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METHODOLOGIES FOR REDUCTION OF OUTPUT UNCERTAINTY OF RIVER WATER QUALITY MODELS

Thesis submitted in fulfillment of the requirements
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SAMENVATTING

In de Europese wetgeving, meer bepaald in de Kaderrichtlijn Water, wordt gesteld dat alle oppervlaktewater een goede ecologische toestand moet behalen, gelijkend op de natuurlijke toestand zonder enige menselijke invloed. De “Clean Water Act”, de belangrijkste wet in de Verenigde Staten met betrekking tot water, heeft als doel het herstel en het behoud van de chemische, fysische en biologische integriteit van het oppervlaktewater. Om de doelstellingen van deze beide wetten te halen, zijn er nog vele maatregelen nodig om de rivierwaterkwaliteit te verbeteren.

Om de huidige toestand te evalueren en voorspellingen te maken over het effect van de maatregelen ter verbetering van de rivierwaterkwaliteit, worden modellen gebruikt. Omwille van verschillende redenen is de onzekerheid op de modelresultaten echter soms zeer groot. Vooreerst is er het probleem van het gebruik van gegevens van slechte kwaliteit als invoer voor het model en voor de kalibratie. Ten tweede zijn de modellen die tegenwoordig gebruikt worden steeds complexer en dat heeft als gevolg dat er ook meer parameters zijn. Omwille van correlatie en afhankelijkheden tussen de parameters, is het niet mogelijk om alle parameters te schatten tijdens de kalibratie. Het gevolg daarvan is dat de onzekerheid nog groter kan worden doordat verkeerde parameters een vaste waarde krijgen of de parameters die niet geschat worden een verkeerde vaste waarde krijgen.

Het doel van dit eindwerk is om goede modelleerpraktijken aan te moedigen en om de onzekerheid op de modelresultaten te verkleinen door op een overzichtelijke manier methodes aan te reiken die de waterbeheerder of ingenieur daarbij kunnen helpen. De methodes ontwikkeld en gebruikt in dit werk zijn eenvoudig en voor de hand liggend, met gemakkelijk te gebruiken software of software die gemakkelijk kan ontwikkeld worden door de gebruiker zelf. De methodes zijn allen toegepast op reële gevallenstudies met name de Dender of de Nete in België.

Reductie van de onzekerheid op de modelresultaten kan bekomen worden op verschillende plaatsen in het modelleerproces. In dit proefschrift werden voor iedere stap enkele belangrijke aspecten gerelateerd aan modelbetrouwbaarheid, behandeld door het toepassen en bespreken van methodes en middelen die het gedrag van het model grondig analyseren en door het nemen van acties om de modelonzekerheid te verkleinen.

De eerste stap van het modelleerproces is het opstellen van het modelstudieplan en de beslissing over welk model het meest geschikt is voor het beschouwde probleem. Het is niet enkel noodzakelijk een model te kiezen dat de huidige toestand van de rivier goed kan weergeven, ook de toekomstige veranderingen in het systeem door het toepassen van bepaalde scenarios moeten kunnen geëvalueerd worden. Met een sensitiviteitsanalyse (SA) werd een evaluatie gedaan voor twee verschillende waterkwaliteitsmodelconcepten, QUAL2E en RWQM1, in het licht van hun gebruik voor beheersbeslissingen. Er werd aangetoond voor de gevallenstudie de Dender, dat de opgeloste zuurstof resultaten van het QUAL2E-gebaseerd waterkwaliteitsmodel vooral gerelateerd waren aan de groei van de algen daar waar het RWQM1 ook de sedimentatie in rekening brengt en processen, uitgevoerd door verschillende

microbiële gemeenschappen, benadrukt en differentieert. Deze studie toont aan dat beheerders zich bewust moeten zijn van de mogelijkheden en beperkingen van het model dat ze gebruiken en dus een model moeten kiezen dat past bij hun specifieke problemen en verwachtingen. Ook is het goed om te weten welke processen belangrijker zullen worden bij de uitvoering van een maatregel zodat bij het opstellen van het model al extra aandacht besteed wordt aan die processen om tot betrouwbaardere resultaten te komen.

Soms is het nodig een model op te stellen van een bekken waar weinig of geen gegevens voorhanden zijn. In een dergelijke situatie is het moeilijk te beslissen welke processen belangrijk zijn en dus in het model moeten aanwezig zijn. De enige data die gemakkelijk te verkrijgen zijn, zijn data die kunnen verzameld worden door directe waarnemingen zoals heuvelachtig landschap, aanwezigheid van algenbloei in de zomer of hoge zomertemperaturen. In dit doctoraatsonderzoek werd een studie gedaan voor modeltoepassingen in niet-bemeten bekkens, waarin de meest belangrijke parameters voor verschillende omstandigheden bepaald werden met een soort van sensitiviteitsanalyse van de sensitiviteitsanalyse. Het besluit is dat het model verschillende sensitiviteit vertoont tegenover de parameters, afhankelijk van de externe omstandigheden. Er kon een tabel opgesteld worden waarin die externe omstandigheden, hier “zachte data” genoemd (data die gemakkelijk kunnen verzameld worden), gerelateerd worden aan de belangrijkheid van de parameters. In die tabel wordt een eerste aanduiding gegeven op welke parameters/processen men moet focussen in een bepaald bekken, gekenmerkt door bepaalde “zachte data”. De meest belangrijke parameterset kennen, is belangrijk voor de kalibratie van het model, optimaal experimenteel ontwerp (OEO), onzekerheidsbepalingen en scenario analyse waarbij andere processen belangrijk kunnen worden in vergelijking met de uitgangstoestand.

De tweede stap is de gegevensverzameling en de meetcampagnes. Het is duidelijk dat het belangrijk is te weten welke gegevens nodig zijn en welke meetdata (plaats, frequentie, hoeveelheid,…) best zijn voor de kalibratie van een model om uiteindelijk zo een klein mogelijke onzekerheid te hebben op de modelresultaten. Er werd een methode van iteratief optimaal experimenteel ontwerp (OEO) voorgesteld om de onzekerheid op parameterschattingen tijdens de kalibratie zo klein mogelijk te maken. Er werd aangetoond dat OEO methodes gebruikt kunnen worden voor een strategie van iteratief sequentiëel ontwerp voor het meten van waterkwaliteitsvariabelen, voor kalibratie van modellen. In een eerste stap is een relatief uitgebreide set van metingen nodig om het riviermodel op te stellen. Gebruikmakende van dit initiële model maakt deze OEO methode het mogelijk efficiënte meetstrategieën te definiëren om betere modelparameterschattingen te bekomen en de onzekerheid op die schattingen kleiner te maken. Voor de verzameling van invoergegevens werd een onzekerheidsanalyse toegepast om meetcampagnes richting te geven. Parameters, diffuse en puntvervuilingen werden afzonderlijk beschouwd zodat informatie over de modelsensitiviteit tegenover deze inputs bekomen werd. De studie gaf aan wanneer en waar best gemeten zou worden.

De derde stap bestaat uit de opbouw van het eigenlijk model. Ook in deze stap van het modelleerproces kunnen verschillende acties ondernomen worden om minimale onzekerheid

op de resultaten te verzekeren. Grondige controles dienen uitgevoerd te worden op de invoergegevensbestanden door de uitvoering van testsimulaties en door evaluatie van de massabalansen. Dit werd echter niet in detail besproken in dit eindwerk.

Een kalibratie en validatie wordt uitgevoerd in de vierde stap. Er zijn twee problemen bij het kalibreren. Ten eerste kunnen niet alle parameters geschat worden door het bestaan van correlaties en afhankelijkheden tussen de parameters. In dit werk werd een SA toegepast om de belangrijkste parameters te bepalen, gerelateerd aan het probleem van de modelstudie. De SA toonde aan dat voor schatting tijdens de kalibratie ongeveer 10 parameters voldoende zijn om tot goede overeenkomsten te komen tussen modelresultaten en metingen, voor de periodes waar de opgeloste zuurstof concentraties onder kritieke waardes gaat. Ten tweede moet het probleem aangepakt worden van het vastzetten van parameters die echter beter geschat zouden worden. Een praktisch voorbeeld toont de gevolgen aan van het gebruik van een verkeerde parameter subset voor de kalibratie van een model. Er werd aangetoond dat kalibreren met verschillende subsets geheel andere resultaten kan opleveren en kan leiden tot afwijkende conclusies.

In de laatste stap dient de simulatie met evaluatie van de modelresultaten uitgevoerd te worden. Eens het model gekalibreerd en gevalideerd is, kan het gebruikt worden voor scenario-evaluaties en de vergelijking van scenarios. Onzekerheidsbanden rond de resultaten dienen zoveel mogelijk mee berekend te worden. De onzekerheid op de modelresultaten kan immers te hoog zijn om een significant verschil te vinden tussen twee scenarios. Twee praktische voorbeelden, de evaluatie van de kosteneffectiviteit van beluchting in de Dender en de bepaling van het effect van het aanplanten van schaduwplanten langsheen de Nete, werd voorgesteld. Onzekerheidsanalyse op de resultaten voor de Dender, voor het scenario “met beluchting”, toonde aan dat het mogelijk is dat de opgeloste zuurstof in de rivier nog beneden bepaalde kritieke waardes duikt, zelfs als het ontworpen beluchtingsysteem in werking is, maar dan wel enkel voor korte periodes. De onzekerheidsanalyse toont ook dat de twee opties met of zonder beluchting significant verschillend zijn. Voor de studie op de Nete voor beschaduwing, kon er besloten worden dat beschaduwen effectief de waterkwaliteit van een oppervlaktewater kan beïnvloeden, vooral voor rivieren die te kampen hebben met te grote algenbloei gedurende de zomerperiodes. Algenbloei werd gereduceerd door beschaduwing tot 20%. Voor de studie op de Nete werden echter geen positieve effecten gevonden voor de minimum, maximum en gemiddelde concentraties van opgeloste zuurstof, chemische zuurstofvraag, fosfaten, ammonium en nitraten in het water.

De algemene conclusie van deze studie is dat men de onzekerheid op de resultaten kleiner kan maken door het toepassen van verschillende methodes op de modellen. Ook werden een aantal suggesties voor betere meetcampagnes geformuleerd. Meetcampagnes die erop gericht zijn het model beter te kalibreren voor de lage opgeloste zuurstofgehaltes in de rivier zouden best gediend zijn met metingen in de lenteperiode. Wanneer men het model wil kalibreren voor puntvervuilingen, dan zijn metingen tijdens droge periodes best. Voor de kalibratie van het model voor de studie van diffuse pollutie zijn metingen tijdens periodes met regen en hoge waterdebieten nodig.

SUMMARY

In European legislation, especially in the Water Framework Directive (WFD), it is stated that all water bodies need to have a good ecological status, close to the pristine conditions. Pristine water means that the water is kept natural and healthy as it was in ancient times, before any influence of humans. In the Clean Water Act (CWA), the principal governing law for water in the United States, the objective is the restoration and maintenance of the chemical, physical and biological integrity of the nation's water. To reach the goals of the WFD or the CWA, a lot of measures are still needed to improve the water quality.

To evaluate the present situation and to predict the effects of measures taken to improve the river water quality, models are used. For several reasons, the uncertainty on the model results is sometimes very high. First there is the problem of the use of poor quality data as inputs or for the calibration of model parameters. Second, the models used nowadays are more complex and as such they contain more parameters. Because of correlation and parameter dependencies, it is not possible to estimate all parameters. Hence, some parameters need to be fixed while only the most important parameters are changed during the calibration. As a consequence, the uncertainty on the model predictions becomes even larger because of fixing wrong subsets of parameters or due to setting a subset of the model parameters on wrong values taken from literature.

It is the aim of this dissertation to promote good modelling practices and to provide in a systematic way methods that help the water manager or engineer to minimise the uncertainty on the model results. The methods developed and applied in this work are simple, straightforward, with easy to use software or with software that can easily be developed by the user. The methods and tools were applied on real case studies, either the river Dender or the river Nete, both in Belgium.

Reduction of the output uncertainty of a model can be achieved during many stages of the modelling process. In this work, for every modelling step, some important issues related to model reliability were answered by discussing and applying methods and tools that help to analyse the behaviour of the model and perform actions to reduce output uncertainty.

The first step in the modelling process is the model study plan and the decision of the most adequate model for the problem under consideration. It is not only necessary to decide for a model that can describe the current state of the river well, but also it must be capable of evaluating the probable changes in the system when the model is used for scenario analysis. With a sensitivity analysis two different water quality concepts, QUAL2E and RWQM1, were evaluated with regard to their use in management decisions. It was shown that for the case study on the Dender river, the DO model results of QUAL2E-based water quality models mainly relate to the algae processes whereas the RWQM1 is also taking into account sedimentation and stresses processes performed by different microbial communities. This study shows that managers should be aware of the possibilities and limitation of the model they use and choose a model that fits their problem and expectations. Also, knowing which

processes will become important after execution of a scenario can make that during model set up extra attention is paid towards those processes in order to get more reliable results.

Sometimes one needs to make a model of a basin with few or no available data. In such situation it is difficult to decide what processes are important and need to be included in the model. The only data that are easily obtained are data which can be gathered by direct observation like hilly region, algae bloom in summer, high summer temperatures. In this work a study for model application in ungauged basins is performed in which the most important parameters are identified for different circumstances by using a kind of sensitivity analysis of a sensitivity analysis. It is concluded that the model shows different sensitivities to the parameters in different external circumstances. A table could be established in which external circumstances, here called soft data, i.e. data that are easily collected, are related to the importance of the parameters. In this table a first indication is given of which parameters/processes one should focus on in a particular catchment characterised by the soft data. Knowing the most influential set of parameters is important for calibration of a model, optimal experimental design, uncertainty estimations and scenario analysis where other processes can become important compared to the base case.

The second step involves data gathering and measurement campaigns. It is obvious that it is important to know what input data is needed and what kind of measurement data (frequency, location, amount, …) for calibration is best suited to have minimal uncertainty of the output results. A method of iterative optimal experimental design (OED) was proposed to minimise uncertainty of parameter estimates during calibration. It is shown that OED methods can be used for an iterative, sequential design of a strategy for measuring water quality variables in a river, in view of the calibration of water quality models. In a first stage a relatively extensive set of measurements is needed to set up a model for the river. Using this initial model, the OED method enables the definition of efficient measurement strategies, to find better model parameter estimates and reduce the uncertainty of those estimates. For the collection of input data, an uncertainty analysis is performed to guide measurement campaigns. Parameters, diffuse and point pollution inputs were considered separately, providing information on the model sensitivity towards these three. This study showed important periods and locations for measurements.

The third step comprises of the set-up of the model. Also in this step of the modelling process different actions exist to assure minimal output uncertainty. There is the need of profound checks of the input files, performance of test runs and checking mass balances. In this work, no additional research related to this step in the modelling process is performed.

A calibration and validation of the model is performed in the fourth step of the modelling process. Two problems arise during the calibration. The first one is that not all parameters can be estimated because of correlation and dependencies. In this work a sensitivity analysis was applied to identify the most important parameters related to a modelling problem. The SA revealed that only around 10 parameters need to be changed during calibration to obtain good fits between simulated and measured values, for the periods with dissolved oxygen

concentrations below a critical value. Second, the problem of fixing wrong parameter subsets on literature values should be dealt with. A practical example shows the consequences of using the wrong parameter subset for the calibration of the model. It was demonstrated that calibrating with different subsets of parameters gives very different model predictions and can lead to different conclusions.

In the last step a simulation and evaluation of the model results needs to be performed. Once the model is calibrated and validated the model can be used for scenario analysis and comparison of different scenarios. Next to the simulation results, uncertainty calculations are needed as well because uncertainty on the results can be too high to find a significant difference between the results of two scenarios. Two practical examples, the evaluation of the cost-effectiveness of in-stream aeration for the Dender river and the assessment of the effect of shading along the Nete river are presented. Uncertainty analysis on the results for the Dender, for the scenario 'with aeration' shows that it is possible for the dissolved oxygen content of the river to drop below a critical level even when the designed aeration system is installed, albeit for very short periods. The uncertainty analysis also shows that the two options, "with" or "without aeration" are significantly different. For the Nete case study about shading, it could be concluded that shading can effectively influence the water quality of a surface water body, in particular in streams that suffer from excessive algal growth during the summer periods because algal growth is reduced by shading up to 20%. In this case study however, no significant positive effects of shading on the minimum, maximum and average concentrations of DO, COD, phosphates, ammonium and nitrates in the water were identified.

The overall conclusion of this PhD study is that by applying different methodologies on the models, uncertainty on the results can be made smaller and a number of suggestions for better measurement campaigns were formulated. Measurement campaigns that aim to calibrate the model better for the low DO concentrations in the river should preferably be organised in spring. When calibrating the model for the Dender river for point pollution, measurements during dry periods are needed. For calibration of the model to study diffuse pollution, measurements during periods with rainfall and high flows are needed.

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AIM	Analytically Integrated Magnus
ANOVA	Analysis Of Variance
AnnAGNPS	Annualized Agricultural Non Point Source
ASM	Activated Sludge Model
AWP	General Water Plan
B	behavioural
BBI	Belgian Biotic Index
BMPs	Best Management Practices
BOD	Biological Oxygen Demand
cBOD	carbonaceous Biological Oxygen Demand
CCE	competitive complex evolution
CDF	cumulative distribution functions
Chl a	Chlorophyl a
CLT	Central Limit Theorem
COD	Chemical Oxygen Demand
cut-HDMR	cut-High Dimensional Model Representation
CWA	Clean Water Act
DEM	Digital elevation map
DO	dissolved oxygen
1D	one dimensional
2D	two dimensional
3D	three dimensional
EE	elementary effects
ESWAT	Extended Soil and Water Assessment Tool
EU	European Union
EVAP	evaporation
FAST	Fourier amplitude sensitivity test
FF	fractional factorial
FF	factor fixing
FIM	Fisher Information Matrix
FM	factor mapping
FORM	First Order Reliability Method
FP	factors prioritising
GIS	Geographical Information System(s)
GLUE	Generalized Likelihood Uncertainty Estimation
GFM	Green's Function Method
GUI	Graphical User Interface
GVA	Gross Value Added

GWQP	General Water Quality Plan
HDMR	High Dimensional Model Representation
HRU's	Hydrological Response Units
HSPF	Hydrologic Simulation Program Fortran
IMP	impervious
INF	infiltration
LHS	Latin Hypercube sampling
MSL	Model Specification Language
NB	non behavioural
OAT	One-factor-At-a-Time
ODE	Ordinary Differential Equation
OED	Optimal Experimental Design
OED-PE	Optimal Experimental Design for Parameter Estimation
PEST	Parameter estimation
RSA	Regional Sensivity Analysis
RSC	Standardized Regression Coefficient
RS-HDMR	Random Sampling High Dimensional Model Representation
RSRC	Ranked Standardised Regression Coefficient
RWQM	River Water Quality Model
SA	Sensitivity analysis
SCE	Shuffled Complex Evolution
SDP	State Depending Parameter
SOD	sediment oxygen demand
SORM	Second Order Reliability Method
SWAT	Soil and Water Assessment Tool
SWIM	Soil and Water Integrated Model
TMDL	Total Maximum Daily Load
UA	Uncertainty analysis
UPM	Urban Pollution Management
USDA	United States Department of Agriculture
VIF	Variation Inflation Facor
VLM	Flemish Institude for Landuse
VMM	Flemish Environmental Agency
WEST	World-wide Engine for Simulation, Training and automation
WFD	Water Framework Directive
WWTP	Waste Water Treatment Plants

CHAPTER I
INTRODUCTION

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- Vandenberghe V., van Griensven A., Bauwens W. and Vanrolleghem P.A. (2006). Effect of different river water quality model concepts used for river basin management decisions Water Science & Technology, 53(10), 277-284.

CHAPTER I: INTRODUCTION

1. River water quality

Water is an integral part of life on this planet. More than three-fourths of the Earth's surface is covered by water. Most of the water on Earth, about 97%, is salt water found in oceans that men cannot drink or use for crops because of the salt content. One can remove salt from ocean water, but desalination is still very expensive. Only about 3% of the Earth's water is fresh. Two thirds of this is in solid form, found in ice caps and glaciers. Because it is frozen, the fresh water in ice caps is not available for use by people or plants. That leaves about 1% of all the Earth's water in a form available to life. This fresh water is found in lakes, rivers, streams, ponds, and in the ground. Because it is at the same time such a valuable and a very sparse product, care has to be taken to keep the fresh water quality optimal. This is reflected in legislation concerning water quality.

In European legislation, especially in the Water Framework Directive (WFD) (EU, 2000), it is stated that all water bodies need to have a good ecological status, close to the pristine conditions. In the Clean Water Act (CWA) (P.L. 95-217, 1977), the principal governing law in the United States for water, the objective is the restoration and maintenance of the chemical, physical and biological integrity of the nation’s water. Pristine water means that the water is kept natural and healthy as it was in ancient times, before any influence of humans that polluted rivers. Pollution is caused by releasing waste into the river, by the creation of sewer networks with outlets to the river, and intensification of agriculture that uses pesticides and fertilizers which finally reach the river water etc…; and also by construction of dams and sluices, by straightening of river bends, reinforcement of the banks to make navigation possible. The latter ones are no source of pollution, but they change the hydrological state and morphology of the water body. Due to all these influences, the river water quality and ecology is now at some places far away from pristine situations: oxygen drops, excessive algae blooms, too high concentrations of nutrients, heavy metals, pesticides or other toxic compounds deteriorate water quality while fauna and flora in the water are suffering. While considerable progress has been made, to reach the goals of the WFD or the CWA, a lot of measures are still needed to improve water quality.

