WFD) was to make an initial registry of the condition of European water bodies. For the majority of the surface waters it is still uncertain if the environmental goals specified by the WFD can be attained (Vogt and Guhl, 2005). This statement is based to a large extent on existing data and knowledge by experts familiar with the particular water bodies. However, the data and knowledge base is limited and much of the uncertainty in making a complete assessment is due to the lack of existing relevant environmental data. In addition, the data that do exist are very heterogeneous due to the wide spectrum in sampling and analysis methods used in making the measurements.

According to Article 8 of the WFD the European member states are required to have monitoring programs set up by 22. December 2006 for the monitoring of the water conditions. The monitoring programs must provide adequate and transparent descriptions of the local and regional conditions of the waters. Thus, the existing monitoring programs need to be revamped to meet the established monitoring goals. In order to evaluate the spatial and temporal relationships of the water conditions holistically with the limited resources available additional methods need to be drawn upon to fulfil the requirements of the monitoring programs. In this context computer modelling can serve an important role. Suggestions are made by Lindenschmidt, Schöl and Christoffels (2005) how to improve and extend data sampling programs to compliment water quality computer modelling used for surveillance and prognoses of river water quality. Case studies show the applicability of models to describe water quality and how existing monitoring programs can be extended to fill data gaps that are crucial for model calibration and validation. The studies include the:

i) importance of data of high temporal resolution in describing phytoplankton dynamics in the Saale River,

ii) effect of water drainage from mines on the water quality of the Erft river, and

iii) significance of the zoobenthos in describing the quality status of the Model river.

The importance of quantifying uncertainties in the measurements and modelling approaches is addressed and it is recommended that the analyses be extended to incorporate risk assessments.

9 Literature

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Appendix: Petersen matrices of processes and variables for each EUTRO complexity

Complexity 1:

Process	Variable number & name								Process rate
	1	2	3	4	5	6	7	8	
					TBOD	***DO***			
Reaeration						1			$K_2\theta_2^{T-20}\left(DO_{sat}-DO\right)$
Total Oxidation					-1	-1			$K_D\theta_D^{T-20}\bullet TBOD$
Settling					-1				$\frac{v_{s3}\left(1-f_{D5}\right)}{D}TBOD$
Sediment O_2-demand						-1			$\frac{SOD}{D}$

Variables:

DO	=	Dissolved oxygen	mg O_2/L
$TBOD$	=	Ultimate total biological oxygen demand	mg O_2/L

Parameters:

D	=	Depth	m
f_{D5}	=	Fraction dissolved *TBOD*	-
SOD	=	Sediment oxygen demand	g $O_2/(m^2 \cdot d)$

Constants:

K_2	=	Reaeration rate at 20°C	1/d
K_D	=	Deoxygenation rate at 20°C	1/d
v_{s3}	=	Settling velocity of organic matter	m/d
θ_2	=	Reaeration temperature coefficient	-
θ_D	=	Deoxygenation temperature coefficient	-

Functions:

DO_{sat}	=	Saturated dissolved oxygen	mg O_2/L
T	=	Water temperature	°C

Complexity 2:

Process	Variable number & name								Process rate
	1	2	3	4	5	6	7	8	
	NBOD				***CBOD***	***DO***			
Reaeration						1			$K_2\theta_2^{T-20}\left(DO_{sat}-DO\right)$
C-Oxidation					-1	-1			$K_D\theta_D^{T-20}\bullet CBOD$
N-Oxidation	-1					$-\frac{64}{14}$			$K_N\theta_N^{T-20}\bullet NBOD$
C-Settling					-1				$\frac{v_{s3}\left(1-f_{D5}\right)}{D}CBOD$
N-Settling	-1								$\frac{v_{s3}\left(1-f_{D1}\right)}{D}NBOD$
Sediment O_2-demand						-1			$\frac{SOD}{D}\theta_S^{T-20}$

Variables:

$CBOD$	=	Ultimate carbonaceous biological oxygen demand	mg O_2/L
DO	=	Dissolved oxygen	mg O_2/L
$NBOD$	=	Ultimate nitrogenous biological oxygen demand	mg O_2/L

Parameters:

D	=	Depth	m
f_{D1}	=	Fraction dissolved *NBOD*	-
f_{D5}	=	Fraction dissolved *CBOD*	-
SOD	=	Sediment oxygen demand	g $O_2/(m^2 \cdot d)$

Constants:

K_2	=	Reaeration rate at 20°C	1/d
K_D	=	Carbonaceous deoxygenation rate at 20°C	1/d
K_N	=	Nitrogenous deoxygenation rate at 20°C	1/d
v_{s3}	=	Settling velocity of organic matter	m/d
θ_2	=	Reaeration temperature coefficient	-
θ_D	=	Carbonaceous deoxygenation temperature coefficient	-
θ_N	=	Nitrogenous deoxygenation temperature coefficient	-
θ_S	=	*SOD* temperature coefficient	-

Functions:

DO_{sat}	=	Saturated dissolved oxygen	mg O_2/L
T	=	Water temperature	°C

Complexity 3:

Process	Variable number & name								Process rate
	1	2	3	4	5	6	7	8	
	NH_4^+	***NO_3^-***			***CBOD***	***DO***	***ON***		
Reaeration						1			$K_2\theta_2^{T-20}\left(DO_{sat}-DO\right)$
C-Oxidation					-1	-1			$K_D\theta_D^{T-20}\bullet CBOD$
ON-Mineralisation	1						-1		$K_{71}\theta_{71}^{T-20}\bullet ON$
Nitrification	-1	1				$-\frac{64}{14}$			$K_{12}\theta_{12}^{T-20}\bullet NH_4^+$
C-Settling					-1				$\frac{v_{s3}\left(1-f_{D5}\right)}{D}\bullet CBOD$
ON-Settling							-1		$\frac{v_{s3}\left(1-f_{D7}\right)}{D}ON$
Sediment O_2-demand						-1			$\frac{SOD}{D}\theta_S^{T-20}$
Phytoplankton growth						$\frac{32}{12}$			$K_{1C}\theta_{1C}^{T-20}\bullet PHYT$
Phytoplankton respiration						$-\frac{32}{12}$			$K_{1R}\theta_{1R}^{T-20}\bullet PHYT$

Variables:

$CBOD$	=	Ultimate carbonaceous biological oxygen demand	mg O_2/L
DO	=	Dissolved oxygen	mg O_2/L
NH_4^+	=	Ammonium nitrogen	mg N/L
NO_3^-	=	Nitrate nitrogen	mg N/L
ON	=	Organic nitrogen	mg N/L

Parameters:

D	=	Depth	m
f_{D5}	=	Fraction dissolved *CBOD*	-
f_{D7}	=	Fraction dissolved *ON*	-
SOD	=	Sediment oxygen demand	g $O_2/(m^2 \cdot d)$

Constants:

K_{12}	=	Nitrification rate at 20°C	1/d
K_{1C}	=	Phytoplankton growth rate	1/d
K_{1R}	=	Phytoplankton respiration rate	1/d
K_2	=	Reaeration rate at 20°C	1/d
K_{71}	=	N-mineralisation rate at 20°C	1/d
K_D	=	Carbonaceous deoxygenation rate at 20°C	1/d
v_{s3}	=	Settling velocity of organic matter	m/d
θ_{12}	=	Nitrification temperature coefficient	-
θ_{1C}	=	Phytoplankton growth temperature coefficient	-
θ_{1R}	=	Phytoplankton respiration temperature coefficient	-
θ_2	=	Reaeration temperature coefficient	-
θ_{2D}	=	Denitrification temperature coefficient	-
θ_{71}	=	N-mieralisation temperature coefficient	-
θ_D	=	Carbonaceous deoxygenation temperature coefficient	-
θ_N	=	Nitrogenous deoxygenation temperature coefficient	-
θ_S	=	*SOD* temperature coefficient	-

Functions:

$PHYT$	=	Phytoplankton concentration	mg C/L
DO_{sat}	=	Saturated dissolved oxygen	mg O_2/L
T	=	Water temperature	°C

Complexity 4:

Process	Variable number & name								Process rate
	1	2	3	4	5	6	7	8	
	NH_4^+	NO_3^-	*IP*	*PHYT*			*ON*	*OP*	
Phosphorus limitation									
Phyt. growth			$-a_{PC}$	1					$G_{P1} \bullet PHYT$
Phyt. death				-1				a_{PC}	$D_{P1} \bullet PHYT$
Phyt. settling				-1					$\frac{v_{S4}}{D} PHYT$
OP-Mineralisation			1					-1	$K_{83}\theta_{83}^{T-20} \bullet OP$
OP-Settling								-1	$\frac{v_{S3}(1-f_{D8})}{D} OP$
IP-Settling			-1						$\frac{v_{S5}(1-f_{D3})}{D} IP$
Nitrogen limitation									
Phytoplankton growth	$-a_{NC} \bullet P_{NH4}$	$-a_{NC} \bullet (1-P_{NH4})$		1					$G_{P1} \bullet PHYT$
Phytoplankton death				-1			a_{NC}		$D_{P1} \bullet PHYT$
Phytoplankton settling				-1					$\frac{v_{S4}}{D} PHYT$
ON-Mineralisation	1						-1		$K_{71}\theta_{71}^{T-20} \bullet ON$
ON-Settling							-1		$\frac{v_{S3}(1-f_{D7})}{D} ON$
Nitrification	-1	1							$K_{12}\theta_{12}^{T-20} \bullet NH_4^+$

Additional equations

Phytoplankton growth rate :

$$G_{P1} = K_{1C} \cdot X_{RT} \cdot X_{RI} \cdot X_{RN}$$

where:

Phytoplankton temperature adjustment:

$$X_{RT} = \theta_{1C}^{T-20}$$

Phytoplankton light limitation (Di Toro):

$$X_{RI} = \frac{e}{K_E \cdot D} f\left[exp\left\{-\frac{I_A}{I_S} exp\left(-K_E \cdot D\right)\right\} - exp\left(-\frac{I_A}{I_S}\right)\right]$$

Phytoplankton nutrient limitation:

$$X_{RN} = \left.\frac{DIP}{K_{mP} + DIP}\right|_{P-limitation} \quad \text{or} \quad X_{RN} = \left.\frac{DIN}{K_{mN} + DIN}\right|_{N-limitation}$$

Phytoplankton death rate : $$D_1 = K_{1R}\theta_{1R}^{T-20} + K_{1D} + K_{1G}Z(t)$$
Ammonium preference factor: $$P_{NH4} = NH_4^+\left(\frac{NO_3^-}{\left(K_{mN} + NH_4^+\right)\left(K_{mN} + NO_3^-\right)}\right) + NH_4^+\left(\frac{K_{mN}}{\left(NH_4^+ + NO_3^-\right)\left(K_{mN} + NO_3^-\right)}\right)$$

Variables:

IP	=	Inorganic phosphorus	mg P/L
NH_4^+	=	Ammonium nitrogen	mg N/L
NO_3^-	=	Nitrate nitrogen	mg N/L
ON	=	Organic nitrogen	mg N/L
OP	=	Organic phosphorus	mg P/L
$PHYT$	=	Phytoplankton carbon $= CHLA \bullet a_{CCHL}$	mg C/L

Parameters:

D	=	Depth	m
f_{D3}	=	Fraction dissolved *IP*	-
f_{D7}	=	Fraction dissolved *ON*	-
f_{D8}	=	Fraction dissolved *OP*	-

Constants:

a_{CCHL}	=	Carbon to chlorophyll ratio	mg C/mg Chla
a_{NC}	=	Nitrogen to carbon ratio	mg N/mg C
a_{PC}	=	Phosphorus to carbon ratio	mg P/mg C
I_S	=	Saturated light intensity	langleys/day
K_{12}	=	Nitrification rate at 20°C	1/d
K_{1C}	=	Phytoplankton growth rate	1/d
K_{1D}	=	Phytoplankton death rate	1/d
K_{1G}	=	Phytoplankton grazing rate	L/(mg C·d)
K_{1R}	=	Phytoplankton respiration rate	1/d
K_{71}	=	*ON*-mineralisation rate at 20°C	1/d
K_{83}	=	*OP*-mineralisation rate at 20°C	1/d
K_{mN}	=	½-saturation for N-limitation on phyto. uptake	mg N/L
K_{mP}	=	½-saturation for P-limitation on phyto. uptake	mg P/L
v_{S3}	=	Settling velocity of organic matter	m/d
v_{S4}	=	Settling velocity of phytoplankton	m/d
v_{S5}	=	Settling velocity of inorganic sediment	m/d
θ_{12}	=	Nitrification temperature coefficient	-
θ_{1C}	=	Phytoplankton growth temperature coefficient	-
θ_{1R}	=	Phytoplankton respiration temperature coefficient	-
θ_{71}	=	*ON*-mineralisation temperature coefficient	-
θ_{83}	=	*OP*-mineralisation temperature coefficient	-