2. River water quality modelling and monitoring

To evaluate the present situation and to predict the effects of measures taken to improve river water quality, models are used. Before making a model of a river, data is gathered: hydrometeorological data, quality measurements in the river, land use, management practices on land, point pollution measurements, flow and water level data. Depending on the desired outcome and use of the model, a simple conceptual model or a very complex physically based

model can be used and the amount of data needed follows the desired degree of complexity and accuracy of the model results. Most of the time, the necessary data are not all available. This means that simpler models would be better suited for use (models that only need those data that are available) or, that additional data gathering and monitoring campaigns are necessary if they stick to their known models. This is a clear source of problems: the institute or company the modeller is linked to, has a licence for only one model or sticks to its own home-made models while additional monitoring campaigns are expensive. The fact that modellers and information gatherers are not working at the same time on the same project in the same institute can also be seen as a problem. People start making assumptions, extrapolations and make use of statistical relationships that are insufficiently backed up. Next to the problem of missing data there is the problem of wrong or inaccurate data. Many data are available that have not received a thorough quality check. The use of poor quality data as inputs or for the calibration, consequently, results in ignored uncertainty on the model predictions.

These days it is the aim of models to cope also with the changes in society, climate, land use, etc. and therefore a lot of processes are considered. This goes together with more complexity and as such more parameters in the model. Because of correlation and parameter dependencies, it is not possible to estimate all parameters from the limited data. Hence, some parameters need to be fixed while only the most important parameters are changed during the calibration. This has as a consequence that the uncertainty on the model predictions becomes even larger because of fixing wrong subsets of parameters or due to setting a subset of the model parameters on wrong values taken from literature. Therefore, every step of the modelling process should be processed with much care and research. The modelling process is pictured in figure I.1.

3. Objectives

This dissertation has to be situated in the field of real applications of river water quality modelling for water management. It is the overall objective to promote good modelling practices and to provide, in a systematic way, methods that help the water manager or engineer to minimise the uncertainty on his/her model results. Therefore, the methods developed in this work are simple, straightforward, with easy to use software or with software that can easily be developed by the user. The developed methods and tools are applied and tested on real case studies, either the river Dender or the river Nete, both in Belgium. The methods and conclusions of these case studies are kept general and described in such a way that they form guidelines for further modelling work, applicable to other river basins.

Reduction of the output uncertainty of a model can be done during many stages of the modelling process (figure I.1). In this work, for every step, some important issues related to model reliability are answered by discussing and applying methods and tools that help to analyse the behaviour of the model and perform actions to reduce output uncertainty.

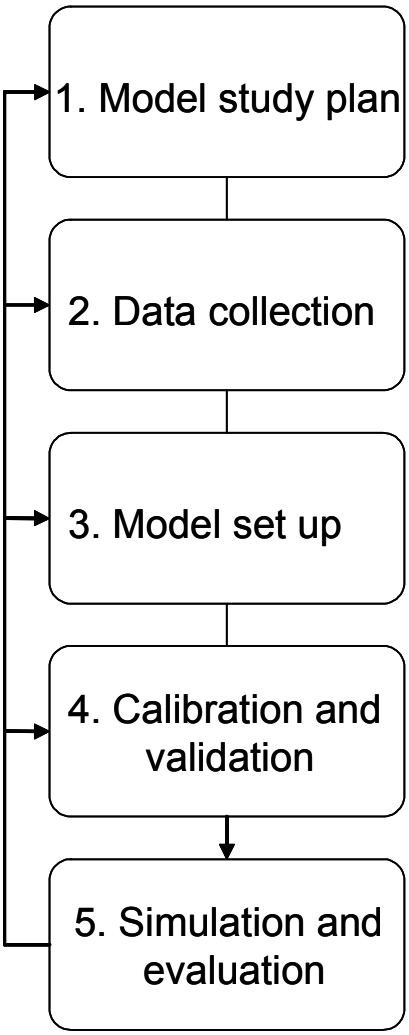


Figure I.1: The modelling process (adapted from Refsgaard et al. (2004))

Step 1. The model study plan and the decision of the most adequate model for the problem under consideration

It is not only necessary to choose a model that can model well the current state of the river, but there comes an additional question: What model concept should be used, in view of evaluating the probable changes in the system when the model is used for scenario analysis? To find the answer, with a sensitivity analysis an evaluation is done for two different water quality concepts with regard to their use in management decisions.

Sometimes one needs to make a model of a basin with few or no data available. In such situation it is difficult to decide what processes are important and needs to be included in the model. The only data that are easily obtained are data which can be gathered by direct observation like hilly region, algae bloom in summer, high summer temperatures. In this work a study for model application in ungauged basins is performed in which the most important

parameters for different circumstances are identified with a kind of sensitivity analysis of a sensitivity analysis.

Step 2. Data gathering and measurement campaigns

It is obvious that it is important to know what input data is needed and what kind of measurement data (frequency, location, amount, …) for calibration is best suited to have minimal uncertainty of the output results. A method of iterative optimal experimental design is proposed to minimise uncertainty of parameter estimates during calibration and for the collection of input data an uncertainty analysis to guide measurement campaigns is applied.

Step 3. The set-up of the model

Also in this step of the modelling process different actions can be done to assure a minimal output uncertainty. There is the need of profound checks of the input files, performance of test runs and checking mass balances. In this work, no additional research related to this step in the modelling process is performed.

Step 4. Calibration and validation of the model

Two problems arise during the calibration. First of all not all parameters can be estimated because of correlation and dependencies. In this work a sensitivity analysis is applied to identify the most important parameters related to a modelling problem. Secondly, the problem of fixing wrong parameter subsets on literature values should be dealt with. A practical example shows the consequences of using the wrong parameter subset for the calibration of the model.

Step 5. Simulation and evaluation of the model results with an uncertainty analysis (UA) to evaluate the trustworthiness of the model outcomes

Once the model is calibrated and validated the model can be used for scenario analysis and comparison of different scenarios. The uncertainty on the results can be too high to find a significant difference between the results of two scenarios. Two practical examples, the evaluation of the cost-effectiveness of in-stream aeration for the Dender river and the assessment of the effect of shading along the Nete river are presented. In this part it is the aim to show the role of uncertainty bounds around the results in the evaluation and to answer the question whether the difference between the scenarios is statistically significant or not.

4. Research approach

There exist many different methods for sensitivity analysis and uncertainty analysis. The purpose of this research was therefore not to reinvent the wheel, but to show the strength and usefulness of different existing model evaluation methods, implemented in non-commercial software and to adopt them to the specific needs of the river water quality models used.

The sensitivity analysis is performed with the aid of the UNCSAM (Janssen et al., 1992) program, a program that calculates sensitivity indicators based on regression and correlation. The PEST (Doherty, 2000) program and the SCE-UA (Shuffled Complex) method (Duan et al., 1992) were used for the calibration of the Dender model. The Nete model was calibrated manually. Uncertainty analysis was performed based on the 5% and 95% confidence bounds, calculated in Microsoft Excel and the optimal experimental design was executed with a linkage of software tools where all the links and the executables are programmed in Perl code.

The models of the two case studies, Dender and Nete were made with different tools.

The river water model for the river Dender had already been implemented in ESWAT (Extended Soil and Water Assessment Tool). The SWAT code was extended by (van Griensven and Bauwens, 2001) to be able to also consider urban drainage and to allow the calculation of urban processes. For the river Nete, the model was implemented in WEST® (World-wide Engine for Simulation, Training and Automation) (Ghermandi, 2004; MOSTforWATER NV). WEST® is a multi-platform modelling and experimentation system. It allows one to construct models and conduct virtual experiments (simulations) on any kind of system that can be represented by differential and algebraic equations. The waste water treatment models, a runoff/sewer model and tanks-in-series river models are now implemented in this package (Meirlaen et al., 2001; Solvi et al., 2005). The advantage of the use of this model is that WEST has an open structure in which the user is allowed to change existing models and define new ones as needed. In that way, for example, the algal growth model in RWQM1 could be changed for the model of the Nete.

5. Outline of the thesis

After the introduction (chapter I), this dissertation starts with a literature review (chapter II). In there, the reader will find a general part about legislation and modelling which comprises of ‘Water quality regulations’ (II.1), ‘Water pollution’ (II.2), ‘Water system modelling’ (II.3) and a part about Modelling methodologies with ‘Sensitivity analysis’ (II.4), ‘Uncertainty analysis’ (II.5) and ‘Optimal experimental design’ (II.6). Before the chapters of the own research, chapter III and IV describe the ‘Materials and Methods’ and the ‘Case studies’ used in the research part. Chapter V is the own research about ‘calculation and reduction of output uncertainties”, after an introduction (V.1) in which all of the studies done here are situated in the modelling process, in eight subparts different methods are presented for the calculation and reduction of output uncertainties, ‘Effect of different river water quality model concepts used for river basin management decisions’ (V.2), ‘Sensitivity analysis to identify ‘soft data’ for the evaluation of a river water quality model’ (V.3) ‘Optimal experimental design in river water quality modelling’ (V.4), ‘The evaluation of uncertainty propagation into river water quality predictions to guide future monitoring campaigns’(V.5), ‘Sensitivity analysis to define the most sensitive parameter subset for auto-calibration of a river water quality model’ (V.6), ‘Importance of the selection of model parameter subsets’ (V.7), ‘Cost-effectiveness of in-stream aeration to improve river water quality’ (V.8) and ‘Assessment of the effect of shading

on river water quality for the Nete river' (V.9). The last chapter contains the 'Conclusions and perspectives' (chapter VI).

CHAPTER II
LITERATURE REVIEW

Parts of this chapter were published as:

- Vandenberghe, V., van Griensven, A. and Bauwens, W. (2001). Sensitivity analysis and calibration of the parameters of ESWAT: Application to the river Dender. Water Science and Technology, 43(7), 295-301
- Vandenberghe, V. , van Griensven A. and Bauwens W. (2002). Detection of the most optimal measuring points for water quality variables: application to the river water quality model of the river Dender in ESWAT, Water Science and Technology, 46(3), 1-7
- Vandenberghe, V., Bauwens, W. and Vanrolleghem, P.A. (2004). The Evaluation of Uncertainty Propagation into River Water Quality Predictions to Guide Future Monitoring Campaigns. Environmental Monitoring and Software, 22, 275-232.
- Vandenberghe V., van Griensven A., Bauwens W. and Vanrolleghem P.A. (2006). Effect of different river water quality model concepts used for river basin management decisions Water Science & Technology, 53(10), 277-284.

CHAPTER II: LITERATURE REVIEW

1. Water quality regulations

In the early stages, water quality regulation was based on physical and chemical water quality criteria. However, this is not reliable unless it is supplemented by biological criteria. Currently, the physicochemical method is thus supplemented by biological and ecological criteria for the purpose of restoring and maintaining the ecological integrity of water resources. Among such water quality criteria, the new EU Water Framework Directive (WFD) (CEC, 1999) and the Clean Water Act (CWA) of the USA are the most important water quality regulations in use today.

1.1. EU Water Framework Directive (WFD)

The historical development of the European Union (EU) water legislation is presented elsewhere (Blöch, 2001; Kallis and Butler, 2001; Tyson et al., 1993; Zabel et al., 2001), and can be summarized into three "waves". In the "first wave" of EU water regulations, before 1980 (after the Treaty of Rome was signed in 1972), the main concern was directed to the protection of "public health" and harmonization of environmental rules to avoid market distortion. This first legislation can be broadly characterized into two types (Somsen, 1990): water use directives and water pollutant directives. The water use directives include drinking water directives (CEC, 1975 and 1980a), the water for bathing directive (CEC, 1976a), fish and shellfish harvesting directives (CEC, 1978; CEC, 1979). Water pollutant directives include the dangerous substance directives for surface waters (CEC, 1976b) and for groundwater (CEC, 1980b). This legislation addressed only a limited number of waters such as those rivers and lakes used for drinking water abstraction. As the ecological degradation was not addressed in this early water legislation, the nutrient load from urban systems and agricultural sites resulted in considerable deterioration of the ecosystems mainly due to eutrophication, disappearance of wetlands and salination of coastal groundwater. This ecological problem resulted in the "second wave" of EU water legislation in which two important water legislations were adopted: the Urban Wastewater Directive (CEC, 1991a), which addresses the water pollution from all settlements and the Nitrates Directive (CEC, 1991b), which addresses the water pollution by nitrates from agriculture. Whereas the Urban Wastewater Directive had already achieved considerable progress in getting the surface water cleaner, the nitrate level still remained high in rivers, and the implementation of the nitrate directive was indicated to be unsatisfactory because the EU water policy was fragmented in terms of objectives and means to control water pollution.

Consequently, a new single piece of framework legislation was proposed, which involves a range of instruments, scientific and technical cooperation at regional and European level. This brings about the "third wave" or the current period of EU water legislation, the so-called new European water policy or the Water Framework Directive (WFD). This new directive is established with the following key objectives (Blöch, 2001):

- protection of all waters such as surface water and groundwater;
- achieving "good" ecological and chemical status for all water by a set deadline of 15 years;
- water management based on a river basins approach;
- emissions and discharges control by a "combined approach" of emission limit values and quality standards;
- getting the price right: mandatory pricing policy for water, contributing to the wise use of water and thus to resource protection, and
- getting the citizen involved more closely: strengthen public participation.

Summarizing, the ultimate goal of the directive is to achieve a "good" ecological and chemical status in the surface waters and "good" chemical status in groundwater. Surface water is of good ecological quality if there is only slight departure from the biological community that would be expected in conditions of minimal anthropogenic impact. This indicates that the standard process is provided in the WFD for defining local standards accordingly. To achieve the ultimate objective, the directive introduced other mandatory approaches as indicated above: river basin approach, combined approach, setting water price and strengthen public participation. The river basin approach is the main innovation of the directive in the sense that rivers and lakes will need to be managed by the natural geological and hydrological unit instead of according to only administrative or political boundaries. This approach is generally agreed as the most effective way to address water pollution by all possible sources.

1.2. USA: the Clean Water Act of 1972

Increasing environmental concerns resulting from water quality degradation in the United States led to the passage of the Federal Water Pollution Control Act Amendments of 1972 (PL 92 92-500) and amendments passed in 1977 (PL 95-217) and in 1987 (PL 100-4), collectively referred to as the CWA (Chen et al., 1993). The objectives of the Clean Water Act (CWA) include:

- restoring and maintaining the chemical, physical, and biological integrity of the nation's waters;
- achieving water quality suitable for protection and propagation of aquatic life and to provide for water recreation, and

- achieving the ultimate goal of eliminating the discharge of pollutants (zero discharge).

The Total Maximum Daily Load (TMDL) concept is used as a guiding principle to restore the polluted waters. It accounts for all sources of pollution: since 1999 both point and non-point source pollution are considered. Before that time TMDL only considered point source pollution. The TMDL is the amount of specific pollutants that a river, stream or lake can assimilate while still meeting the water quality standards. The Clean Water Act requires that regulatory agencies determine total maximum daily loads for every water body that does not meet water quality standards. The TMDL is calculated for water bodies and the control measures are implemented to ensure that this level is never exceeded. It is developed in two steps: calculation of the maximum amount of a pollutant that a water body can take in and still meet the water quality standards, and a distribution of that amount to the pollutant's sources. To implement the TMDL, the regulations agency works with local governments and the public to determine how to reduce pollutant loads to bring the impaired water into compliance. The implementation of TMDL most often involves putting Best Management Practices (BMPs) in place or upgrading the wastewater treatment plants. Being based on the river basin approach, the water legislation in the EU and the USA share the same approach in addressing the protection of all waters from all sources of pollution. Indirectly, the water legislation in both EU and USA may influence wider international developments in water policy, as they will provide a major reference to other countries in reforming their water policies and institutions.

1.3. Developing countries

When discussing water quality regulation in developing countries, it is important to note the difference between developing and poor developing countries, as these two groups of countries differ in setting their priorities. In developing countries like in Malaysia, South Africa and Thailand numerous efforts haven been initiated to overcome environmental degradation (Ujang and Buckley, 2002), e.g. setting new regulations and policies, and initiating university-industry collaboration on pollution prevention and cleaner production. It is also indicated that the water quality policy development in developing countries is progressing in a similar way to the developed countries (EU, USA and Japan), i.e. they are moving towards the river basin approach.

In poor developing countries on the other hand, the situation is different in the sense that economic activities are declining, leading to political instability and environmental degradation. In many situations, water resources are limited and water quality is deteriorating, particularly in the case of Africa and South Asia. In these countries, water pollution issues are therefore not the main concern because other issues such as national security, food availability and epidemic control are more pressing. The general problems in these countries are also outlined in Ujang and Buckley (2002) and summarised as follows:

- lack of environmental awareness among the majority of policy makers and the general public create a situation where water and wastewater management sectors are perceived to be less important than other sectors such as military empowerment, food security, road improvement, electricity, mass education and health care facilities;
- insufficient expertise, leading to gaps between ideal policies and implementation;
- inappropriate policies on the conservation of water resources, e.g. no legislation for deforestation activities in water catchment areas;
- insufficient funding for water supply and sanitation programmes because of competing public expenditure due to rapid urbanization and population growth;
- insufficient water resources, especially in arid and urban areas, and
- inappropriate management systems and institutional support for providing water supply and sanitation facilities.

It should be noted that water quality management needs to be developed in line with economic development otherwise the environmental issues may limit the progress of the economy. Many examples can be given. Developing artificial ponds or lakes for water supply and irrigation services in arid and semi arid regions is particularly an important one. If the artificial pond or lake is not protected from pollution due to agricultural runoff, the water quality of the lake or pond will deteriorate with time due to high salinity or contamination by pesticides/herbicides. Such water quality deterioration will in turn affect the economic activities such as irrigation and drinking water supplies.

2. Water Pollution

Water pollution is a large set of adverse effects upon water bodies caused by human activities. There exist two main types of water pollution: point pollution and diffuse pollution. Also other natural causes of pollution exist such as volcanoes, algae blooms, storms, and earthquakes, but these are not further discussed in this literature study.

2.1. Point pollution

Point pollution is characterised by a fixed location and a discharge structure like a discharge pipe or a sewer overflow construction. The main point pollution discharges are the industrial loads and the loads coming from wastewater treatment plants (WWTPs). Further there is still pollution coming from unconnected households. The emissions or large point pollution sources are most often well known due to regular measurements. The emissions of smaller industries are often just estimated on the basis

of average values of water discharge per sector. Unconnected households are also estimated with an average pollution load per inhabitant. Emission limits are fixed in legislation. Table D1 in Appendix D gives the emission limits as stated in European legislations.

2.2. Diffuse pollution

Diffuse pollution also referred to as non-point pollution results from the release of a variety of substances in many different situations. It includes:

- nutrients such as nitrogen and phosphorus from over-application of fertilisers and manures;
- faecal and other pathogens from livestock and from overloaded and badly connected drainage systems;
- soil particles from arable and livestock farming, upland erosion, forestry, urban areas and construction and demolition sites;
- pesticides, veterinary medicines and biocides from industrial, municipal and agricultural use, poor storage and handling, and run-off;
- organic wastes (slurries, silage liquor, surplus crops, sewage sludge and industrial wastes) that are poorly stored or disposed of and spread to land;
- oil and hydrocarbons from car maintenance, disposal of waste oils, spills from storage and handling, road and industrial run-off;
- chlorinated solvents from industrial areas where the use of solvents is ubiquitous;
- metals, including iron, acidifying pollutants and chemicals from atmospheric deposition, abandoned mines, industrial processes etc.

Rural areas should not always necessarily be considered as pollutant areas. Non-intensive grazing for instance has beneficial effects on erosion reduction and does not cause excessive nutrient loads to the receiving systems. In Europe, an evolution towards more intensive practices took place during the past decades and has caused an increase of nutrient release into the environment (Poirot, 1999). Under the Common Agricultural Policy of the EU, the Gross Value Added (GVA) of the agricultural sector has raised sharply over the last 25 years. This was mainly due to the increased investments giving an increase of the volume of production (Barthelemy and Vidal, 1999). The measures have generally led to a reduction of permanent grassland in favour of wheat, maize, the appearance of oilseed and protein crops and annual crops as fodder. The livestock production also follows a trend to intensification, where the small extensive holdings are replaced by modern and specialised ones. These "non-land-bound" farms resulted in a considerable growth in the livestock sector (Boschma et al., 1999). In particular, the pig husbandry constitutes the most intensive type. The intensification in livestock

production and crop culture has lead to a high application of nutrients to agricultural land. Livestock manure is the second most important source in the EU. The Netherlands and Belgium had the highest input of nitrogen from manure per hectare coming mostly from pig production (Pau Val and Vidal, 1999). Within the European soils, 115 millions of hectares suffer from water erosion and 42 million hectares from wind erosion (Montarella, 1999). Most agricultural activities are considered to be non-point sources. This is not the case for the large "non-land-bound" farms that are agricultural enterprises where a large number of animals are kept and raised in confined areas. The feed is here generally brought to the animals, rather than that the animals are grazing or otherwise seeking feed in pastures, fields or rangeland. Such activities are treated in a similar manner to other industrial sources of pollution. Whereas point-source pollution can be measured by monitoring the discharge and the water quality, diffuse pollution sources are very difficult to monitor because the sources are distributed along the river.

3. Water system modelling: actual situation

Integral water system management needs a good foundation when it comes to juridical questions, decision-making, the set up of water management plans and the realisation of the decisions in practice. To completely understand the causes of perturbations in the water system (bad water quality, poor ecology, flooding, …) and to restore the natural equilibriums, it is best to work in an integrated way and to work in a complete cycle of optimal measuring networks, accessible data and useful numerical models. This would allow to comprehend the water system in all its aspects and provide the necessary input for integral water management (reports of actual situation, evaluations, scenario calculations,…). The integration of all possible knowledge around water systems is still a big challenge. At the moment however, it is mostly the case that the different subsystems (sewers, wastewater treatment plants, receiving water, groundwater) are supervised by different organisations and there is little communication between them. When looking at modelling, everyone uses different models, there is no linkage between models for different subsystems, reliability analysis is rarely done, and the need of input data for all those models is not structured and as such gathered data is mostly not complying with the data needs. New European projects (www.CD4WC.info, www.tiszariver.com, www.SMURF-project.info,…) tried to overcome this by studying the interactions among the different subsystems, gathering all knowledge into a central database, working out a case study for improvement of an urban river. In all those projects one of the main conclusions was the need for more and better input data for the models. Methods that help formulating which data collections are most useful for a certain model, can fill this gap. At the end of each model use, the user can then use these methods to not only indicate the need for more data but also to exactly formulate the desired accuracy, frequency, place and period of the data collection.

3.1. Water quality modelling

One of the models used for the subsystem 'receiving water' is the water quality model. This dissertation is focussing all its efforts on water quality modelling. Water quality models try to support the decision making process in a scientific and technical manner. Those models make it possible to quickly and systematically run simulations over large simulated periods and the results and conclusions are based on scientific assumptions. Models allow visualising the results in an attractive manner, which makes the transfer of knowledge easier. Simulations of future scenarios are also possible with the aid of models.

In most modelling applications, research is based on the following research themes:

- the oxygen balance
- eutrophication
- pollution by heavy metals
- pollution by pesticides

In the past, scenarios were mainly based on the reduction of pollution loads, nowadays also scenarios with actions taken in the receiving water itself are evaluated. Evaluations of reduction in point pollution and diffuse pollution showed often that the receiving water quality is not improving as expected according to the effort related to the reduction of those pollution sources. With the aid of models, those effects can be investigated a priori before large investments are done that do not give the desired effect.

3.2. Water quality models

Models are usually grouped into categories based on the environment modelled, the purpose of the model, the number of dimensions considered, how the processes are decribed, whether the data used are discrete observed measurements or statistical distributions and whether temporal variability is considered (see figure II.1). The above subdivisions give information about the limitations of a particular model. When looking at the purposes of the models, one knows that hydrochemical models are designed to model the chemical and biological processes and the main aim is to represent water chemistry. A mixing zone model will only represent that portion of the system that is immediately downstream or adjacent to a discharge point into the water and a time-of-travel model provides the user with the time of arrival of pollutants downstream of an accident and so is only used to simulate simple pollution incidents.

The dimensions simulated by a particular model will provide information on both the complexity of a model and also on its suitability to specific applications. A 0D model

does not represent the processes of dispersion of contaminants in any direction but simply represents the volumes and concentrations assuming that the water body is completely and instantaneously mixed. A one-dimensional (1D) model represents the water flow and the advection and dispersion of solutes in just one direction (i.e. downstream in a river model) and so the stream is assumed to be completely and instantaneously mixed across its width and depth. Following from this, a two-dimensional (2D) model will either simulate dispersion across the width or the depth of the stream but not both. Three-dimensional models (3D) account for the water flows and solute transport in all directions. These models are complex and sophisticated and usually are reserved for large (deep and wide) estuaries where the mixing patterns are complex (Cox, 2003).

The difference between mechanistic and empirical models is often not clear-cut and mechanistic descriptions will often contain empirically derived components. Empirical models make no attempt to explicitly model hydrochemical processes. The model inputs are related directly to its outputs by one or more experimentally obtained relationships. They do not represent any mechanism and are as such often referred to as black-box models. They can cope with a large number of inputs with minimal computation requirement. Mechanistic models quantitatively describe the relationship between the variables and the underlying principles of cause and are physically based. A last division can be made according to the time variation: dynamic and steady state models. Dynamic models describe the behaviour of a system over time whereas the outputs of steady-state models do not change in time.

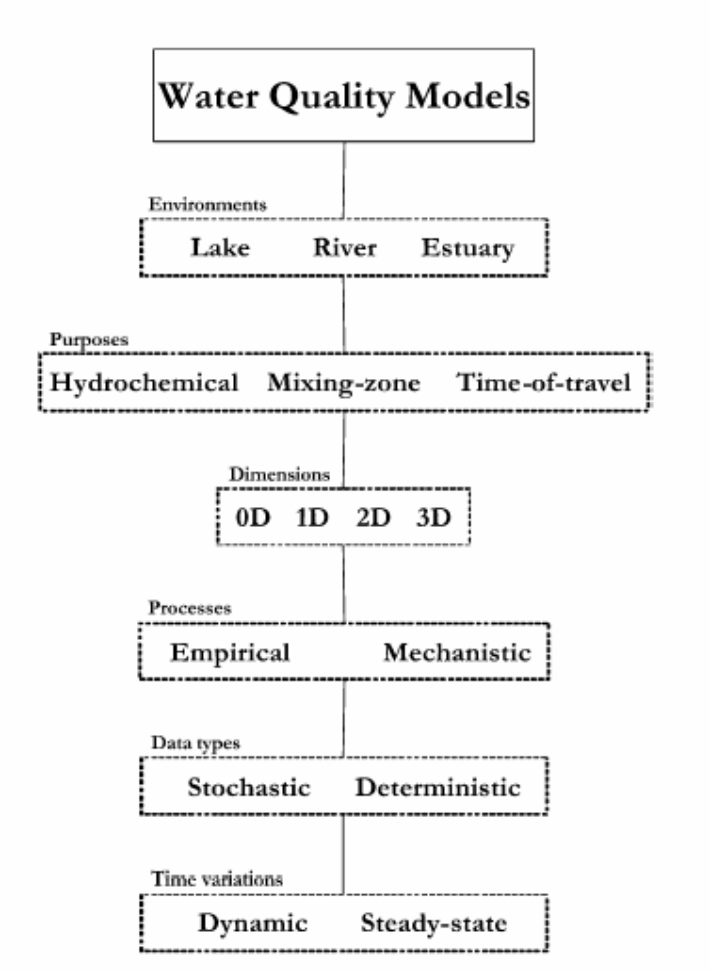


Figure II.1 Different categories of water quality models

Two main trends in mechanistic river water quality modelling can be identified. These are represented by the traditional QUAL2E model that is based on the original Streeter–Phelps equations and the recently developed RWQM1 (River Water Quality Model nr 1) based on the mass balance-based approach adapted in the ASM (Activated Sludge Model) for waste water treatment plants (WWTP).

Qual2E

During the 1980s and 1990s the standard model in water quality was QUAL2E (Brown and Barnwell, 1987; Shanahan et al., 1998). QUAL2E is an example of a multiconstituent river ecosystem model. This model is able to predict a variety of water quality constituents including conservative substances, algal biomass and Chlorophyll-a, ammonia, nitrite, nitrate, phosphorus, carbonaceous biological oxygen demand

(cBOD), sediment oxygen demand, dissolved oxygen (DO), coliforms and radionuclides.

The main state variables are BOD and DO. By adding new variables and constituents, the model became a three layer model (Masliev et al., 1995)

- The phenomenological level: the traditional Streeter-Phelps state variables (BOD and DO)
- The biochemical level: the extended Streeter-Phelps model variables (ammonia, nitrate, nitrite and sediment oxygen demand (SOD)
- The ecological level: the algae model variables (organic nitrogen, organic phoporus, dissolved phosphorus and chla)

The QUAL2E model is until now the most widely known model for river water quality. A large number of eutrophication models are based on its process descriptions and it is implemented in a large number of simulation programs, e.g. SWAT (Arnold et al., 1996), QUAL2K (Park and Lee, 2002), WASP5 (Ambrose and Martin, 1993), ISIS (Wallingford, 1994), DUFLOW-EUTRO (Aalderink et al., 1995), MIKE11 (DHI, 1992),… QUAL2E was designed for steady state conditions, but it is also coupled to complex hydrodynamic models to be applicable for unsteady state conditions, e.g. ESWAT(van Griensven et al., 2000), CE-QUAL-RIV1 (U.S. Army Corp of engineers, 1995), CE-QUAL-ICM (Cerco and Cole, 1995), WASP5 (Masliev et al., 1995; Shanahan et al., 1998) point toward problems with the use of QUAL2E, like non-closed mass balances, e.g. the decay of algal biomass is not included in the BOD, processes in the sediments are not linked to the river column processes. Further, the variable BOD as a measure for organic carbon, only has a biological meaning, is hard to estimate and not a quantitative mass value.

RWQM1

In order to overcome some of the problems with QUAL2E, a new model has recently been developed, the River Water Quality Model No.1 (RWQM1) (Reichert et al., 2001b). The main goal of this effort, however, was to formulate a suite of standardised, consistent river water quality models and guidelines for their use. Moreover, RWQM1 was aimed to be compatible with the existing ASM models since they are both COD-based models, so no conversion between variables are needed anymore when modelling in an integrated way whereby connection of ASM based models and a river model is needed. RWQM1 introduced bacterial biomass as an explicit component. In this way, bacterial concentration can vary in time, allowing a better description of the observed water quality changes without modifications of the parameters. It also introduces some new processes that were not included in QUAL2E like pH equilibrium reactions, precipitation and predation processes. No anaerobic processes are included in the

general model structure. RWQM1 is designed to have closed mass and elemental balances. For every organic component a fixed composition is given, described by the mass fractions αC (carbon), αH (hydrogen), αO (oxygen), αN (nitrogen), αP (phosphorus) and αX (all the other elements), which moreover sum to one. With the aid of the chemical oxidation reaction and a choice of a reference compound for every element considered, the COD of each form of organic matter can be determined. For all reactions the ionic charge balance is closed as well.

The RWQM1 model is implemented in the following software platforms: WEST (MOSTforWATER NV), Aquasim (Reichert, 1994) and ESWAT (van Griensven and Bauwens, 2001).

3.3. The modelling process

In this section the process to make a model of a water body is described. Focus is here on the different steps that preferably should be taken when modelling for the purpose of WFD compliance.

A modelling study will involve several phases and several actors. A typical WFD modelling study will involve the following four different types of actors (Scholten et al., 2004):

- The water manager, i.e. the person or organisation responsible for the management or protection of the water resources, and thus of the modelling study and the outcome (the problem owner).
- The modeller, i.e. a person or an organisation that works with the model conducting the modelling study. If the modeller and the water manager belong to different organisations, their roles will typically be denoted consultant and client, respectively.
- The reviewer, i.e. a person that is conducting some kind of external review of a modelling study. The review may be more or less comprehensive depending on the requirements of the particular case. The reviewer is typically appointed by the water manager to support the water manager to match the modelling capability of the modeller.
- The stakeholders/public. A stakeholder is an interested party with a stake in the water management issue, either in exploiting or protecting the resource. Stakeholders include the following different groups: (i) competent water resource authority (typically the water manager, cf. above); (ii) interest groups; and (iii) general public.

The WFD modelling process may, according to the HarmoniQuA project (Refsgaard et al., 2004, www.harmoniqua.org; Scholten et al., 2004) be decomposed into five major steps (figure II.2).

- STEP 1 (Model Study Plan). This step aims to agree on a Model Study Plan comprising answers to the questions: Why is modelling required for this particular model study? What is the overall modelling approach and which work should be carried out? Who will do the modelling work? Who should do the technical reviews? Which stakeholders/public should be involved and to what degree? What are the resources available for the project? The water manager needs to describe the problem and its context as well as the available data. A very important task is then to analyse and determine what are the various requirements of the modelling study in terms of the expected accuracy of modelling results. The acceptable level of accuracy will vary from case to case and must be seen in a socio-economic context. It should, therefore, be defined through a dialogue between the modeller, water manager and stakeholders/public. In this respect an analysis of the key sources of uncertainty is crucial in order to focus the study on the elements that produce most information of relevance to the problem at hand. This is achived with a sensitivity analysis.
- STEP 2 (Data and Conceptualisation). In this step the modeller should gather all the relevant knowledge about the study basin and develop an overview of the processes and their interactions in order to conceptualise how the system should be modelled in sufficient detail to meet the requirements specified in the Model Study Plan. Consideration must be given to the spatial and temporal detail required of a model, to the system dynamics, to the boundary conditions and to how the model parameters can be determined from the available data. The need to model certain processes in alternative ways or to differing levels of detail in order to enable assessments of model structure uncertainty should be evaluated. The availability of existing computer codes that can address the model requirements should also be addressed.
- STEP 3 (Model Set-up). Model Set-up implies transforming the conceptual model into a site-specific model that can be run in the selected model code. A major task in Model Set-up is the processing of data in order to prepare the input files necessary for executing the model. Usually, the model is run within a Graphical User Interface (GUI) where many tasks have been automated. The GUI speeds up the generation of input files, but it does not guarantee that the input files are error-free. The modeller performs this work.
- STEP 4 (Calibration and Validation). This step is concerned with the process of analysing the model that was constructed during the previous step, first by

calibrating the model, and then by validating its performance against independent field data. Finally, the reliability of model simulations for the intended domain of applicability is assessed through uncertainty analyses. The results are described so that the scope of model use and its associated limitations are documented and made explicit. The modeller performs this work.

- STEP 5 (Simulation and Evaluation). In this step the modeller uses the calibrated and validated model to make simulations to meet the objectives and requirements of the model study. Depending on the objectives of the study, these simulations may result in specific results that can be used in subsequent decision making (e.g. for planning or design purposes) or to improve understanding (e.g. of the hydrological/ecological regime of the study area). It is important to carry out suitable uncertainty assessments of the model predictions in order to arrive at a robust decision. As with the other steps, the quality of the results needs to be assessed through internal and external reviews.

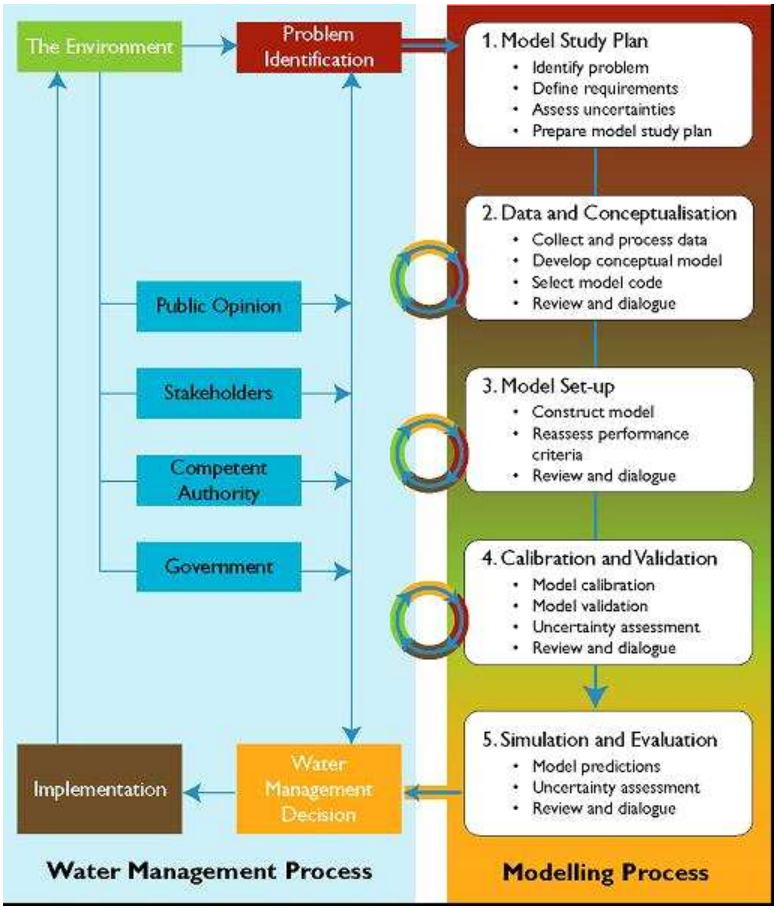


Figure II.2. The modelling process in water management (Refsgaard et al., 2004)

Sensitivity analysis can be used as an aid in identifying the important uncertainties for the purpose of prioritizing additional data collection or research (Frey et al., 2004). In

addition, sensitivity analysis can play an important role in model verification and validation throughout the course of model development and refinement (Fraedrich and Goldberg, 2000; Wagener, 2003). Sensitivity analysis also can be used to provide insight into the robustness of model results when making decisions (Saltelli et al., 2000).

Modelers conduct sensitivity analysis for a number of reasons including the desire to determine:

1. Input parameters that contribute most to output variability, thereby requiring additional research to increase knowledge of parameter behaviour in order to reduce output uncertainty;

2. If parameter interactions are present, which (group of) parameters interact with each other;

3. Which parameters are insignificant and can be held constant or eliminated from the final model; and

4. The optimal regions within the parameter space for use in subsequent calibration studies.

Sensitivity analysis methods have been applied in various research fields, including complex engineering systems, economics, physics, social sciences, medical decision making, and others (e.g., (Helton, 1993)).

As can be seen in figure II.2 sensitivity and uncertainty assessments should be done in step 1, 4 and 5. Sensitivity analysis can find the parameters that are important in the calibration. Uncertainty assessment can either help to detect the most important sources of uncertainty or to quantify the uncertainties on the model results. Further in this literature review methods for sensitivity analysis and uncertainty analysis will be discussed.

4. Sensitivity analysis

4.1. Introduction

Sensitivity analysis (SA) is “The study of how the uncertainty in the output of a model (numerical or otherwise) can be apportioned to different sources of uncertainty in the model input” (Saltelli et al., 2000). This definition is general enough to cover a variety of strategies for sensitivity analysis, while committing the strategy to some sort of quantitative partition of the output uncertainty (no matter how this uncertainty is defined) into factors-related components.

Originally, SA was created to deal simply with uncertainties in the input variables and model parameters. Over the course of time the ideas have been extended to incorporate

model conceptual uncertainty, i.e. uncertainty in model structures, assumptions and specifications. As a whole, SA is used to increase the confidence in the model and its predictions, by providing an understanding of how the model response variables respond to changes in the inputs, be they data used to calibrate the model, model structures, or factors, i.e. the model independent variables. SA is thus closely linked to uncertainty analysis (Beven, 2007; Refsgaard et al., 2007), which aims to quantify the overall uncertainty associated with the response as a result of uncertainties in the model input.

Often the terms sensitivity and uncertainty analysis are mixed as both are sometimes using the same techniques. One can say that SA focuses on the inputs and studies the influence of variations on parameters, initial conditions and inputs on model outputs, whereas UA is more related to uncertain aspects in the modelling process and its influence on the model outputs.

In order to apply sensitivity analysis, it is paramount to understand in which ways parameters and factors can be varied. For example, it may be necessary to run the model(s) with a multiple set of parameters (e.g. a floodplain model with different surface roughness parameters) to observe the change in the prediction variable (e.g. flood inundation extent). In sensitivity analysis this is understood as Experimental Design, which will be discussed in part II.4.3.

Fundamentally, sensitivity analysis can be grouped in four major subdivisions, which are graphical methods, screening methods, local methods and global methods:

Graphical methods include different ways to plot results of model outcome and parameters (e.g. scatter plots) or of other sensitivity analyses themselves (e.g. in the form of histograms).

Screening methods are often preliminary numerical experiments whose purpose is to isolate the most important factors amongst a large number that may affect a particular model response. By using screening methods, factors can also be ranked in their order of importance. However, the percentage of the output variation that each factor is accounting for cannot be quantified.

Local methods investigate how small changes of parameters affect the model output. Therefore, these analysis techniques evaluate this partial derivative at one specific set of parameter values, also called the nominal parameter set. For some local methods, differential equations need to be solved and will require complex manipulations of the model equations. However, this is often not practically feasible because the models are too complicated or the model equations are not directly accessible (e.g. because they are compiled in executable commercial code).

Global methods evaluate the effect on the model output by varying all parameters at the same time, in a multivariate fashion. Properties of global methods should be the

inclusion of the influence of range and shape of the probability distributions of the input factors; the sensitivity estimates of individual factors are evaluated by varying all other factors as well (multidimensional averaging); and global methods should be model-independent, i.e. they should work irrespective of the non-linearity, interaction structure and possible discontinuity of the model at hand.

An important approach to sensitivity, which has developed in the last few years, falls within the emulation context. More about model emulators is given in II.4.4 of this chapter. The basic idea is to represent in a direct way the relationship between model output and model parameters or factors without the need to run the model multiple times. If the emulation exercise is successful, one can obtain a simple relationship between the model parameters or factors and the model output that fits well the original model and is less computationally demanding. Given the emulator, this can be used to compute any measure of interest, including sensitivities.

4.2. Examples

The methodologies, which will be introduced in what follows, have been demonstrated on two examples. These are purely mathematical functions, which have been used earlier to demonstrate sensitivity analysis techniques (Ratto et al., 2004; Saltelli et al., 2004).

4.2.1. Example 1

The first example is a simple additive combination of two factors. The example is taken from Saltelli et al. (2004):

$$Y = X_1^2 + X_2^2$$

with

$$X_j \sim U(-0.5, 0.5)\,|_{0.2<Y<0.25}$$

Y: Predicted variable

X_j: Factors j

U: Uniform distribution

4.2.2. Example 2

This example uses the Sobol g-function that is a non-linear and non-additive model. It has been used in previous studies to test global sensitivity analysis models (Ratto et al., 2004; Saltelli et al., 2004).

$$Y = \prod_{j=1}^{k} g_j(X_j)$$

where

$$g_j(X_j) = \frac{\left|4X_j - 2\right| + a_j}{1 + a_j}$$

with $a_j \geq 0$ and $X_j \approx U(0,1)$

Y: Predicted variable

X_j: Factors j

U: Uniform distribution

This allows to tune the importance of the factors by changing a. The smaller a is the more important it should be. For this structure eight input factors have been considered (k=8) with a_j=[0,1,4.5,9,99,99,99,99].

4.3. Experimental design of SA (Sampling)

Different sampling procedures exist, the most important ones are: screening design (one-at-a-time, Morris, fractional factorial), random sampling, Latin Hypercube sampling, correlation control and quasi-random sampling. The two first ones are used in the screening methods, which are explained in section 4.3.1 and the others can be used for the global methods, explained in section 4.3.3.

4.3.1. Screening design

Probably the simplest way to sample parameters for doing a sensitivity analysis is to use a `one-at-a-time' (OAT) design, where only one parameter changes values between consecutive simulations. Hence, if there is any change in value of the output between two consecutive simulations, it can only be attributed to a change in the parameter x_i that has been changed. OAT sampling is inefficient when the number of parameters k is large and only a few of them are influential. Each simulation changes the value of one parameter. If only a few parameters are influential, most of the simulations would be devoted to determining the very small effects of non-influential parameters. These simulations would be duplicates as far as the values of influential parameters are concerned. Very little new information would be generated.