Functions:

f	=	Fraction of day that is daylight	-
I_A	=	Average daily surface solar radiation	langleys/day
K_E	=	Extinction coefficient	1/m
T	=	Water temperature	°C
Z	=	Zooplankton population	mg C/L

Complexity 5:

Process	Variable number & name								Process rate
	1	2	3	4	5	6	7	8	
	NH_4^+	***NO_3^-***	***IP***	***PHYT***	***CBOD***	***DO***	***ON***	***OP***	
CBOD & Oxygen									
Reaeration						1			$K_2\theta_2^{T-20} \bullet \left(DO_{sat} - DO\right)$
C-Oxidation (low O_2 – limitation)					-1	-1			$K_D\theta_D^{T-20} \cdot CBOD \cdot \left(\frac{DO}{K_{BOD} + DO}\right)$
C-Settling					-1				$\frac{v_{s3}\left(1 - f_{D5}\right)}{D} \bullet CBOD$
Sediment O_2-demand						-1			$\frac{SOD}{D}\theta_S^{T-20}$
Nutrients									
OP-Mineralisation			1					-1	$K_{83}\theta_{83}^{T-20} \bullet OP \bullet \left(\frac{PHYT}{K_{PHY} + PHYT}\right)$
OP-Settling								-1	$\frac{v_{S3}\left(1 - f_{D8}\right)}{D} OP$
ON-Mineralisation	1						-1		$K_{71}\theta_{71}^{T-20} \bullet ON \bullet \left(\frac{PHYT}{K_{PHY} + PHYT}\right)$
ON-Settling							-1		$\frac{v_{S3}\left(1 - f_{D7}\right)}{D} ON$
Nitrification (low O_2 – limitation)	-1	1				$-\frac{64}{14}$			$K_{12}\theta_{12}^{T-20} \cdot NH_4^+ \cdot \left(\frac{DO}{K_{NIT} + DO}\right)$
Denitrification (high O_2 – limitation)		-1			$-\frac{5}{4} \bullet \frac{32}{14}$				$K_{2D}\theta_{2D}^{T-20} \cdot NO_3^- \cdot \left(\frac{K_{NO3}}{K_{NO3} + DO}\right)$
Phytoplankton (phosphorus limitation)									
Phyt. growth			$-a_{PC}$	1		b^*			$G_{P1} \cdot PHYT$
Phyt. resp.				-1		$\frac{32}{12}$		a_{PC}	$K_{1R}\theta_{1R}^{T-20} \cdot PHYT$
Phyt. death			$a_{PC} \bullet \left(1 - f_{OP}\right)$	-1	a_{OC}			$a_{PC} \bullet f_{OP}$	$K_{1D} \cdot PHYT$

Phyt. grazing				-1				a_{PC}	$K_{1G} \cdot Z \cdot PHYT$
Phyt. settling				-1					$\frac{v_{S4}}{D} PHYT$
Phytoplankton (nitrogen limitation)									
Phyt. growth	$-a_{NC} \bullet P_{NH4}$	$-a_{NC} \bullet (1-P_{NH4})$		1	a_{OC}	b^*			$G_{P1} \bullet PHYT$
Phyt. resp.				-1		$\frac{32}{12}$	a_{NC}		$K_{1R}\theta_{1R}^{T-20} \cdot PHYT$
Phyt. death	$a_{NC} \bullet (1-f_{ON})$			-1			$a_{NC} \bullet f_{ON}$		$K_{1D} \cdot PHYT$
Phyt. grazing				-1			a_{NC}		$K_{1G} \cdot Z \cdot PHYT$
Phyt. settling				-1					$\frac{v_{S4}}{D} PHYT$

$^* \; b = \frac{32}{12} + \frac{48}{14}\frac{14}{12}(1-P_{NH4})$

Additional equations

Phytoplankton growth rate :

$$G_{P1} = K_{1C} \cdot X_{RT} \cdot X_{RI} \cdot X_{RN}$$

where:

Phytoplankton temperature adjustment:

$$X_{RT} = \theta_{1C}^{T-20}$$

Phytoplankton light limitation:

$$X_{RI} = \frac{e}{K_E \cdot D} f\left[exp\left\{-\frac{I_A}{I_S} exp\left(-K_E \cdot D\right)\right\} - exp\left(-\frac{I_A}{I_S}\right)\right] \text{(Di Toro)}$$

or

$$X_{RI} = \frac{e}{K_E \cdot D}\left[exp\left\{-\frac{I_0}{I_S} exp\left(-K_E \cdot D\right)\right\} - exp\left(-\frac{I_0}{I_S}\right)\right] \text{(Smith)}$$