It is possible that there are no influential parameters for sensitivity analysis to reveal. This happens when sensitivity analysis indicates that many parameters have similar small effects, but cannot give further insight into this model's behaviour. All of the parameters are equally non-influential. Usually, however, there are a few parameters

that stand out from the rest. So with large numbers of parameters, it is desirable to find a more efficient approach than changing one parameter at a time.

In fractional factorial design (FF), a fraction of a full factorial design is 'cleverly' selected to generate a smaller, feasible design that can still produce useful results. In general, if one starts with a full factorial design on two levels for n parameters, requiring $k = 2^n$ simulations, it can be converted into a fractional factorial (FF) design for k-1 parameters.

Morris design is perhaps one of the most efficient ways to sample parameters for screening purposes. It allows estimating sensitivity measures at the cost of $r(k+1)$ model runs, where k is the number of parameters and $r \approx 8$ (see dedicated part in section 4.4.1 on the Morris screening method).

4.3.2. Random sampling

Here the input factor is sampled randomly according to the joint probability distribution. This is a technique easy to explain, provides unbiased estimates for means, variances and distribution functions and is easy to implement. The problem is that the sample of parameter values has to be sufficiently large and that the term 'sufficiently' is not well defined. When the underlying models need a long time to evaluate then the required sample size to achieve a certain purpose may be too large to be computational practicable.

4.3.3. Latin Hypercube Sampling (LHS)

The Latin Hypercube Sampling method uses a stratified sampling approach (McKay et al., 1979) to ensure the full coverage of the range of each variable. It subdivides the distribution of each parameter into N ranges, each with a probability of occurrence equal to 1/N. Random values of the parameters are generated such that each range is sampled only once. . It is possible to combine two-level FF and LH sampling, to secure the advantages of both (see e.g. Saltelli et al. (2007)).

4.3.4. Correlation control

Control of correlation within a sample can be very important. If two or more parameters are correlated, then it is necessary that the appropriate correlation structure is incorporated into the sample if meaningful results are to be obtained in subsequent uncertainty/sensitivity studies. What is present in most situations is some idea of the extent to which parameters tend to move up or down together and more information about variable linkage is not available. Therefore the measures of correlation can not be determined quantitatively but an idea of which variables are related is present. So for

most uncertainty/sensitivity analysis problems, rank correlation is probably the most natural measure of congruent variable behaviour.

4.3.5. Quasi-random sampling with low-discrepancy sequences

Using a pseudo-random generator for sampling is much simpler than using a complex design: as many values as necessary can be generated, and if more parameters or more simulations are desired, it is a simple matter to generate more. Unfortunately samples generated randomly tend to have clusters and gaps. Where a cluster occurs, function values in that vicinity are overemphasized in statistical analysis. Where a gap arises, function values within that gap are not sampled for statistical analysis. The net effect is that mean values estimated with random samples have an uncertainty that diminishes slowly as $1/\sqrt{N}$. To reduce an estimated uncertainty by a factor of 10, the analyst must increase N by a factor of $10^2 = 100$.

A mathematical measure called discrepancy characterizes the lumpiness of a sequence of points in a multidimensional space. The discrepancy of a sequence of points is the maximum absolute difference over a specified set of regions between the area fraction and the point fraction. Smaller discrepancy values are better for sensitivity analysis (the distribution is less lumpy).

Random sequences (and also LH samples) of k-dimensional points have a relatively high discrepancy (see e.g. Saltelli et al. (2007)). But there are infinite sequences of k-dimensional points that behave much better with respect to this measure. They are called low-discrepancy sequences.

They have the property that as the sequence length N gets very large, the discrepancy shrinks at the theoretically optimal rate. As a result, an estimated mean for a function $y = f(x_1,...x_k)$ evaluated on points $(x_{i1},...,x_{ik})$, $i = 1,...,N$ from such a sequence will converge much more quickly than would an estimated mean based on the same number of random points. While the rate of stochastic convergence for pure pseudo-random Monte Carlo methods is $N^{-1/2}$, the actual rate of convergence of quasi-Monte Carlo methods can be N^{-c} with $c \leq 1$ (Sobol, 1993). This means that the rate of convergence can be doubled, in such cases where c approaches one.

Samples made from a finite subset of such sequences are called quasi-random samples. These samples are not random, in the sense of being completely unpredictable. In fact, to maintain an even spread of points, an algorithm that generates low-discrepancy sequences must somehow bias the selection of new points to keep them away from the points already present. But they are like random points in the sense that they are uniformly distributed across the entire sample space.

4.4. Methods of sensitivity analysis

This section introduces different methodologies to perform sensitivity analysis. Categories of sensitivity analysis are introduced and followed by a more detailed explanation of each methodology.

4.4.1. Screening methods

Screening methods are preliminary numerical experiments whose purpose is to isolate the most important factors amongst a large number of factors that may affect a particular model response. By using screening methods, factors can be ranked in order of importance. However, the percentage of the output variation that each factor is accounting for cannot be quantified.

One-At-a-Time (OAT)

This is the simplest class of screening designs. Here a set of simulations is performed in which only one parameter is modified between two consecutive simulations. Therefore, changes in the model outcome can for sure be assigned to that modified parameter and the magnitude of the change is an indication of the sensitivity.

OAT can be classified into five categories (Saltelli et al., 2000)

- Standard OAT, which varies one factor from a standard condition (from a nominal value to an extreme value)
- Strict OAT, which varies one factor from the condition of the last preceding experimental run
- Paired OAT, which produces two observations and hence one simple comparison at a time
- Free OAT, which makes each new run under new conditions
- Curved OAT, which produces a subset of results by varying only one easy-to-vary factor

Many OAT experiments are local, that is, the factors are changed over small intervals around their nominal values. Results of such a local experiment are dependent on the choice of this point because the model behaviour is identified only locally in the input space. If the model results show strong non-linearity then a change in the selected nominal values provides totally different results.

Morris sampling

A sampling design that is not dependent on the choice of the specific point in the input space is that proposed by Morris (1991) (see figure II.3). The sampling design takes a number r of incremental changes for each input factor randomly selecting the initial

point on a grid of p-levels in the k-dimensional space of input factors. This provides a set of r 'elementary effects' (EE) for each input factor. In the original Morris work, taking the average (μ) and the standard deviation (σ) of the set of EE's allows to determine which factors have negligible effects, linear and additive effects or non-linear or interaction effects. Morris´ computational cost is of r(k+1) model runs for k input parameters. Campolongo et al. (2007) have developed and refined Morris' original work. The sampling strategy of Morris is improved to avoid oversampling of some levels and undersampling of others that often occurs in the standard Morris procedure. Moreover, only the mean of the absolute values of the elementary effects is computed (μ^*). For screening purposes, this is actually the only measure needed, since this alone is able to provide negligible input factors ($\mu^* \approx 0$). Moreover, it is rather resilient against type II errors, i.e. if a factor is seen as non-influential by μ^*, it is unlikely to be seen as influential by any other measure (Campolongo et al., 2007; Saltelli et al., 2004)).

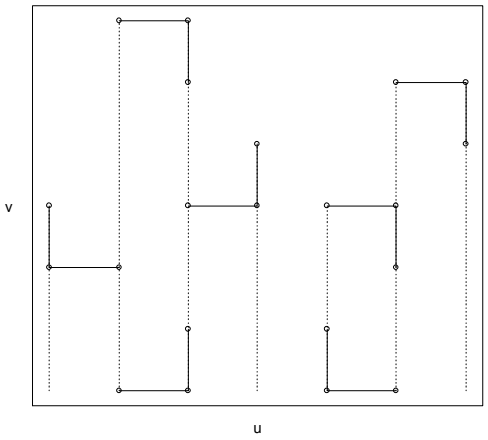


Figure II.3: Morris' OAT design

Advantages and Disadvantages

Screening procedures do not give any quantitative information about the sensitivity, so they are very useful as a first screening when the number of parameters is too high to perform a quantitative analysis. The low computational cost is one of the main advantages of the screening methods.

4.4.2. Local methods

Local sensitivity analysis methods refer to small changes of parameters. A factor is called sensitive if small changes produce significant changes in the output. On the other hand, a factor is called insensitive if changes of the factor produce insignificant changes in the model output. This variation can be analytically solved if the analytical solution

of the model equation is known. Unfortunately, this is rarely the case and numerical methods have to be used in order to approximate the sensitivity function. The sensitivity functions describe the effect of the disturbance in the parameters on the considered output in time. Since sensitivity functions are used in several applications like uncertainty analysis and optimal experimental design, model reduction, etc., it is of great importance that a correct approximation of the sensitivity function is calculated to produce accurate results. Various techniques for local sensitivity analysis will be described here, which are (a) the finite difference method, (b) the direct differential method, (c) Green's function method, (d) the polynomial approximation method and (e) automatic differentiation.

The finite difference method

The simplest way of calculating local sensitivities is to use the finite difference approximation. This technique is also called the brute force method or indirect method. It is very easy to implement because it requires no extra code beyond the original model solver. In this method an infinitesimal variation (perturbation) of the parameters, inputs or initial conditions is applied. It should be noted that only one parameter is perturbed at a time while all others are kept at their nominal value. The finite difference technique was found to be too computationally intensive, especially in cases with a large number of input factors (De Pauw and Vanrolleghem, 2003a).

Direct method for sensitivity analysis

Atherton et al. (1975) developed the direct method for sensitivity analysis. Differentiation of the equations with respect to the model factors yields a set of sensitivity differential equations. The solution of these equations results in the sensitivity functions. The direct differential method sensitivity analysis method relies on the fact that the sensitivity differential equations (obtained after differentiating the ordinary differential equation (ODE) system equations with respect to the parameters) are coupled with the equations of the ODE system. Both systems of differential equations are coupled through the jacobian matrix of the right hand side of the ODE system with respect to the states and the parameters. The implementation of this method is difficult, but the advantage is that less numerical simulations are needed and numerical problems of the finite difference technique are avoided.

Green function's method

The difficulties of solving the large sets of differential equations led to the development of the Green's function method, also called the variational method (Hwang et al., 1978). This method makes use of the fact that the sensitivities can be expressed in integral, rather than differential form. There are a number of variations of the Green's function method. Probably the most used method is the GFM/AIM method (Green Function's method/Analytically Integrated Magnus). It is beyond the scope of this document to go into more detail on these solving techniques. In all Green's function methods, the numerical effort is proportional to the number of variables and not the number of parameters. So this method should be preferred when the number of parameters is large compared to the number of variables. When the number of variables is much larger than the number of parameters, direct differential methods should be used.

Automatic differentiation

Recently, a technique called automatic differentiation has gained a lot of attention. Automatic differentiation techniques are based on the fact that every function, no matter how complicated, is executed on a computer as a sequence of elementary functions. By applying the chain rule of differentiation repeatedly to the composition of these elementary operations, one can compute the derivative information exactly and in a completely automated fashion. This method produces compilable code that evaluates derivatives up to machine precision with a minimum of human effort.

Advantages and Disadvantages

All the above techniques except for the finite difference technique have one thing in common. They all require complex manipulations of the model equations. In many studies this is not practically feasible because the models are too complicated or the model equations are not directly accessible (e.g. because they are compiled in executable commercial code). This is the basic reason why the finite difference method, although inefficient, is still used very often.

4.4.3. Global methods

Two key global properties are essential for global sensitivity methods (Saltelli et al., 2000):

- the inclusion of the influence of range and shape of the probability distributions of the input factors;

- the sensitivity estimates of individual factors are evaluated varying all other factors as well (multidimensional averaging).

Finally, global methods should be model-independent, i.e. they should work irrespective of the non-linearity, interaction structure and possible discontinuity of the model at hand. Four methods are presented here: variance based methods, regression analysis, regionalised sensitivity analysis and enthropy.

4.4.3.1 Variance based methods

Variance-based methods quantify sensitivity by decomposing the variance of model outputs into factor related components. In particular, the variance is decomposed into main effects and interaction effects. The main effect of a parameter quantifies the portion of the variance of the model output that is explained by that parameter, by allowing all other parameters to be varied at the same time. It can also be interpreted as the expected reduction in the variance (i.e. in the uncertainty) of the model output that could be obtained if we were able to fix that parameter to its 'true', albeit unknown, value. For this reason, the main effect provides the answer to the Factors Prioritization setting. The total effect of a parameter measures the residual variance of the model output that remains by removing the portion explained by all other parameters, i.e. quantifies the variance (i.e. the uncertainty) in the model output that would be left by fixing any other factor to its 'true', albeit unknown, value. The total effect of a parameter can also be seen as the sum of its main effect and all its interaction terms with any other model parameter. When a parameter has a null total effect, this provides a sufficient condition for assessing its irrelevance in the model. For this reason, the total effect provides the answer to the Factors Fixing setting. The total effect, main effect and interaction effects are normalized by the unconditional variance to obtain sensitivity indices. The variance-based analysis allows for an analytical solution of example 2:

Table II.1: Sensitivity indices of example 2

Factor	Main effect	Total effect
X_1	0.7165	0.7871
X_2	0.1791	0.2422
X_3	0.0237	0.0343
X_4	0.0072	0.0105
$X_{5,6,7,8}$	0.0001	0.0001
sum	0.927	-

Table II.1 shows that the main effects (i.e. the additive part of the model) account for about 93% of the entire output variation, implying that only 7% is due to interaction terms. Analysing the total effects, one can see that interaction terms involve parameters X_1, X_2 and X_3.

There are several methods available for the estimation of variance-based indices: the 'classic' ones are the Sobol' method, FAST and extended FAST. Moreover, reliable estimates of main effects and low order interaction effects can be obtained by applying parametric and non-parametric smoothing techniques (RS-HDMR, SDP, spline, see section 4.4.4 on emulation).

FAST

FAST is a methodology which allows to estimate the entire set of main effect sensitivities by Fourier transformation (Koda et al., 1979; McRae et al., 1982b), using a single sample of size N.

When using FAST, V_i is computed by exploring the k-dimensional space of the input factors with a search curve defined by a set of parametric equations

$$x_i = G_i(\sin(\omega_i s))$$

with $i = 1,2,...k$, where s is a scalar varying in $(-\infty,+\infty)$ and the ω_i are a set of different angular frequencies associated with each factor and the G_i are properly selected transformation function. Scanning the above equation for different values of s results in a curve in the k-dimensional hypercube whereby each dimension is explored with a different frequency ω_i. Fourier analysis allows then the computation of $V_{X_i}\left(E_{\mathbf{X}_{-i}}\left(Y|X_i\right)\right)$ based on the signal at ω_i and its harmonics. The implementation of the method requires care, mostly in avoiding interferences, based on accurate selection of the set of k frequencies ω_i (Koda et al., 1979; McRae et al., 1982b). Extensions of the FAST method are described in Saltelli et al. (1999) and Tarantola et al. (2006).

In classic FAST only the main effect terms V_i are computed. Extended FAST (Saltelli et al., 1999) allows the computation of higher order terms, in particular it allows to compute the entire set of main and total effects, at the cost of kN model runs.

The Sobol' method

The Sobol' method is a Monte Carlo procedure that allows to compute any term of the variance decomposition, each at the cost of N model runs (Sobol, 1993). Following Saltelli (2002), the cost of estimating the entire set of main and total effects is of (2+k)N model evaluations, which roughly halves the computational cost with respect to the original Sobol' algorithm. The method of Sobol' is based on decomposing the variance of model output into terms of increasing dimensionality, as in the classical Analysis Of Variance (ANOVA) of factorial experimental designs. The indices can be used for estimating the influence of individual variables or groups of variables on the model output.

ANOVA-representation

Consider an integral function f(x) defined in I^n. We shall study its representation in the form

$$f(x) = \sum_{s=1}^{n} \sum_{i_1}^{n} f_{i_1 \dots i_s}(x_i, \dots, x_{i_s})$$

where $1 \le i_1 < \dots < i_s \le n$.

The formula can also be given as

$$f(x) = f_0 + \sum_i f_i(x_i) + \sum_{i<j} f_{ij}(x_i, x_j) + \dots + f_{12\dots n}(x_1, x_2, \dots, x_n) \qquad (1)$$

The total numbers of summands in (2) is 2^n.

Formula (1) is called the ANOVA representation (comes from Analysis Of Variance) of f(x) if

$$\int f_{i_1 \dots i_s}(x_{i_1}, \dots, x_{i_s}) dx = 0 \quad \text{for } k = i_1, \dots, i_s$$

and from this follows that the members in (1) are orthogonal and can be expressed as integrals of f(x). Thus:

$$\int f(x)dx = f_0$$

$$\int f(x)\prod_{k\neq i} dx_k = f_0 + f_i(x_i)$$

$$\int f(x)\prod dx_k = f_0 + f_i(x_i) + f_j(x_j) + f_{ij}(x_i, x_j)$$

and so on.

Assume now that f(x) is square integrable, then squaring (1) and integrating over I^n you get

$$\int f^2(x)dx - f_0^2 = \sum_{s=1}^{n} \sum_{i_1<\ldots<i_s}^{n} \int f_{i_1\ldots i_s}^2 dx_{i_1}\ldots dx_{i_s}$$

The constants $D_{i_1\ldots i_s} = \int f_{i_1\ldots i_s} dx_i \ldots dx_s$, $D = \int f^2 d - f_0^2$, are called variances and

$$D = \sum_{s=1}^{n} \sum_{i_1<\ldots<i_s}^{n} D_{i_1\ldots i_s} .$$

The ratios $S_{i_1\ldots i_s} = \frac{D_{i_1\ldots i_s}}{D}$ are called global sensitivity indices.

The integer s is often called the order or the dimension of this index. All the $S_{i_1}\ldots S_{i_s}$ are non-negative and their sum is

$$\sum_{s=1}^{n} \sum_{i_1<\ldots<i_s}^{n} S_{i_1\ldots i_s} = 1$$

The introduction of $S_{i_1}\ldots S_{i_s}$ is more or less evident. The main breakthrough of the computation of global sensitivity measures with the method of Sobol´ is the computation algorithm, a Monte Carlo algorithm.

The ANOVA representation for subsets of variables looks like $D = D_y + D_z + D_{yz}$

Where $D_y = \sum_{s=1}^{m} \sum_{(i_1<\ldots<i_s)\in K} D_{i_1\ldots i_s}$ is the variance corresponding to the subset y. The inner sum is extended over all groups $(i_1,\ldots,i_s)$ where all the $i_1,\ldots,i_s$ belong to K. Same for D_z. D_{yz} quantifies how much the model output variance depends on interactions between the two subgroups y and z. The total variance corresponding to the subset y is $D_y^{tot} = D - D_z$.

The Monte Carlo based approach

For the computation of S_y and $S_y^{tot} = 1 - S_z$ one has to estimate four integrals:

$\int f(x)dx$, $\int f^2(x)dx$, $\int f(x)f(y,z')dxdz'$ and $\int f(x)f(y',z)dxdy'$.

When one considers now two independent random points ξ and ξ' uniformly distributed in I^m and let ξ = (η,ζ) and ξ'= (η',ζ') then each Monte Carlo trial requires three computations of the model: f(η,ζ), f(η,ζ') and f(η',ζ). After N trials, crude Monte Carlo estimates are obtained:

$$\frac{1}{N}\sum_{j=1}^{N} f(\xi_j) \xrightarrow{P} f_0 \quad , \quad \frac{1}{N}\sum_{j=1}^{N} f(\xi_j) f(\eta_j, \zeta_j') \xrightarrow{P} D_y + f_0^2$$

$$\frac{1}{N}\sum_{j=1}^{N} f^2(\xi_j) \xrightarrow{P} D + f_0 \quad , \quad \frac{1}{N}\sum_{j=1}^{N} f(\xi_j) f(\eta'_j, \zeta_j) \xrightarrow{P} D_z + f_0^2 \quad .$$

Advantages

Extremely robust, these global methods work with any type of discontinuous (even randomised) mapping between input factors and the output. Sobol' estimator is unbiased. They do not rely on any hypothesis about the smoothness of the mapping. The only key assumption is that variance (i.e. the second moment) is an adequate measure for quantifying the sensitivity of the model output. Computing main effects and total effects for each factor, while still being far from a full factors mapping, gives a fairly instructive description of the system. Moreover, they provide unambiguous and clear answers to well specified sensitivity settings (prioritisation and fixing).

Disadvantages

The computational cost is relatively high, which implies that these methods cannot be applied to computationally expensive models.

They do not provide any mapping, i.e. they decompose the output uncertainty but they do not provide information about, e.g., the input factors responsible for producing Y values in specified regions, such as extreme high/low or any behavioural classification.

4.4.3.2 Regression Analysis

In a regression analysis a relationship between the conditional expected variable y given some input variables x is established (see e.g. Iman et al., 1985). The simplest form of regression analysis is correlation analysis. In table II.2 a correlation analysis for example 1 is presented together with the p-value that is testing the hypothesis of no correlation against the alternative that there is a non-zero correlation. It can be seen that this simple analysis fails to identify sensitivities and predominantly suggests insensitive model factors.

Nonlinear regression approaches include approaches such as Neural Networks (Zeng and Yeung, 2003) or random forests (Pappenberger et al., 2006). Many other models can be postulated as a relationship. However, more complex approaches should be treated with care as they usually exhibit larger uncertainties in the identification (for a discussion on that topic see Young et al., 1996). Smoothing procedures to estimate the decomposition of the model output into additive factor related components (RS-HDMR, SDP and spline, see further) can be seen as nonlinear extensions of the regression analysis into the sensitivity analysis context.

The regression coefficient can be used as a measure of sensitivity. In general, the sensitivity of a factor can be quantified by computing a measure of fit (such as the correlation coefficient, Kendall's coefficient of concordance or top down coefficient of concordance, see Helton et al., 2005), the distribution of this measure of fitness and the significance level. The measures of fit are estimated from a random sample and are themselves random variables. Therefore, if a measure of fit is not significantly different from zero, then there is no statistical significant relationship between the variables (typical tests include the Student's t-test or the Kolmogorov-Smirnov test). If the measure of fit is statistically significant then there is evidence that a relationship exists. The lower the significance level for which the hypothesis that the measure of fit is zero can be rejected (usual levels are 0.05 or 0.1), the stronger is the evidence of a relationship (Frey et al., 2004; Frey and Patil, 2002). If linear regression is used nonlinear monotonic data can be transformed into linear relationships by for example taking the logarithm or rank transforming the data. The usage of ranked transformed correlation coefficients such as Spearman correlation coefficient can significantly improve the resolution of the sensitivity analysis (Helton et al., 2005; Helton et al., 2006). However, nonlinear methods should be preferred if such transformation does not improve the analysis.

The coefficients of a regression analysis are often identified by least squares optimization and thus have to fulfil assumptions such as the independence of input variables and a normal distribution of errors.

Helton et al. (2006) advocate that any regression analysis should be performed in a step-wise manner, with a regression model first constructed with the most influential variable

followed by the next most important variable. The importance is identified by computing the coefficient of determination for a regression model containing only a single variable. Variable importance is then indicated by the order in which the factors are chosen, the changes of the coefficient of determination that are caused by added additional factors and a standardized regression coefficient (e.g. the Pearson correlation coefficient).

Table II.2: Correlation analysis of example 2 using Spearman, Pearson and Kendall correlation. The PVal is the p-value testing the hypothesis of no correlation against the alternative that there is a non-zero correlation

	Factor 1		Factor 2		Factor 3		Factor 4	
	Corr	Pval	Corr	Pval	Corr	Pval	Corr	Pval
Spearman	0.02	0.30	0.01	0.50	0.01	0.68	0.00	0.73
Pearson	0.02	0.27	0.02	0.64	0.02	0.46	0.00	0.90
Kendall	0.01	0.27	-0.01	0.43	0.00	0.71	0.00	0.73
	Factor 5		Factor 6		Factor 7		Factor 8	
	Corr	Pval	Corr	Pval	Corr	Pval	Corr	Pval
Spearman	0.00	0.99	0.00	0.98	0.00	0.98	0.00	0.00
Pearson	0.00	0.78	0.00	0.79	0.00	0.76	0.00	0.00
Kendall	0.00	0.99	0.00	0.99	0.00	0.99	0.00	0.00

Advantages

Regression analysis is conceptually simple and is part of many software packages (Helton et al., 2006). The technique allows the evaluation of the sensitivity of individual model inputs without neglecting the influence of other factors (Cullen and Frey, 1999). The methodology has a large degree of flexibility (multiple ways of transforming data and assumption of different model relationships).

Disadvantages

If the key assumptions of the regression analysis are not met, then, the results will not be robust. Moreover, a functional relationship between the input and the selected outputs has to be assumed (not model-free).

In the case of correlated inputs, the problem of multicollinearity can affect the robustness. This is the case when two variables are highly correlated and thus essentially convey the same information. Any couple of highly correlated variable would exhibit very similar sensitivity, due to the correlation, irrespective to the possibly extremely different effect onto the model output itself.

A second assumption of regression analysis is that the errors are distributed normally, which is not the case for many real world examples. Therefore, if the functional relationship used for the regression is not correct, this can give biased and misleading results. Neter et al. (1996) have shown that the result of regression analysis depends largely on the functional form chosen a priori and that such an analysis can lead to results which are counter-intuitive or statistically insignificant.

4.4.3.3 ***Regionalised Sensitivity Analysis***

The Regionalised Sensitivity analysis (RSA) has been originally developed in the context of environmental models by Spear and Hornberger (Spear and Hornberger, 1980) and further developed by Beven and Binley (1992). The paper by Spear and Hornberger (Spear and Hornberger, 1980) is one of the first landmark papers in Monte Carlo analysis and thus this method requires to execute the model multiple times using factor set sampled from their joint distributions. It has been applied to many environmental and water resource system applications (Chang and Delleur, 1992; Hornberger and Cosby, 1985; Lence and Takyi, 1992; Osidele and Beck, 2004). The Regional Sensitivity Analysis procedure involves three fundamental tasks: (1) Running the model in a Monte Carlo framework (2) a qualitative definition of system behaviour and (3) a binary classification of model output (Osidele and Beck, 2004). The definition of system behaviour involves the setting of thresholds and boundaries in which the model output has to lie. This expected behaviour can be derived from hard data such as measurements or soft data such as empirical information (for discussion on hard and soft data see e.g. Seibert and McDonnell, 2002). For example, a predicted flow hydrograph is expected to lie within a certain range of limits (Pappenberger and Beven, 2004). Such a constrain should take account of all model errors (e.g. input, parameters, model structure), the errors in the measurements and the commensurability errors; van Straten and Keesman, 1991). All model simulations which fall outside the qualitative definition of the system behaviour are called nonbehavioural (NB) and all model simulations which fulfil the constraints are termed behavioural (B) (Spear and Hornberger, 1980). The subjectivity within this separation is based on an understanding of the system (Freer et al., 2003). The distributions of the factors which are classified as NB and the once which are classified as B can be compared by a Kolmogrov-Smirnov test (Saltelli et al., 2004).

The importance of the uncertainty of each factor is inversely related to the significance level for rejecting H_0. A low significance level means that there is stronger evidence for a significant discrepancy between the factor distributions for B and NB. On the contrary, a high significance level indicates that the H_0 hypothesis cannot be rejected and the possibility that this factor or process is redundant in the model structure. Input factors can be grouped into three sensitivity classes, based on the significance level for rejecting H_0:

[1] critical (<1%); [2] important (>1% & <10%); and [3] possibly insignificant (>10%). (Osidele and Beck, 2004; Saltelli et al., 2004).

In figure II.4 the behavioural (0.25> y >0.2), non-behavioural (0.2>y) and prior distribution of example 1 is plotted and is defined as the entire sampled space. For more details see Saltelli et al. (2004). The hypothesis that the two distributions are the same cannot be rejected (significance level, 0.05).

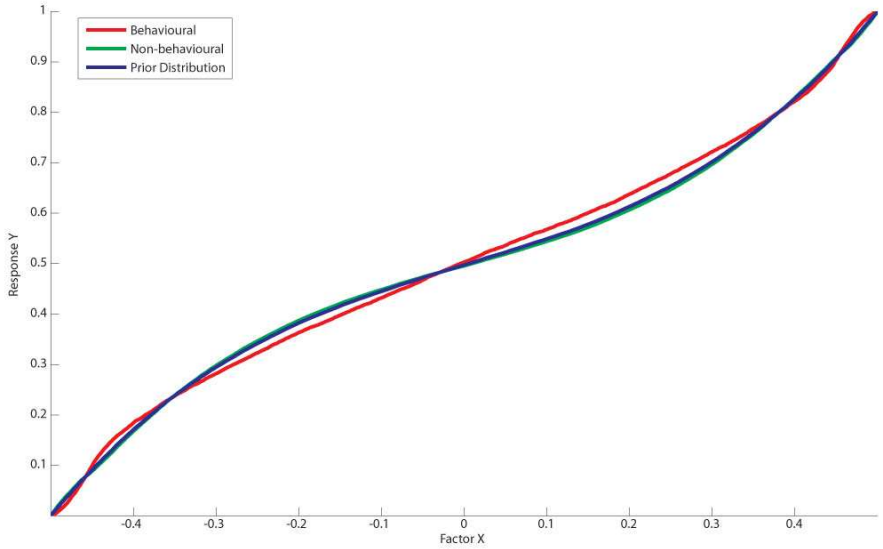


Figure II.4: Regional Sensitivity Analysis of example 1. Behavioural is defined as 0.25> y >0.2, non-behavioural as 0.2>y

The method has been further developed by Beven and Binley (1992) within the Generalized Likelihood Uncertainty Estimation (GLUE) framework. In the RSA application all behavioural and nonbehavioural factor sets are regarded as equally likely representations of the modelled system whereas within the GLUE framework the performance of each simulation is taken into account. Similar to RSA the Monte Carlo runs of the model are classified into behavioural and nonbehavioural. However, a model performance (e.g. a Nash-Sutcliffe of a flow hydrograph) is computed for all behavioural runs. These model performances are binned according to their ranked performance (for example in 10% steps, meaning that the best 10% of all models are treated together as well as the 10%-20% 'best' models etc.). The performances of each bin are normalized (by for example dividing through the sum) and a cumulative distribution function (cdf) against the factor values is plotted. The larger the area such an ensemble of cdfs encloses, the more sensitive a factor can be considered. The sensitivity measure can be quantified either by the area or the significance level on which the hypothesis that the area is equal to zero can be rejected (see Pappenberger et al., in press). Figure II.5 shows the result of the analysis for example 2 (assuming that all factors are behavioural and that the response variable is a performance measure). It can be seen that factor 1 and 2 show sensitivity by having a spread in the cumulative distribution functions. The different cdf's are based on subdividing the model response in bins of 10% (e.g. the lowest 10% of model response, all response with values between 10% and 20% etc.)

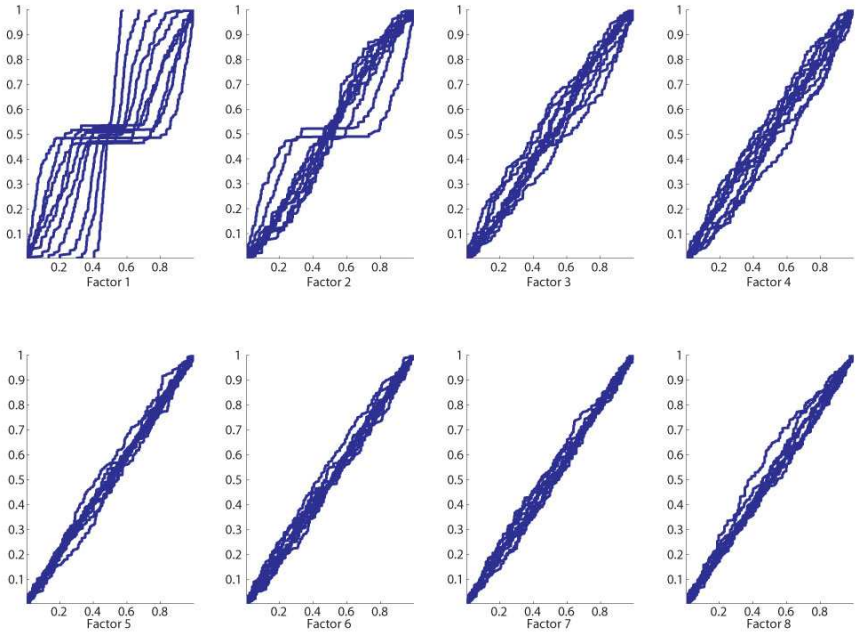


Figure II.5: Regional Sensitivity Analysis of example structure 2.

Advantages

The method has the advantage that it is conceptually simple and easy to implement. The result has an easy to understand qualitative meaning and the methodology is model free (no assumptions of a model have to be made for the sensitivity analysis).

Disadvantages

In its current form, the methodology cannot quantify higher order effects (problem of multicollinearity) or search for interacting structures, except for stylised structures detectable through correlation analysis within the B or NB samples. It has also to be noted that only a hypothesis rejection is sufficient to make a decision. The acceptance of a hypothesis in this kind of test does not imply that there is no importance of that particular factor.

Saltelli et al. (2004) argue that the fraction of behavioural models is too small for large models and that this implies a lack of statistical power. However, one could argue that this is due to overparameterization /complexity combined with the difficult task to search the entire model response space adequately or simply that the model is inadequate for the task in question.

4.4.3.3 Entropy

Krykacz-Hausmann (2001) argued that sensitivity should be measured as a deviation of the factor distribution from being uniform (if the factor has been sampled from a uniform prior distribution). The author developed a sensitivity measure which is based on the Kullback-Leibler Entropy (Kullback and Leibler, 1951) and was extended by Liu at al. (2004). Entropy is a measure of disorder in the universe or of the availability of the energy in a system to do work. The Kullback–Leibler entropy is a measure of the difference between two probability distributions: from a "true" probability distribution P to an arbitrary probability distribution Q.

Liu et al. (2004) point out that this entropy shares many properties of a metric measure such as non-negativity, additivity and convexity despite not being a metric measure. The K-L entropy can be understood as a measure, which expresses the lack of overlapping between probability density functions (within given limits). Liu et al. (2004) define total and main effect indices in analogy to the Sobol method. The concept of entropy and sensitivity is also exploited (in a slightly different formulation) in methodologies such as the dynamic identifiability analysis (Wagener et al., 2003) for rainfall-runoff models and its numerical expression by Horritt (2005) for flood inundation models.

Advantages

It has been argued that variance-based methods rely too heavily on the assumption that the second moment is sufficient to describe the uncertainties and sensitivities encountered. These assumptions may be invalid if the distribution is highly skewed due to nonlinear functions or inputs (Liu et al., 2004). This methodology proposes a way to overcome this limitation by taking account of the full probability density function.

Disadvantage

The mathematical framework on which first and higher order effects as well as total effects are calculated is less rigid than for the variance-based methods (despite being designed to be an improvement to those methods). It can be argued that the main order effect as formulated by Liu et al. (2004) actually contains properties of the total effect (if the definitions of the Sobol method are used). The method relies on a structured sampling design which maybe difficult to achieve in some practical applications, e.g. due to numerical instabilities.

4.4.4. Sensitivity and model emulators

An important approach to sensitivity analysis, which has developed in the last few years, falls within the emulation context. The basic idea is to represent in a direct way the relationship between the model factors and the model results, whose form is usually unknown to the analyst. If the emulation exercise is successful, one can obtain a simple relationship between the model factors and the model output that fits well the original model and is less computationally demanding. Given the emulator, this can be used to compute any measure of interest, including sensitivities.

There is a vast literature in this framework. Local approximation methods provide a first class of emulator that matches the properties of the model at a base point and in the nearby region (Taylor series). Interpolation methods look at 'nice' functions that go through a set of data points spanning the entire domain of the mapping. The approximation is then identified by fixing a set of parameters (e.g. the coefficients of the polynomials) using a set of data points (Lagrange, Chebyshev interpolation). The cut-High Dimensional Model Representation (cut-HDMR) expansion (see later) is an example of this. Regression methods differ from interpolation whereby a set of more data points than the amount of parameters is used to identify the approximating function. For univariate models, the interpolation approach can be extended by applying piecewise polynomials, constructing functions that are only piecewise smooth. Splines (the cubic spline is the most popular) are a powerful and widely used piecewise polynomial interpolation, which are smooth where the polynomial pieces connect. In the multivariate case, which is the most interesting, radial basis function networks can be seen as the equivalent of univariate piecewise interpolation.

All the above approaches can be referred to as model approximation methods: see Storlie and Helton (2006) for a review of smoothing methods for sensitivity analysis purposes.

There are strong links between regression analysis and the theory of variance based sensitivity analysis. Let $g(\cdot)$ be the generic function approximating the true model $Y = f(X_1,...,X_k)$ and let us assume a quadratic loss function $\mathrm{E}[(\mathrm{Y} - \mathrm{g}(\cdot))^2]$ as a measure of 'fit' for g. If we were to approximate f with a function of one single parameter X_i, which is the function $g_i^*(X_i)$ that provides minimum loss?

It is well known from standard school texts on statistics that the univariate function

$$g_i^* = E(Y|X_i) \quad (2)$$

i.e. the conditional expectation of Y given X_i, is the minimum loss approximation to f. The above expression tells us that at any p-location $X_i = x_{i,p}$, the value of g* is

obtained by integrating (averaging) Y over all the remaining $(X_1,...,X_{i-1,}X_{i+1},...X_k)$ input factors.

Equation (2) can be generalised to any subset of the input factors, by

$$g_i^* = E(Y|X_{i1},...,X_{il})$$

Both equations are linked to the HDMR decomposition of f:

$$Y = f(X_1, X_2,...X_k) = f_0 + \sum_i f_i(X_i) + \sum_{\substack{ij \\ i<j}} f_{ij}(X_i, X_j) + ... + f_{12...k}$$

with here the various terms that can be expressed as:

$$f_0 = E(Y)$$
$$f_i(X_i) = E(Y \mid X_i) - f_0$$
$$f_{ij}(X_i, X_j) = E(Y \mid X_i, X_j) - f_1 - f_2 - f_0$$

we explicitly highlight the link between the terms of the HDMR and the minimum loss approximating functions $g(\cdot)$. Each term of the decomposition tells the analyst how much Y moves around its mean level f_0 as a function of single input factors or groups of them.

Coming back to the emulation problem, we require that the smoothing function(s) of increasing order approximate and ultimately converge to $g_i^*(.)$. This assures that, given a truncation of the full HDMR expansion, the emulator obtained is the optimal one in a least squares sense among all possible models of the same order of interaction.

cut- High Dimensional Model Representation (cut-HDMR)

The papers by H. Rabitz and co-workers (Rabitz et al., (1999) and Rabitz and Aliş (2000)) can be seen as precursory applications of the emulation approach in SA. There, the emulator is given by the so-called cut- High Dimensional Model Representation (cut-HDMR) expansion, obtained by evaluating the model on quadrature points falling on lines, planes and hyper-planes passing through a `base' point in the input factor space, and truncating the order of the hyper-planes . Then, all the required integrals are computed on the truncated cut-HDMR function. This helps to reduce the computational cost of the analysis with respect to variance based methods, albeit still not sufficiently to treat computational expensive models. Moreover, the cut-HDMR approach still depends significantly on the dimensionality of the problem.

Random Sampling-HDMR (RS-HDMR)
The same research group who worked on cut-HDMR presented the so-called Random Sampling-HDMR (Liu et al., 2004), where the HDMR terms are estimated by smoothing a Monte Carlo sample of the mapping with orthogonal polynomials. Due to the curse of dimensionality problem, a truncated HDMR is estimated, usually up to order three, using polynomials of order up to 2-3. RS-HDMR can be seen as the first implementation of the emulation concept within the sensitivity context. RS-HDMR allows to significantly reduce the computational cost of sensitivity analysis.

Bayesian and Kriging Emulators
The theoretical foundations of model emulation are grounded in statistical theory of stochastic processes. The general framework is originally due to Sacks et al. (1989). Oakley and O'Hagan (2004) have demonstrated its application in SA, where a Bayesian approach is applied to produce a Gaussian process emulator of the computational model and, subsequently, to compute sensitivity indices in an extremely efficient way, with a computational cost of only a few hundreds of runs for a reasonable number of input variables. Kriging emulators (Kleijnen, 2007a) are similar to Gaussian, except that they do not rely on Bayesian interpretation.

Their computational efficiency is linked to certain limitations and hypotheses: namely, that the model response needs to be smooth and the number of input variables should not be very high (< 30). Moreover, Gaussian/kriging emulators can be prone to the curse of dimensionality and to the smoothness assumptions of the function under analysis. This is because Gaussian emulators try to interpolate and predict the $f(\cdot)$ mapping by applying a Gaussian kernel of the same k-dimensionality as the input parameter space. Therefore, as k increases, the number of hyper-parameters to be estimated (linked to the covariance structure of the k-dimensional Gaussian kernel), increases strongly, possibly implying problems with identification and over-parameterization. Under such hypotheses and caveats, the GP emulator works in an extremely efficient way and a few hundred runs are sufficient to describe with good accuracy most of the model behaviour. More details on Gaussian emulator can be found in Oakley and O'Hagan (2004).

State Depending Parameter (SDP)
This is a non-parametric methodology and it is based on an approach to State Depending Parameter (SDP) modelling. It was applied for sensitivity analysis and emulation by Ratto et al. (2004). The estimation is performed with the help of the `classical' recursive (non-numerical) Kalman filter (Kalman, 1960) and associated fixed interval smoothing algorithms.

As for the RS-HDMR, the emulator is based on a truncated ANOVA-HDMR expansion up to the order 3 and, as in the previously published approaches, it normally estimates

all the main effects with only a few hundred Monte Carlo realisations (< 1,000), almost independently of the dimensionality k of the problem.

Splines

The spline approach is based on the SDP method introduced above. The methodology estimates the relationship of the state dependent parameters over hermite cubic splines (Pappenberger and Stauch, 2006). For this, an interval of the random input variable X_i is divided into m-1 subsections resulting in m node locations, each with node values $Y_1 \ldots Y_m$. For each subinterval of the random variable X_i, the polynomials $pol(X_{i,m})$ are estimated as cubic hermite interpolating polynomials based on four interpolation conditions (see De Boor, 2001). The shape preserving algorithm by Fritsch and Carslon (1980) is applied and the values of the knots of the cubic spline optimised using a Levenberg-Marquart nonlinear least square minimisation (Stauch et al., in press) (see also chapter of materials and methods). The optimisation procedure duplicates the backfitting algorithm for the SDP procedure

The number of nodes and location has been fixed after several initial tests, but could be optimised Bitterlich et al. (2004). However, initial tests suggest that this is not always necessary.

Advantages and disadvantages

All emulation approaches allow to perform quantitative global sensitivity analysis, like variance-based analysis, with a much lower computational effort compared to classical Monte Carlo estimation approaches (FAST, Sobol'). This is because they try to make best use of the smoothness properties of the function under analysis. These methods are less simple to code with respect to classical methods, although they are conceptually simple. The RS-HDMR (polynomial regression), SDP (non-parametric, recursive regression) and spline approaches can also be seen as extensions of the regression approach for the estimation of low order HDMR expansions. As such (and irrespective of the emulation context), they can be used for estimating main effect variance-based sensitivity indices, for such models where the number of model evaluations required by classical Monte Carlo methods are unaffordable.

4.4.5. Choice of the method

After this summation of all the methods for SA, out of all the advantages and disadvantages and the obtained answers from every SA method, two ways of how to choose the right SA will be presented here (Pappenberger, 2007).

4.4.5.1 According to sensitivity aim/setting

Saltelli et al. (2004) have argued that the effectiveness of a sensitivity analysis is greater if the purpose of the analysis is specified unambiguously beforehand. Over time, practitioners have identified cogent questions for sensitivity analysis. These questions define the setting, which in turn allows for the selection of the strategy. The most typical settings are:

Factors prioritization (FP)

Assume that, in principle, the uncertain input factors can be 'discovered', i.e. determined or measured, so as to find their true value. One legitimate question is then "which factor should one try to determine first in order to have the largest expected reduction in the variance of the model output"? The variance-based *main effect* provides the answer to the Factor Prioritization setting.