Phytoplankton nutrient limitation:

$$X_{RN} = min\left(\frac{DIN}{K_{mN} + DIN}, \frac{DIP}{K_{mP} + DIP}\right) \text{ or } X_{RN} = \frac{DIN}{K_{mN} + DIN} \cdot \frac{DIP}{K_{mP} + DIP}$$

Ammonium preference factor:

$$P_{NH4} = NH_4^+\left(\frac{NO_3^-}{\left(K_{mN} + NH_4^+\right)\left(K_{mN} + NO_3^-\right)}\right) + NH_4^+\left(\frac{K_{mN}}{\left(NH_4^+ + NO_3^-\right)\left(K_{mN} + NO_3^-\right)}\right)$$

Variables:

$CBOD$	=	Ultimate carbonaceous biological oxygen demand	mg O_2/L
DO	=	Dissolved oxygen	mg O_2/L
IP	=	Inorganic phosphorus	mg P/L
NH_4^+	=	Ammonium nitrogen	mg N/L
NO_3^-	=	Nitrate nitrogen	mg N/L
ON	=	Organic nitrogen	mg N/L
OP	=	Organic phosphorus	mg P/L
$PHYT$	=	Phytoplankton carbon $= CHLA \bullet a_{CCHL}$	mg C/L

Parameters:

D	=	Depth	m
f_{D3}	=	Fraction dissolved IP	-
f_{D5}	=	Fraction dissolved $CBOD$	-
f_{D7}	=	Fraction dissolved ON	-
f_{D8}	=	Fraction dissolved OP	-

Functions:

f	=	Fraction of day that is daylight	-
I_A	=	Average daily surface solar radiation	langleys/day
I_0	=	Incident light intensity just below water surface	langleys/day
K_E	=	Extinction coefficient	1/m
SOD	=	Sediment oxygen demand	g/m^2/day
T	=	Water temperature	°C
Z	=	Zooplankton population	mg C/L

Constants:

a_{CCHL}	=	Carbon to chlorophyll ratio	mg C/mg Chla
a_{NC}	=	Nitrogen to carbon ratio	mg N/mg C
a_{OC}	=	Oxygen to carbon ratio	mg O_2/mg C
a_{PC}	=	Phosphorus to carbon ratio	mg P/mg C
f_{ON}	=	Fraction of dead phytoplankton recycled to *ON*	-
f_{OP}	=	Fraction of dead phytoplankton recycled to *OP*	-
I_S	=	Saturated light intensity	langleys/day
K_{12}	=	Nitrification rate at 20°C	1/d
K_{1C}	=	Phytoplankton growth rate	1/d
K_{1D}	=	Phytoplankton death rate	1/d
K_{1G}	=	Phytoplankton grazing rate	L/(mg C·d)
K_{1R}	=	Phytoplankton respiration rate	1/d
K_2	=	Reaeration rate at 20°C	1/d
K_{2D}	=	Denitrification rate at 20°C	1/d
K_{71}	=	*ON*-mineralisation rate at 20°C	1/d
K_{83}	=	*OP*-mineralisation rate at 20°C	1/d
K_{BOD}	=	½-saturation for O_2-limitation on deoxygenation	mg O_2/L
K_D	=	Carbonaceous deoxygenation rate at 20°C	1/d
K_{mN}	=	½-saturation for N-limitation on phyto. uptake	mg N/L
K_{mP}	=	½-saturation for P-limitation on phyto. uptake	mg P/L
K_{NIT}	=	½-saturation for O_2-limitation on nitrification	mg N/L
K_{NO3}	=	½-saturation for O_2-limitation on denitrification	mg N/L
K_{PHY}	=	½-saturation for *PHYT*-limit. on mineralisation	mg C/L
v_{S3}	=	Settling velocity of organic matter	m/d
v_{S4}	=	Settling velocity of phytoplankton	m/d
v_{S5}	=	Settling velocity of inorganic sediment	m/d
θ_{12}	=	Nitrification temperature coefficient	-
θ_{1C}	=	Phytoplankton growth temperature coefficient	-
θ_{1R}	=	Phytoplankton respiration temperature coefficient	-
θ_{71}	=	*ON*-mineralisation temperature coefficient	-
θ_{83}	=	*OP*-mineralisation temperature coefficient	-