Factors fixing (FF)

Another aim of sensitivity analysis is to simplify models. If a model is used systematically in a Monte Carlo framework, so that input uncertainties are systematically propagated into the output, it might be useful to ascertain which input factors can be fixed, anywhere in their range of variation, without sensibly affecting a specific output of interest. This may be useful for simplifying a model in a larger sense, because we may be able then to condense entire sections of our models if all factors entering in a section are non-influential. Saltelli and Tarantola (2002) also showed that the variance-based *total effect* provides the answer to the Factor Fixing setting. A null total effect is a sufficient condition for an input factor to be irrelevant, and therefore to be fixed.

Factors Mapping (FM)

In this case, the analyst is interested to as many information as possible, either global and local, i.e. which values of an input factor (or of group of factors) are responsible for driving the model output in a given region? Which conditions are able to drive a specified model behaviour? In this case, a full array of methods, from local ones, to Monte Carlo Filtering, to model emulators, to variance-based and entropy-based methods can provide useful insights about model properties.

Calibration

In this case, the analyst aims at identifying the portions of the input factors space that allow the model to behave according to available information (data, constraints) about the modelled system. FP and FF settings are linked to calibration and can be used to prepare a calibration step: with FP and FF one can say what can be effectively calibrated (those parameters having large main effects) and what cannot (those having

null total effect). Parameters in the grey area (i.e. small main effect and large total effect) fall under the so-called equifinality conditions. An effective calibration can be performed by first concentrating on the input factors highlighted by the FP setting.

In figure II.6 a decision tree is presented to provide guidance on the choice of methods, Therefore, specifying the aim for the sensitivity analysis becomes crucial for concentrating on specific sensitivity methods:

- FP? Variance based (VB) main effects provide the answer. This setting is also connected to Type I errors, i.e. when one is 'scared' of labelling as important something that is not: if one gets a high main effect, he can be sure that this parameter is really relevant for the model. As far as the computational cost is concerned, the classical Monte Carlo algorithms (Sobol') to estimate main effects require a few thousands of model runs: this might be unaffordable in some cases. In such cases, we point the readers to recently developed smoothing methods (RS-HDMR, SDP, spline) that are not particularly difficult to code and that allow to reliably estimate main effects with few hundreds of model runs.

- FF? Variance based total effects provide the answer. This is also linked to Type II errors, i.e. one is 'scared' of fixing something that can have an effect on the model. In this case, therefore, one is mostly interested at the zero sensitivity indices. From the computational point of view the only reliable route to compute total effects is the classical Monte Carlo algorithm (Sobol'). However, it has been shown that the screening method based on elementary effects (Morris, 1991, as extended by Campolongo et al., 2007), provides an excellent proxy to total effects at a much smaller computational cost: whenever a zero index is found using the Morris approach, it is extremely difficult that any other method detects any effect for such an input factor.

Both the FF and the FP settings can be treated at a quite small computational cost by taking a few hundred runs to perform the screening test by Campolongo et al. (2007) plus another few hundred runs to apply a smoothing technique for estimating the main effects.

- FM? In this case, the suggestion of using as many methods as possible is justified by the fact that one is interested to as many information, both global and local, i.e. which parameter values are responsible for driving the output in a given region? It has to be noted that many methods can be applied using the same sample, for example Monte Carlo Filtering (MCF), regression analysis, smoothing and emulation approaches can be applied on the same Monte Carlo sample.

- In the case of numerical instabilities, MCF can be very useful to map the occurrence of such numerical problems. Moreover, most of the sensitivity methodologies (MCF, Morris, Sobol', smoothing, etc.) can be applied also in such cases when model simulation fails for a portion of the sample.

4.4.5.2 According to the computational Cost

Here the best SA method is presented with a decision tree. The decision tree is a pragmatic approach to sensitivity analysis. For a scientific approach we suggest to use as many methods as possible to highlight differences and have a maximum understanding of the processes, in particular when the aim of the analysis is a 'mapping'. This can be easily achieved as most methods can be based on the same sampling design. Figure II.6 shows a decision tree based on the computational cost and learning curve of performing a sensitivity analysis. Explanation for each field is given below. The decisions are based on the most widely agreed approaches.

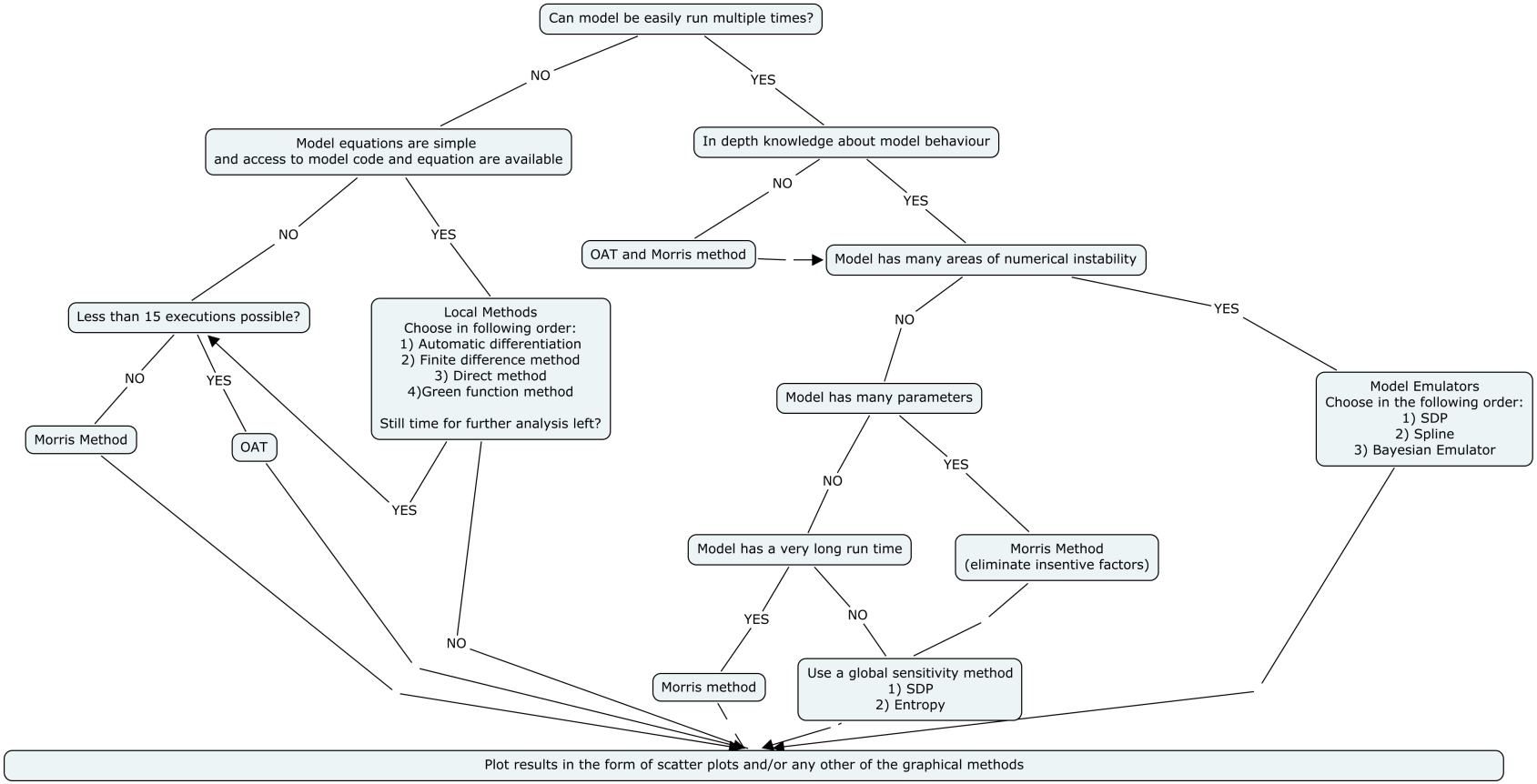


Figure II.6: Decision tree to choose a sensitivity analysis method

Explanation of fields

Can the model be run easily multiple times?

The model can be executed externally e.g. from another programming language without the use of a Graphical User Interface. The model output is parsed back or the output files are sufficiently documented so they can be read from an external controller (e.g. another programming language)

Model structure is 'simple' e.g. Manning equation

No numerical analysis or complex direct solution schemes are required to compute these equations.

In depth model knowledge

The user is greatly familiar with the model and has used it many times before

Model has many areas of numerical instability

For many parameter sets, the model does not converge to a solution. 'Many' has to be defined in respect to the model run time and the number of model parameters.

Model has a long runtime and / or many parameters

The more parameters a model has the more runs are necessary to describe the response surface adequately.

The question about the sample dimension depends highly on the type of model used and should be based on previous experience. In general, a few hundreds/one thousand of model runs is in many cases sufficient for deriving useful information about the most important model characteristics. This is due to the fact that there is always an upper bound to the number of important input factors. This implies that there is always a small subset of input factor (usually not larger than 10) that produce most of the output variation, which makes the 'effective' dimension of the problem much smaller than the *k*-dimensional input space considered by the modeller. As a very bold statement, we argue that a model with more than 20 parameters and an execution time of more than 10 minutes should be considered as computing intensive (if executed on a single CPU).

5. Uncertainty analysis

One definition for uncertainty analysis is ´the means of calculating and representing the certainty with which the model results represent reality´. The important questions one should consider are whether prior theory adequately matches observed behaviour and whether the predictions obtained from models are meaningful and useful (Beck, 1987).

The difference between the model results and reality arises from:

- uncertainty of the values of the parameters that appear in the identified structure of the dynamic model for the system behaviour; model parameter error (ε1)

- uncertainty of the model structure, i.e. uncertainty about the relationships among the variables characterising the dynamic behaviour of systems and uncertainty associated with predictions of the future behaviour of the system; model structure error (ε2)
- numerical errors, truncation errors, rounding errors and typographical mistakes in the numerical implementation (ε3)
- boundary condition uncertainties (ε4)
- sampling errors (i.e. the data not representing the required spatial and temporal averages) (ε5)
- measurement errors (ε6)
- human reliability, human mistakes (ε7)

The model inputs can have errors ε4, ε5 and ε6, while calibration data only can have errors ε5 and ε6. An error-free model should have results that equate error-free observations and therefore we can summarise the relationship between the actual model results and the actual observations by

$$M - \varepsilon 1 - \varepsilon 2 - \varepsilon 3 - \varepsilon 4 = O - \varepsilon 5 - \varepsilon 6 - \varepsilon 7$$

It is the goal of the modeller to achieve an error free model by reducing the errors (ε1-ε4). However, the model structure errors ε2, numerical errors ε3, and the boundary condition errors ε4 are difficult to control by the modeller. So the aim becomes to compensate as far as possible for ε2-ε4 by identification of the optimum effective parameter values. As such the best parameter estimates compensate for the other errors.

As a result, uncertainty analysis in water quality modelling mainly focussed on model parameter variability (Schnoor, 1996). Recently also the other errors gain more attention, this mainly driven by the problem of ungauged basins and how to deal with all the different sources of uncertainty to produce a model for such basins which gives results with realistic uncertainty bounds. It would also be ideal if one could come up with the magnitude of different uncertainty causes in view of reducing those uncertainties by additional measurements or ameliorations to model structure.

In the next section, the different methods will be given with the pro's and contra's and with indication of which uncertainty can be detected with the method.

In order to quantify uncertainty, the distribution of model inputs should be propagated through the model to obtain distributions on model outputs. Propagation techniques may be analytical, approximation, or numerical.

5.1. Analytical propagation techniques

For simple models in which the output is a function of a linear combination of model inputs with no dependency, the propagation of probability distributions through the model is straightforward. For such cases the Central Limit Theorem (CLT) can be used. CLT can be stated in a variety of ways. One way is the application of the CLT for the sum of independent random variables. The distribution of the sum of independent random variables approaches a normal distribution as the number of random variables becomes large (De Groot, 1986). It is not required to assume a specific shape for the probability distribution for each of the variables in the sum. The CLT for the sum of independent variables can be summarized as:

$$\mu_s = \sum_{i=1}^{n} \mu_{x,i}$$

where μ_s is the mean of the sum and $\mu_{x,i}$ are the means of each of the variables being added together. The variance of the sum is equal to the sum of the variances:

$$(\sigma_s)^2 = \sum_{i=1}^{n} (\sigma_{x,i})^2$$

The same approach can be used for models with log normal distributional input, using a logarithmic transformation.

Advantages. Analytical propagation techniques based on the CLT are straightforward and easy to implement to simple models in which the model output is a linear sum or products of model inputs.

Disadvantages. Although the results of the CLT approach are useful in some cases for propagating the mean and the variance through a simple linear model, they do not imply anything about the shape of the model output distribution (Cullen and Frey, 1999). Moreover, the implications of the CLT are relevant only if the conditions of the CLT exist for a particular situation. Thus, if a model contains both products and sums of inputs, or for which some of the inputs are dominant over others, or for which some of the inputs are not statistically independent, the analytical propagation techniques based on the CLT cannot be used.

5.2. Approximation methods based upon Taylor series

There are a number of methods based upon the use of the Taylor series expansions for propagating the mean and other central moments of random variables through a model. The basic approach is to take a general function, such as:

$$y = h(x_1, x_2, ..., x_n)$$

and then expand the function about the point [E(x_1), E(x_2), …, E(x_n)] using a multivariate Taylor series expansion. The series is usually truncated at a specified set of higher order

terms. For example, the mean of the output distribution, E(y), can be approximated by the following Taylor series expansion (Hahn and Shapiro, 1967):

$$E(y) = h[E(x_1), E(x_2), ..., E(x_n)] + \frac{1}{2} \times \sum_{i=1}^{n} \frac{\partial^2 \bar{h}}{\partial x_i^2} \times (x - x_i)^2 + \{Higher\ order\ terms\}$$

The function *h* and the partial derivatives on the right side are evaluated at the point [E(x_1), E(x_2), …, E(x_n)] and . The variance of the model output, σ_y^2, of statistically independent random variables, is approximated by the following:

$$\sigma_y^2 = \sum \left(\frac{\partial \bar{h}}{\partial x_i} \right)^2 \times \sigma_{x_i}^2 + \sum_{i=1}^{n} \left(\frac{\partial \bar{h}}{\partial x_i} \right) \times \left(\frac{\partial^2 \bar{h}}{\partial x_i^2} \right) \times \mu_3(x_i) + \{Higher\ order\ terms\}$$

where, $\mu_3(x_i)$ is the third central moment of each input random variable.

Advantages. Based upon a sufficient number of central moments for a model output, it may be possible to select a parametric probability distribution model that provides a good representation of the output distribution (Cullen and Frey, 1999). Once a parametric distribution of the output is specified, predictions can be made regarding any percentile of the model output. Thus, as an advantage of approximation methods based upon Taylor series, it may only be necessary to propagate the moments of each probability distribution of the model inputs instead of the entire probability distribution.

Disadvantages. Approximation methods based on Taylor series typically have three major limitations (Cullen and Frey, 1999). First, as a primary limitation in application of these techniques, the model function should be differentiable. Therefore, these methods cannot be applied to problems with discrete or discontinuous behaviours. Second, these methods are computationally intensive as they typically require the evaluation of second order (and potentially higher) derivatives of the model. Third, although these techniques are capable of propagating the central moments of the input distributions, information regarding the tails of the input distributions cannot be propagated. In environmental exposure and risk assessment problems where the shape of the tails is critical, this limitation can be problematic.

5.3. Numerical propagation techniques

The most common techniques for numerical propagation of uncertainty are sampling-based methods. Some of the sampling-based methods for propagating probability distributions are: (1) Monte Carlo and Latin Hypercube Sampling methods; and (2) the Fourier Amplitude Sensitivity Test (FAST); and (3) reliability based methods.

Monte Carlo Simulation

In Monte Carlo simulation, a model is run repeatedly, using different values for each of the uncertain input parameters each time (Ang and Tang, 1975; Hahn and Shapiro, 1967; Morgan and Henrion, 1990). The values of each of the uncertain inputs are generated based on the probability distribution for the input. With many input variables, one can envision Monte

Carlo simulation as providing a random sampling from a space of *m* dimensions, where *m* is the number of inputs to a model.

As a general approach for applying Monte Carlo simulation to a model, for each input a probability distribution should be specified. Random samples are generated from each of the probability distributions. One sample from each input distribution is selected, and the set of samples is fed into the model. The model is then executed, as it would be for any deterministic analysis. The process is repeated until the specified number of model iterations has been completed. Thus, instead of obtaining a single number for model outputs as in a deterministic simulation, a set of samples is obtained. These can be represented as cumulative distribution functions (CDFs) and summarized using typical statistics such as mean and variance. Most numerical simulation methods, including random Monte Carlo, require the generation of uniformly distributed random numbers between 0 and 1 (Cullen and Frey, 1999). Given a uniformly distributed random variable, several methods exist from which to simulate random variables that are described by other probability distributions (e.g., normal, lognormal, and gamma). These methods include the inverse transformation, composition, and function of random variables (e.g., (Ang and Tang, 1975)). In addition methods exist for simulation of jointly distributed random variables, which enables one to represent correlations between two or more simulated random variables.

• ***Advantages.*** Advantages of Monte Carlo methods in propagating probability distributions of inputs flow from the fact that their output provides more information compared to analytical and approximate methods. Moreover, because Monte Carlo methods provide a probability distribution of the output, they avoid the problem of compounding conservative values of input variables and obtaining only worst case scenario's (Burmaster and Harris, 1993). Additional advantages follow from the information provided by Monte Carlo simulation. For example, results based on Monte Carlo simulations can typically also be used for sensitivity analysis, permitting the risk assessors to determine where additional data will be most useful in reducing uncertainty (Finley and Paustenbach, 1994).

• ***Disadvantages.*** Because Monte Carlo simulation requires multiple iterations of a model, such simulations can be computationally intensive if the model requires a large run time per simulation. Furthermore, depending on the data quality objectives of the analysis, it may be necessary to perform a large number of simulations. Sample sizes of more than 1000 are most of the time already too time consuming.

Although not a limitation of the method itself, in practice results based on Monte Carlo simulations are easy to misuse by stretching them beyond the limits of credibility. For example, problems can arise when inexperienced analysts use commercial simulation packages due to ease of application and lack of familiarity with underlying assumptions and restrictions. Typical misapplications of Monte Carlo simulation include failure to properly develop input distributions and misinterpretation or over-interpretation of results. For example, it is not possible to have a precise estimate of an upper percentile of an output distribution without a large simulation sample size.

Latin Hypercube Sampling Methods

An alternative to random Monte Carlo simulation is Latin Hypercube Sampling (LHS) (McKay et al., 1979). In LHS methods, parameter ranges are first divided into ranges of equal probability, and one sample is taken from each equal probability range. However, the order of samples is typically random over the course of the simulation, and the pairing of samples between two or more random input variables is usually treated as independent. In median LHS, one sample is taken from the median of each equal-probability interval, while in random LHS one sample is taken at random within each interval (Morgan and Henrion, 1990).

• ***Advantages.*** LHS typically has the same advantages as Monte Carlo simulation. Furthermore, LHS ensures better coverage of the entire range of the distribution. Because the distributions are more evenly sampled over the entire range of the probable values in LHS, the number of samples required to adequately represent a distribution is lower for LHS compared to random Monte Carlo simulation (Iman and Conover, 1982; McKay et al., 1979; Morgan and Henrion, 1990). Moreover, compared to Monte Carlo simulation, LHS reduces the statistical fluctuation in simulations of random variables for a given sample size (Cullen and Frey, 1999).

• ***Disadvantages.*** Because LHS is not random in pairing of values of the input random variables, it is not practical to use LHS to characterize the effect of statistical sampling error using the bootstrap technique (Cullen and Frey, 1999) With the bootstrap, the observations need to be randomly reassigned, and estimates recomputed. There are specific situations in which median LHS cannot provide correct results, such as when sampling from a periodic function if the sample intervals are spaced with the same period (Morgan and Henrion, 1990), but this is a rare problem in practice.

Fourier Amplitude Sensitivity Test

FAST has been developed for uncertainty and sensitivity analysis (Cukier et al., 1973; Cukier et al., 1978; Schaibly and Shuler, 1973). The FAST method applies a functional transformation to each input, assigns each input a distinct integer frequency, and introduces a common independent variable to all inputs (Cukier et al., 1978; McRae et al., 1982a). The inputs vary simultaneously with this independent variable in such a way that output becomes a periodic function of the independent parameter. Fourier analysis is performed on the output, which produces Fourier amplitudes for each frequency. FAST provides a way to estimate the expected value and variance of the output variable and the contribution of individual factors to this variance (Saltelli et al., 2000). See also literature section II.4 on SA.

• ***Advantages.*** The FAST method is superior to local sensitivity analysis methods because it can apportion the output variance to the variance in the inputs. It also can be used for local sensitivity analysis with little modification (Fontaine et al., 1992). It is model independent and works for monotonic and non-monotonic models (Saltelli et al., 2000). Furthermore, it can allow arbitrarily large variations in input parameters. Therefore, the effect of extreme events can be analyzed (eg. Helton, 1993; eg. Lu and Mohanty, 2001). The evaluation of sensitivity estimates can be carried out independently for each factor using just a

single set of runs (Saltelli et al., 2000). The FAST method can be used to determine the difference in sensitivities in terms of the differing amount of variance in the output explained by each input and, thus, can be used to rank order key inputs.

- ***Disadvantages.*** The FAST method suffers from computational complexity for a large number of inputs. The classical FAST method is good only for models with no important or significant interactions among inputs (Saltelli and Bolado, 1998). However, the extended FAST method developed by Saltelli et al., (1999) can account for high-order interactions. The reliability of the FAST method can be poor for discrete inputs (Saltelli et al., 2000). Current software tools for FAST are not readily amenable to application to complex risk assessment models.

Reliability Based Methods (FORM and SORM)

First order reliability methods, also known as FORM, estimate the probability of an event under consideration. FORM can provide the probability that an output exceeds a specific value, also known as probability of failure (Hamed et al., 1995; Karamchandani and Cornel, 1992; Lu et al., 1994). The failure probability can be expressed by:

$$P_f = P(Z(X) \le 0) = \int_{Z(X)\le 0} f_x(\xi) \times d\xi$$

where, Z(**X**) is the output function and **X** is a set of *k* random variables (x_1, x_2, …, x_k). If Z(**X**) is a deterministic function of the random variables, **X**, it can be linearized in the neighborhood of some point $x^* = (x_1^*, x_2^*, ..., x_k^*)$ as:

$$Z(X) = Z(x^*) + \sum_{i=1}^{k} \frac{\partial Z}{\partial x_i} \times (x_i - x_i^*) + \{Higher\ order\ terms\}$$

The point x^* is chosen as the design point, which is defined as the point with greatest probability density, satisfying $Z(x^*) = 0$. This point is found by an optimization procedure. For the case of independent inputs and by neglecting higher order terms, the output mean and variance can be estimated as:

$$\mu_z \approx Z(x^*) + \sum_{i=1}^{k} (\mu_i - x_i^*) \times \frac{\partial Z(x^*)}{\partial x_i}$$

$$\sigma_Z^2 \approx \left\{ \sum_{i=1}^{k} \sigma_i^2 \times \left(\frac{\partial Z}{\partial x_i}\right)^2 \right\}$$

where, μ_i and σ_i^2 are the mean and variance of input x_i. Various methods have been suggested to improve the accuracy of FORM calculations and to give a rough estimate of the quality of approximation. The second order reliability method (SORM) uses second-order terms in estimation of the mean and variance of the output, and hence, provides more accuracy (Fiessler et al., 1979).

• ***Advantages.*** FORM and SORM typically require only the knowledge of the moments of component reliabilities, that is, no distribution function must be specified. Moreover,

generation of random numbers is not required; therefore, there is no sampling error in propagation. Finally, they can be applied to dependent as well as correlated inputs, although the equations for dependent variables would be more difficult to derive due to their complexity.

• ***Disadvantages.*** FORM and SORM are approximate and a finite error is associated with the use of only up to first and second order terms, respectively. Furthermore, the accuracy of these methods is not readily quantifiable.

5.4. Comparison of selected methods for propagation of probability distributions of inputs

The ideal method(s) for propagation of probability distributions of inputs should: (1) not be dependent on the functional form of the model; (2) provide insight regarding the entire range of the output distribution; (3) require few iterations of the model; (4) not only propagate the probability distributions, but also provide insights regarding sensitivity of the model output to the inputs; and (5) be typically available in commonly used software packages. Based on the discussions provided for advantages and disadvantages of typical methods for propagation of probability distributions of inputs, sampling based numerical methods including Monte Carlo simulation and LHS are preferred. These methods can be used for a wide variety of models and can accommodate a wide variety of assumptions regarding input distributions. Furthermore, these methods enable characterization of the probability distribution for the model output. The sample values generated as part of a Monte Carlo or Latin hypercube simulation can be used as the basis for sensitivity analysis with a wide variety of sensitivity analysis methods. Both of these methods are commonly available and are widely used. The main potential disadvantage is the need for repeated iterations of a model. As computing power increases, this limitation typically decreases in practice.

6. Optimal experimental design for parameter estimation

Quantitative measurements are needed to calibrate and to statistically assess the performance of a proposed mathematical model describing the system under investigation. To successfully identify model structure and reliably estimate model parameters, an experimental design can be used because it can drastically improve the estimation accuracy. In this dissertation, model structure uncertainty is not discussed, so this subject is also left out in this section. Since quantitative time-resolved measurements are time and cost intensive, improvements and measurements will reduce the experimental costs needed to achieve a prespecified accuracy.

In this section an overview of different techniques to design experiments that give the most valuable information for parameter estimation is given. First a distinction is made between structural and practical identifiability of the parameters. Then the methods that are commonly used in optimal experimental design (OED) are described and at the end of this section the studies that for now exist about OED in hydrological modelling are presented.

6.1. Structural versus practical identifiability

It is important to differentiate between structural and practical identifiability of parameters because a structurally unidentifiable parameter will not benefit from any optimal experimental design technique whereas practically unidentifiable parameters can become better identifiable with a good measurement set-up. Hence, in such case, optimal experimental design techniques can therefore be applied.

For the analysis of structural identifiability a known model structure with perfectly noise-free data should be considered (Dochain and Vanrolleghem, 2001). The question to be answered is whether in that case it is evident that all parameters in the model are identifiable. Consider for instance the following simple equation: $y = ax1 + bx2 + c(x1 + x2)$, where x1 and x2 are two variables, y is the measured variable and a, b and c are the model parameters. From this simple example it is obvious that only the parameter combinations (a+c) and (b+c) can be identified unless the value of one of them is a priori known. When a model has parameters that theoretically can be determined uniquely from a noise-free data set, one says the model parameters are structurally identifiable. For linear equations it seems an easy task to decide whether or not the parameters can be identified from the structural point of view. Despite this a number of different tests for parameter identifiability were developed for linear models. An overview of these different methods is given in (Godfrey and Distefano, 1985). For models that are non-linear in the parameters the problem is a lot more complex. In this case several structural identifiability tests exist, but they are usually very complex (Dochain et al., 1995).

While the structural identifiability is studied under the assumption of perfect, i.e. noiseless data, the problem of highly correlated parameters arises when a limited set of experimental, noise-corrupted data is used for parameter estimation. Under such conditions the uniqueness of parameter estimates predicted by the theoretical analyses, may no longer be guaranteed, because a change in one parameter can be compensated almost completely by a proportional shift in another one, still producing a satisfying fit between experimental data and model predictions. In addition, the numerical algorithms that perform the non-linear estimation show poor convergence when faced with this type of ill-conditioned optimization problems, the estimates being very sensitive to the initial parameter values given to the algorithm (Dochain and Vanrolleghem, 2001). The practical identifiability not only depends on the noise level of the data, but also depends on the experimental conditions themselves. Practical identifiability is thus related to the quality of the data and is related to their information content, i.e. whether or not the available data are informative enough to identify the model parameters accurately. Holmberg (1982) shows that the practical identifiability of Monod parameters from batch experiments depends on the chosen initial substrate concentration. The author states that the optimal initial substrate concentration depends not only on the noise level of the data but also on the sampling instants. De Pauw (2003b) performed optimal experimental design for calibration of bioprocess models. Vanrolleghem et al. (1995) performed research to improve the practical identifiability of a biokinetic model of activated sludge respiration. For river water quality modelling Reichert and Vanrolleghem (2001) presented a technique based on the sensitivity ranking and the collinearity index which allows to find practical identifiable subsets of parameters for the River Water Quality Model 1 (RWQM1) (Reichert et al., 2001a).

6.2. Optimal experimental design to maximize the practical identifiability of parameters

The quality of a model calibration can be evaluated by analysing the parameter estimation error covariance matrix C (Equation 1).

$$C = \begin{bmatrix} \sigma^2_{\theta i} & \operatorname{cov}(\theta_i,\theta_j) & \cdots & \operatorname{cov}(\theta_i,\theta_n) \\ \operatorname{cov}(\theta_i,\theta_j) & \sigma^2_{\theta j} & & \\ \vdots & & \ddots & \\ \operatorname{cov}(\theta_i,\theta n) & & & \sigma^2_{\theta n} \end{bmatrix} \quad (1)$$

This matrix is calculated by several parameter estimation algorithms and can also be estimated using different techniques (Dochain and Vanrolleghem, 2001). The diagonal elements are the variances of the parameter estimates and the off-diagonal elements are the covariances between the different parameters. The parameter estimation covariance matrix can be used to calculate confidence intervals, confidence regions and parameter correlations. Small variances will result in small confidence regions and thus more accurate parameter estimations.

The quality of the model calibration largely depends on the quality of the available data and thus on the design of the experiment which was used to obtain the data. Poorly designed experiments result in poor data and will obviously result in poorly estimated parameters (large variances or strong correlations). Designing experiments is a difficult task and is often performed without a clear strategy. This is due to the large amount of choices that can be made and experimental constraints that have to be met when designing an experiment. These choices and constraints include (De Pauw and Vanrolleghem, 2003b):

- Resources, including experimentation time and expenses, might be limited.
- Which measurements have to be performed?
- Which measuring frequencies can or have to be used?
- Where should the measurements be performed?
- Which experimental manipulations should be performed (e.g. temperatures, flow rates, …) and what are the constraints for these manipulations?

In order to design an experiment that will produce high quality data required for an accurate model calibration, optimal experimental design for parameter estimation (OED-PE) can be used. This is a mathematical technique, which provides a solution to the complex problem of constrained choices resulting in an optimal experiment. The basis of OED-PE is the Fisher Information Matrix (FIM) which under certain conditions (uncorrelated white measurement

noise), gives the lower bound of the parameter estimation error covariance matrix according to the Cramer-Rao inequality (Ljung, 1999; Walter and Pronzato, 1999):

$$C(\theta) \geq FIM^{-1} \tag{2}$$

6.2.1. Fisher information matrix

The Fisher Information Matrix (Equation 3) summarises the information content of a certain experiment (Bard, 1974). Two sources of information are considered in its definition: sensitivity functions and measurement error. The summation of these two terms is made at each measurement point (i=0 . N).

$$FIM = \sum_{i=0}^{N} \left(\frac{\partial y}{\partial \theta} \right)^{T} Q^{-1} \left(\frac{\partial y}{\partial \theta} \right) \tag{3}$$

Sensitivity functions indicate how sensitive a certain variable (y) is with respect to a certain parameter (θ). Mathematically this is expressed as the partial derivative of the variable to the parameter ($\partial y/\partial \theta$). A variable is said to be sensitive if small changes in the parameter produce significant changes in the variable. This is explained in the literature chapter "sensitivity analysis".

The second source of information in the FIM is related to the measurement error, which is expressed as a (time-varying) measurement error covariance matrix (Q). This matrix contains the measurement errors and correlations between the measurements. Measurements with large measurement error will obviously contribute less to the information content of the experiment than measurements with small measurement error.

As already discussed, the FIM is the inverse of the parameter estimation error covariance matrix (Equation 2). This relationship is illustrated in Figures II.7a and II.7b for a 2 parameter estimation problem. These figures represent the confidence regions of two parameters (θ1 and θ2). The size, shape and orientation of the confidence ellipse are determined by the eigenvalues and eigenvectors of the FIM. The largest axis of the confidence ellipse is inversely proportional to the square root of the smallest eigenvalue (λ_{min}), while the smallest axis is inversely proportional to the square root of the largest eigenvalue (λ_{max}). In this way properties of the FIM determine the properties of the confidence region and thus the accuracy of the parameter estimates.

The information content of the experiment can be evaluated in different means by considering different properties of the FIM. All of these criteria are based on the shape of the confidence region of the parameters. Actually, each parameter obtained from a parameter estimation procedure is situated within a confidence region. For linear models and for one parameter this will be a symmetric interval, for two parameters the confidence region will be an ellipse,

whereas for n parameters the confidence region will be an n-dimensional ellipsoid. The volume of this ellipsoid is proportional to the inverse of the determinant of the FIM (Walter and Pronzato, 1999). Following criteria exist:

D-optimal criterion (i.e. the volume criterion)
Optimising this criterion will select for the experimental conditions that will minimize the volume of the ellipsoid. This volume is inversely proportional to the determinant of the FIM, i.e. the product of its eigenvalues. Maximizing the determinant of the FIM physically means minimizing the geometric average of the errors on the parameter values.

E-optimal criterion (i.e. the shape criterion)
With this criterion experimental conditions will be selected for which the longest axis of the confidence ellipsoid is shortest, which is equivalent to maximizing the smallest eigenvalue of the FIM.

Modified E-optimal criterion
This criterion is a slight modification of the above criterion, i.e. instead of only taking into account the smallest eigenvalue, the ratio of the largest to the smallest eigenvalue will be minimized. This ratio expresses the stiffness of the FIM. The more important the stiffness becomes, the more difficult it becomes to invert the matrix until finally a singular matrix is obtained i.e. complete correlation between two parameters exist.. The modified E-optimal criterion will thus give rise to a FIM that is as far away as possible from singularity. The modified E design criterion aims at reducing parameter correlations by getting the shape of the confidence region as close to a circle as possible. This is illustrated in Figure II.7b. The best value one can obtain for the modified E criterion is 1, and this has been achieved. However, one must be aware that such optimum only guaranties the confidence region is a circle, but it can be a very large circle (Dochain and Vanrolleghem, 2001).

Modified A-optimal criterion
This criterion will maximize the trace of the FIM, i.e. it allows maximizing the sum of the eigenvalues of the FIM. Physically this criterion will minimize the arithmetic mean of the error on the parameter estimates and assures there is no problem if the FIM is singular..

A-optimal criterion
This criterion will minimize the trace of the inverse of the FIM. Physically this criterion will, as with the modified A-optimal criterion, minimize the arithmetic mean of the error on the parameter estimates.

Table II.3 lists these criteria. The D- and A-optimal design criteria aim at minimizing the volume of the confidence ellipse. This is illustrated in Figure II.7a. Bard (1974) shows that the D-optimal criterion is best suited as design criterion for parameter estimation.

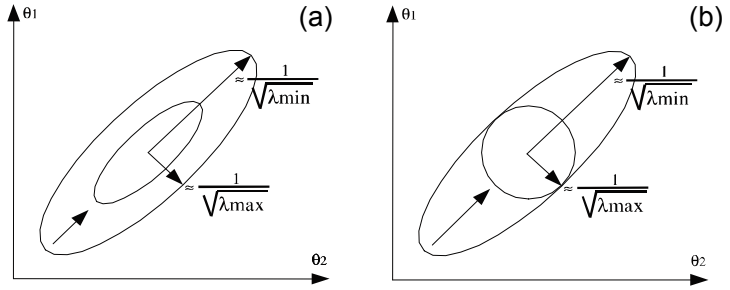


Figure II.7a-b: Effect of different FIM design criteria (D-criterion: left, Modified E criterion, right) on the size and shape of the parameter confidence region

Table II.3: Different optimal design criteria based on FIM properties

Name	Criterion
A-optimal design	$\min[tr(FIM^{-1})]$
Modified A-optimal design	$\max[tr(FIM)]$
D-optimal design	$\max[det(FIM)]$
E-optimal design	$\max[\lambda_{min}(FIM)]$
Modified E-optimal design	$\min[\lambda_{max}(FIM)/\lambda_{min}(FIM)]$

tr(): sum of eigenvalues; det(): product of eigenvalues

6.2.2. Calculation of the FIM

For the practical implementation of the OED, it is necessary to calculate the value of the FIM for each proposed experiment. To calculate the elements of the FIM the sensitivity functions have to be calculated. These sensitivity functions can be calculated analytically, which is a laborious task, or the calculations can be based on a numerical approximation. In the latter case model predictions are calculated where for each simulation run a single parameter is perturbed slightly from its optimal value. This is only one of the possibilities (see literature chapter about SA). As such, at each measurement time instant a number of model predictions are available corresponding to the number of parameters plus one. To obtain the approximated value for the sensitivities, the difference is made between the slightly perturbed predictions and the nominal model predictions. Dividing this difference by the perturbation of the parameter gives the sensitivity. This calculation has to be performed for each response (y_k), for all parameters (θ_p) at each time instant (t_n). The accuracy of the numerical approximation largely depends on the magnitude of the parameter perturbation (De Pauw and Vanrolleghem, 2003a). It is suggested to verify the results by calculating the matrix using a fixed parameter perturbation and subsequently recalculating the matrix using a parameter perturbation half the previous one or to use a perturbation factor. If no difference is noticed in the sensitivities, the fixed value is used for all subsequent calculation. Unfortunately, both methods, analytically and numerically are still (computer) time consuming. Indeed, as indicated above, for every measurement point (i.e. time) the change in the value of the

response (y) has to be calculated for a small change in the parameters, and this for all parameters.

Fortunately, calculation of the FIM can be performed using a third method. Indeed, the elements of the FIM are the elements of the inverse of the covariance matrix of the parameter estimates (Godfrey and Distefano, 1985). This covariance matrix can typically be obtained from mathematical parameter estimation algorithms (for theoretical background on the calculation of the covariance matrix, see chapter "Materials and Methods"). In the "covariance method" for the optimal experimental design of experiments, the steps between simulating the experiment and evaluating the objective functional are different. For the covariance method, experimental data including noise have to be generated. Therefore noise is added to the simulated data. These "created" concentration profiles are then used as virtual experimental data and used as input data for parameter estimation. From the parameter estimation algorithm also the covariance matrix is obtained. This matrix can then be inverted to obtain the FIM. This procedure has to be repeated for each possible next experiment. The possible ways for the calculation of the FIM are given schematically in figure II.8.

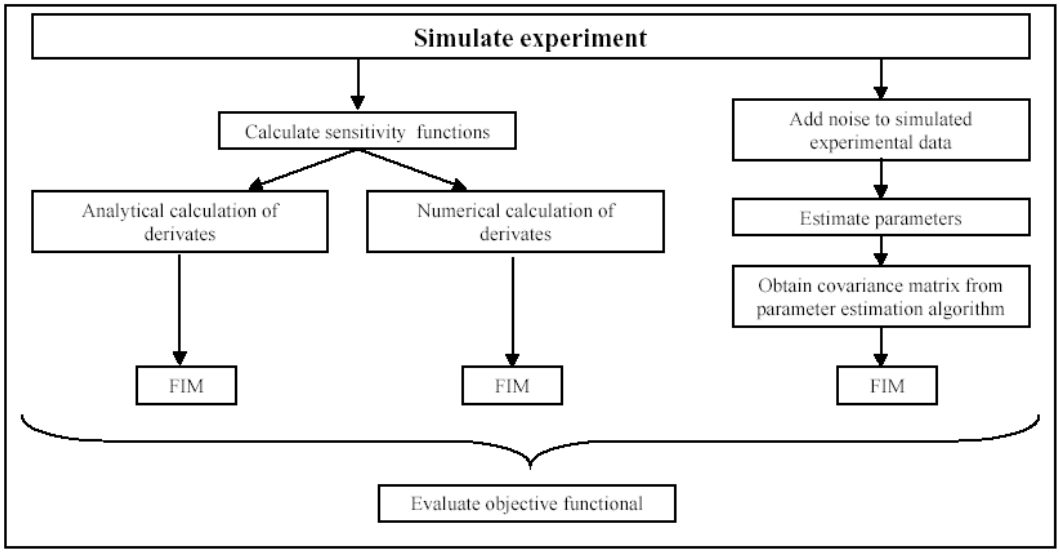


Figure II.8: Possible ways to identify the FIM and calculate the objective functional (from Baetens (2000))

6.3. Iterative optimal experimental design procedure

Before starting experimental design, a preliminary model should be available. Parameter values can be obtained from literature or when no literature values are available, initial parameter values can be based on at least one experiment, i.e. an initial experiment has to be performed. With parameter estimation algorithm an initial set of parameter values is obtained.

Based on the current model an experiment is proposed by choosing certain experimental degrees of freedom. This experiment is then simulated on the computer and an objective

function is evaluated. Typically this objective function is a design criterion from the Fisher Information Matrix (table II.3) which summarizes the information content of the proposed experiment and is also a measure for the accuracy of the parameter estimates (in case this experiment would be performed in reality and the model would be fitted to the acquired data). A (non-linear) optimisation algorithm can be used to propose different experiments (from the experimental degrees of freedom and within the experimental constraints and find an "optimal" experiment in the sense that it for instance maximizes the parameter estimation accuracy and/or minimizes parameter correlations.

Once the "optimal" experiment is found it can be performed in reality. Based on the data of this experiment the model can be refitted and the accuracy of the parameter estimates evaluated. If the required accuracy is not yet reached another iteration can be performed, leading to an even better "optimal" experiment (figure II.9). Finally, a calibrated model is available for its intended use.

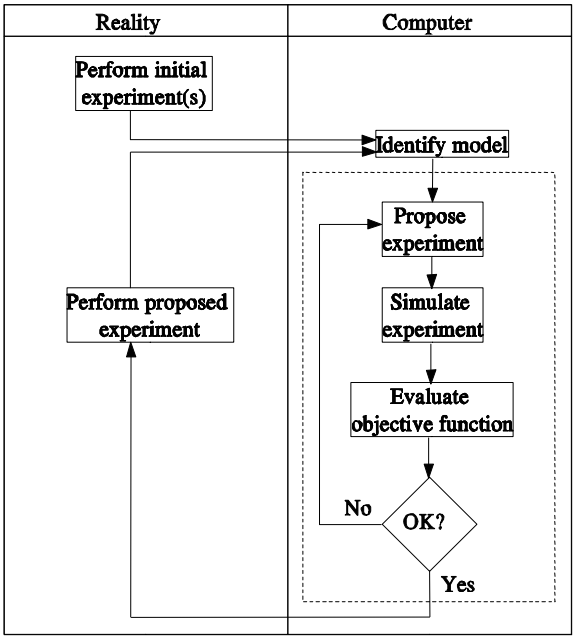


Figure II.9: General procedure for optimal experimental design (from Dochain and Vanrolleghem, 2001)

6.4. OED in hydrology

At the moment only a limited number of studies in the domain of hydrology have addressed the problem of designing experiments by which more informative data can be collected.

In 1983, Szidarovsky (1983), dealt with the optimal location problem for measuring water quality for a single experimental point, and extended this to a second, third and fourth design which pertains to the case of multiple additional points. For the second and third case, an optimal regular observation network was designed to minimize the uncertainty of the estimation process subject to either the given number of additional data, or an upper bound for

the cost of the additional data. In the fourth case, the number or cost of additional points was minimized subject to bounded uncertainty conditions. Finally, a numerical example was used to illustrate the models and algorithms.

A second interesting study was performed by Casman et al. (1988). They describe optimal experimental design for river water quality modelling. In their case the boundary conditions and parameters are not exactly known and they show how sequential design is needed. They illustrated the methods on a simple Streeter-Phelps model.

Tung and Hathorn (1989) performed a study to determine critical locations in a stochastic stream environment. They defined as criteria the variance of dissolved oxygen (DO) deficit and so the probability of violating specified DO standards and took measurements at the place associated with the maximum value of their respective functions. Also here again the mathematical model is restricted to the simple Streeter Phelps model.

More recent research in the field of hydrology is performed on the determination of good measurements for specific parameters. In this context one can find the optimal experimental design for dispersion experiments by Agunwamba (2002). Their design helps to determine the dispersion coefficient more accurate. Research on optimal experimental design is also done for parameter estimation in column outflow experiments (Altmann-Dieses et al., 2002). Experimental conditions, such as irrigation schemes, substance concentrations, and sampling schemes lead to an intricate, nonlinear, constrained optimization problem that is solved by a direct approach based on a structured sequential quadratic programming (SQP) method. Another recent study was performed by Catanai et al. (2004) in which an estimation is done of the, longitudinal and transversal dispersivity coefficients, from a soil column experiment. The dispersivity coefficient is an important parameter for groundwater modelling.

Most of the research on optimal experimental design was done around the late 80's but apparently this kind of research was not extended and was not applied on real studies. Possible explanation of this phenomenon is the large computational need for the calculation of optimal experimental design for environmental systems. Simple and theoretical concepts could be checked but the more complex models with inclusion of natural variability in the experimental conditions could not be examined.

CHAPTER III
MATERIALS AND METHODS

Parts of this chapter were published as:

- Vandenberghe, V., van Griensven, A. and Bauwens, W. (2001). Sensitivity analysis and calibration of the parameters of ESWAT: Application to the river Dender. Water Science and Technology, 43(7), 295-301
- Vandenberghe, V. , van Griensven A. and Bauwens W. (2002). Detection of the most optimal measuring points for water quality variables: application to the river water quality model of the river Dender in ESWAT, Water Science and Technology, 46(3), 1-7
- Vandenberghe, V., Bauwens, W. and Vanrolleghem, P.A. (2004). The Evaluation of Uncertainty Propagation into River Water Quality Predictions to Guide Future Monitoring Campaigns. Environmental Monitoring and Software, 22, 275-232.
- Vandenberghe V., van Griensven A., Bauwens W. and Vanrolleghem P.A. (2006). Effect of different river water quality model concepts used for river basin management decisions Water Science & Technology, 53(10), 277-284.

CHAPTER III: MATERIALS AND METHODS

1. Software for calibration, optimisation, sensitivity and uncertainty analysis

1.1. Pest

PEST is a software for model-independent parameter estimation and uncertainty analysis (Doherty, 2000). The purpose of PEST (which is an acronym for Parameter ESTimation) is to assist in data interpretation, model calibration and predictive analysis. One can use PEST when model parameters and/or excitations need to be adjusted until model-generated numbers fit a set of observations as closely as possible, provided certain continuity conditions are met.

PEST is able to "take control" of a model, running it as many times as it needs to, while adjusting its parameters until the discrepancies between selected model outputs and a complementary set of field or laboratory measurements is reduced to a minimum in the weighted least squares sense. Using PEST has two main advantages over other packages for parameter estimation. First, it doesn't have the difficulty that normally one needs to partially recode the model under consideration or programming tasks are needed in order to communicate with an estimation program; this usually involves recasting the model as a subroutine which is then called by the estimator each time it needs to run the model. PEST communicates with the model through the model's own input and output files. The only requirements for the "model" are that it can be run from the command line and that it reads and write ASCII files. Secondly, it makes use of a particularly robust variant of the Gauss-Marquardt-Levenberg method for nonlinear parameter estimation, so the performance of the estimator is not degraded when optimizing parameters for large numerical models, or for the sometimes-complex models used for simulating environmental processes.

1.1.1. The parameter estimation algorithm

For linear models (ie. models for which observations are calculated from parameters through a matrix equation with constant parameter coefficients), optimisation can be achieved in one step. However for nonlinear problems (most models fall into this category), parameter estimation is an iterative process. At the beginning of each iteration the relationship between model parameters and model-generated observations is linearised by formulating it as a Taylor expansion about the currently best parameter set; hence the derivatives of all observations with respect to all parameters must be calculated. This linearised problem is then solved for a better parameter set, and the new parameters tested by running the model again. By comparing parameter changes and objective function improvement achieved through the current iteration with those achieved in previous iterations, PEST can tell whether it is worth undertaking another optimisation iteration; if so, the whole process is repeated.

Unless a model can calculate them itself, derivatives of observations with respect to parameters must be calculated by PEST using finite differences. During every optimisation iteration the model is ran once for each adjustable parameter, a small user-supplied increment

being added to the parameter value prior to the run. The resulting observation changes are divided by this increment in order to calculate their derivatives with respect to the parameter. This is repeated for each parameter. This technique of derivatives calculation is referred to as the method of "forward differences".

Derivatives calculated in this way are approximate. If the increment is too large the approximation will be poor; if the increment is too small, the round-off errors will reduce the quality of the derivatives accuracy. Both of these effects will degrade optimisation performance. To combat the problem of derivatives inaccuracy, PEST allows derivatives to be calculated using the method of "central differences". Using this method, two model runs are required to calculate a set of observation derivatives with respect to any parameter. For the first run an increment is added to the current parameter value, while for the second run the increment is subtracted. Hence three observation-parameter pairs are used in the calculation of any derivative (the third pair being the current parameter value and corresponding observation value). The derivative is calculated either by (i) fitting a parabola to all three points, (ii) constructing a best-fit straight line for the three points or (iii) by simply using finite differences on the outer two points (the user can choose).

PEST can make the switch from the forward difference method to the central difference method automatically according to a criterion, which is supplied to it prior to the commencement of the run.

1.1.2. Non-linear parameter estimation

Let the relationships between parameters and model-generated observations for a particular model be represented by the function M which maps the n-dimensional parameter space into the m-dimensional observation space. Suppose that for the set of parameters comprised in the vector b_0 the corresponding set of model-calculated observations (generated using M) is c_0, ie.

$$c_0 = M(b_0) \qquad (1)$$

Now to generate a set of observations c corresponding to a parameter vector b that differs only slightly from b_0, Taylor's theorem tells that the following relationship is approximately correct, the approximation improving with proximity of b to b_0:

$$c = c_0 + J(b - b_0) \qquad (2)$$

where J is the Jacobian matrix of M, ie. the matrix comprised of m rows (one for each observation), the n elements of each row being the derivatives of one particular observation with respect to each of the n parameters. To put it another way, J_{ij} is the derivative of the i'th observation with respect to the j'th parameter. Equation 2 is a linearisation of equation 1.

To derive a set of model parameters for which the model-generated observations are as close as possible to our set of experimental observations in the least squares sense, i.e. to determine a parameter set for which the objective function Φ defined by

$$\Phi = (c - c_0 - J(b - b_0))^t Q\, (c - c_0 - J(b - b_0)) \qquad (3)$$

is a minimum, with Q the weighing matrix for the observations and where c in equation 3 now represents the experimental observation vector, the parameter upgrade vector ($b - b_0$) can be calculated on the basis of the vector ($c - c_0$) which defines the discrepancy between the model-calculated observations c_0 and their experimental counterparts c. Denoting u as the parameter upgrade vector, the vector u which minimises Φ of equation 3 is given by

$$u = (J^tQJ)^{-1}J^tQ(c - c_0) \qquad (4)$$

and the parameter covariance matrix becomes

$$C(b) = (J^tQJ)^{-1} \qquad (5)$$

The linear equations represented by the matrix equation 4 are often referred to as the "normal equations". The matrix (J^tQJ) is often referred to as the "normal matrix".

Because equation 2 is only approximately correct, so too is equation 4; in other words, the vector b defined by adding the parameter upgrade vector u of equation 4 to the current parameter values b_0 is not guaranteed to be that for which the objective function is at its minimum. Hence the new set of parameters contained in b must then be used as a starting point in determining a further parameter upgrade vector, and so on until, hopefully, we arrive at the global Φ minimum. This process requires that an initial set of parameters b_0 be supplied to start off the optimisation process. The process of iterative convergence towards the objective function minimum is represented diagrammatically for a two-parameter problem in figure III.1.

It is an unfortunate fact in working with nonlinear problems that a global minimum in the objective function may be difficult to find. For some models the task is made no easier by the fact that the objective function may even possess local minima, distinct from the global minimum. Hence it is always a good idea to supply an initial parameter set b_0 that you consider to be a good approximation to the true parameter set. A suitable choice for the initial parameter set can also reduce the number of iterations necessary to minimise the objective function; Also, the inclusion of prior information into the objective function can change its structure in parameter space, often making the global minimum easier to find (depending on what weights are applied to the articles of prior information). Once again, this enhances optimisation stability and may reduce the number of iterations required to determine the optimal parameter set.

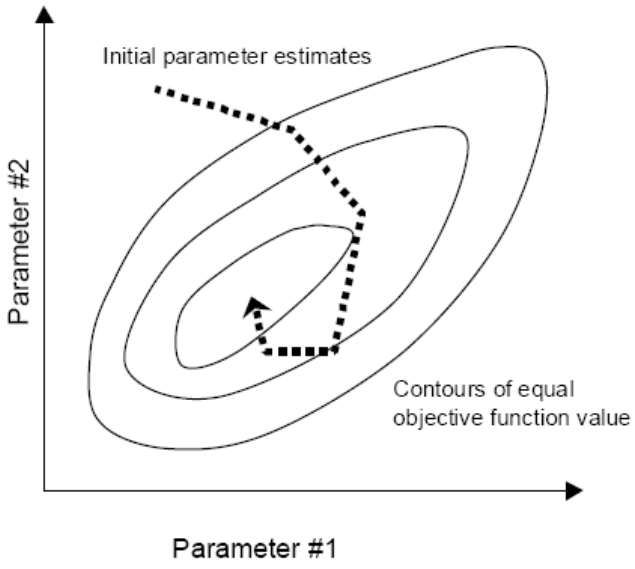


Figure III.1: Iterative improvement of initial parameter values toward the global objective function minimum.

The Marquardt Parameter Equation (4) forms the basis of nonlinear weighted least squares parameter estimation. It can be rewritten as

$$u = (J^tQJ)^{-1}J^tQr \quad (6)$$

where u is the parameter upgrade vector and r is the vector of residuals for the current parameter set. Let the gradient of the objective function in parameter space be denoted by the vector

$$g_i = \frac{\partial \Phi}{\partial b_i}$$

i.e. by the partial derivative of the objective function with respect to the i'th parameter. The parameter upgrade vector cannot be at an angle of greater than 90 degrees to the negative of the gradient vector. If the angle between u and -g is greater than 90 degrees, u would have a component along the positive direction of the gradient v thus cause the objective function to rise, which is the opposite of what we want. However, in spite of the fact that -g defines the direction of steepest descent of Φ, it can be shown that u is normally a far better parameter upgrade direction than -g, especially when parameters are highly correlated. In such situations, iteratively following the direction of the steepest descent leads to the phenomenon of "hemstitching" from side to side of a valley in Φ as parameters are upgraded on successive iterations; convergence toward the global Φ minimum is then extremely slow. See figure III.2.

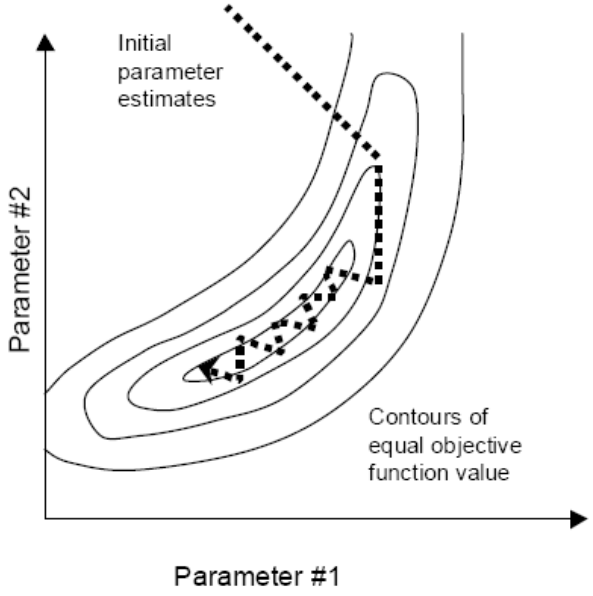


Figure III.2: The phenomenon of "hemstitching"

Nevertheless, most parameter estimation problems benefit from adjusting u such that it is a little closer to the direction of -g in the initial stages of the estimation process. Mathematically, this can be achieved by including in equation 6 the so-called "Marquardt parameter", named after Marquardt (1963), though the use of this parameter was, in fact, pioneered by Levenberg (1944). Equation 6 becomes

$$\mathbf{u} = (\mathbf{J}^t\mathbf{Q}\mathbf{J} + \alpha\mathbf{I})^{-1}\mathbf{J}^t\mathbf{Q}\mathbf{r} \qquad (7)$$

where α is the Marquardt parameter and I is the n × n identity matrix. It can be shown that the gradient vector g can be expressed as

$$\mathbf{g} = -2\mathbf{J}^t\mathbf{Q}\mathbf{r} \qquad (8)$$

It follows from equations 7 and 8 that when α is very high the direction of u approaches that of the negative of the gradient vector; when α is zero, equation 6 is equivalent to equation 5. Thus for the initial optimisation iterations it is often beneficial for α to assume a relatively high value, decreasing as the estimation process progresses and the optimum value of Φ is approached. Where the direction is now favourable, the magnitude may be not.

Under the linearity assumption used in deriving all equations presented so far, it can be shown that the optimal parameter adjustment vector is given by βu, where u is determined using equation 7 and β is calculated as

$$\beta = \frac{\sum_{i=1}^{m}(c_i - c_{0i})w_i^2\gamma_i}{\sum_{i=1}^{m}(w_i\gamma_i)^2}$$

where, once again, the vector c represents the experimental observations, c_0 represents their current model-calculated counterparts, w is the weight pertaining to observation i, and γ is given by

$$\gamma_i = \sum_{j=1}^{n} u_j \frac{\partial c_{0i}}{\partial b_j}$$

i.e.

$$\gamma = Ju$$

where J represents the Jacobian matrix once again. If b_0 holds the current parameter set the new, upgraded set is calculated using the equation

$$b = b_0 + \beta u$$

1.1.3. PEST applications in hydrology

PEST is widely used as a parameter estimation tool coupled with various simulation tools. Baginska et al. (2003) coupled PEST with Annualized Agricultural NonPoint Source (AnnAGNPS) to determine the export of nitrogen and phosphorous through nonpoint sources. Application with Surface-Water Assessment Tools (SWAT) to model snowmelt hydrology was made by Wang and Melesse (2005). Urban runoff models and watershed models such as Hydrologic Simulation Program Fortran (HSPF) have also been coupled with PEST (Doherty and Johnston, 2003; Ovbiebo and Kuch, 1998). PEST has also been successfully applied with temperature and salinity models as in Gao and Meerick (1996). The field of groundwater has found PEST to be a useful tool with application for flow, heat transfer, and mass transfer (Doherty, 2003; Keating et al., 2003; Vesselinov et al., 2001).

The comparison between the results after calibration of a model for the river Dender with PEST and with SCE-UA (explained here further (section 1.3) is discussed in the work of van Griensven (2002). There it was found that PEST often gives different values after calibration depending on the initial parameter values. SCE-UA always finds the same solution. This indicates that PEST gets stuck in local optima. On the other hand, it was seen that SCE-UA always finds the same solution, independently of the search parameters.

1.2. Uncsam

The UNCSAM computer package developed by Janssen et al. (1992) was used to generate random values for each uncertain parameter using the Monte Carlo, Latin Hypercube (McKay et al., 1979) Simulation approach and to perform various regression and correlation analyses among input parameters and model output. UNCSAM offers tools to perform sensitivity and uncertainty analysis on a model in an automised way. The results of the analyses are stored in

ASCII files in the form of tables or plot constructions. The model simulations and the analysis of the simulation results by UNCSAM, need interfacing between UNCSAM and the model. Tools for the interfacing are supplied in the software package.

1.2.1. Sensitivity and uncertainty analysis based on regression and correlation analysis

In the literature study, the chapters about sensitivity and uncertainty analysis, the theory about sensitivity and uncertainty analysis based on regression analysis and correlation analysis is explained. Also the Monte Carlo technique and the Latin Hypercube sampling can be found there in detail. UNCSAM performs a least squares regression and then calculates measures that can be used for sensitivity and uncertainty interpretations. In table III.1 the different measures are given.

Table III.1: Sensitivity and uncertainty measures available in UNCSAM

Method	Original data	Rank transformed data	Formula
Regression	Ordinary regression coefficient (ORC)	Rank transformed regression coefficient (RRC)	$\hat{\beta}_i^{(S)}$
	Standardised regression coefficient (SRC)	Rank transformed standardised regression coefficient (SRRC)	$\hat{\beta}_i^{(s)} = \hat{\beta}_i . \frac{S_{x_i}}{S_y}$
	Normalised regression coefficient (NRC)	Rank transformed normalised regression coefficient (NRRC)	$\hat{\beta}_i \frac{\overline{x}_i}{\overline{y}}$
	Relative partial sum of squares (RPSS)	Rank transformed relative partial sum of squares (RPRSS)	$S_{\hat{y}}^2 - S_{\hat{y}\|i-}^2$
	Rank transformed partial uncertainty contribution (PUC)	Rank transformed (RPUC)	$\sum_{j=1}^{p} \hat{\beta}_i^{(s)} r y_{x_i} r_{x_i x_j}^2$
Correlation	Rank transformed linear correlation coefficient (LCC)	Rank transformed correlation coefficient (RCC)	$r_{\overline{y}_i \overline{x}_i}$
	Partial correlation coefficient (PCC)	Rank transformed Partial correlation coefficient (PRCC)	$r_{xy-z} = \frac{r_{xy} - r_{xz} r_{yz}}{\sqrt{\left(1 - r_{xz}^2\right)\left(1 - r_{yz}^2\right)}}$
	Semi-partial correlation coefficient (SPC)	Semi-partial rank transformed correlation coefficient (SPRC)	$r_{yx\|z} = \frac{\left(r_{yx} - r_{yz} r_{xz}\right)^2}{1 - r_{xz}^2}$
Total influence	Coefficient of Determination (COD)	Rank transformed coefficient of determination (RCOD)	$\frac{S_{\hat{y}}^2}{S_y^2}$

1.3. SCE-UA

The Shuffled Complex Evolution (SCE) algorithm was developed by Duan et al. (1992), using the best features of multiple complex shuffling and competitive evolution (Holland, 1975) based on the simplex search method of Nelder and Mead (1965). The algorithm is freely available as FORTRAN code. As it searches over the whole parameter space, the

algorithm finds the global optimum with a success rate of 100% (Sorooshian et al., 1993). Duan et al. (1992) describes the SCE-UA as an approach that treats the global search as a process of natural evolution. The sampled points constitute a population that is partitioned into several communities (complexes), each of which is permitted to evolve independently (i.e., search the space in different directions). After a certain number of generations, the communities are mixed and new communities are formed through a process of shuffling. This procedure enhances survivability by a sharing of the information (about the search space) gained independently by each search community.

The SCE-UA requires less runs than the random search method and claims to systematically find the global optimum (Sorooshian et al., 1993). A large number of studies (Cooper et al., 1997; Duan et al., 1992; Franchini et al., 1998; Gan and Biftu, 1996; Kuczera, 1997; Sorooshian et al., 1993; Thyer et al., 1999) concluded that in general the global population-evolution based algorithms are more effective than multi-start local search procedures, which in turn perform better than pure local search methods for calibration of rainfall-runoff models.

The SCE-UA method operates according to the following steps (Duan et al., 1992):

1. Sample points are generated from the feasible space (using upper and lower bounds of the parameters). The criterion function values are computed using these sampled points.

2. The sampled points are sorted and ranked in ascending order based on the criterion function values. This will result in the smallest criterion function value generating parameters at the top of the sampled parameter list.

3. The sampled points are partitioned into complexes with predefined size of the complex population.

4. Each complex is evolved independently a predefined number of times. The evolution of the complexes takes place using three types of evolution steps, namely: reflection, contraction and mutation. In the reflection step, the worst point in the subcomplex is reflected through the centroid of the other points. Since the reflected point has a lower criterion value than the worst point, the worst point is discarded and replaced by the new point. Thus an evolution step is completed. If the reflection step does not improve the criterion value, a contraction step in evolution is tried. In the contraction step, the new point lies halfway between the worst point and the centroid of the other points. If after the reflection step, the criterion value is outside the feasible parameter space, the mutation step is initiated. It is also used when both reflection and contraction steps fail to improve the criterion value. In a mutation step, a point is randomly selected in the feasible parameter space to replace the worst point of the sub-complex.

5. The evolved complexes from the previous step are combined into a single sample population. The sample population is sorted in order of increasing criterion value. Steps 3 to 5 are repeated until conditions as defined in step 6 are met.

6. The loop is stopped if the number of evolutionary steps has exceeded a predefined value or the criterion value has not improved by a predefined percentage in a predefined number of steps.

2. Software for river models

2.1. ESWAT

ESWAT is an extension of SWAT (van Griensven, 2002; van Griensven and Bauwens, 2001), the Soil and Water Assessment Tool developed by the USDA (Arnold et al., 1996). ESWAT was developed to allow for an integral modelling of the water quantity and quality processes in river basins. First the SWAT simulator is described here shortly. More detail can found in the user manual, which can be downloaded from http://www.brc.tamus.edu/swat. Next, the extensions made by van Griensven (2002) are described.

2.1.1. SWAT

SWAT98 - the Soil and Water Assessment Tool - was developed by the ARS/USDA as an integrator of the simulators CREAMS, GLEAMS, SWRRB and ROTO (Arnold et al., 1996). It includes modules for river basin scale modelling, hydrologic river routing, sediment, nutrient and pesticide transport. The calculation time step is daily.

SWAT has been developed and used for analysing agricultural management practices, water supply management and climate change effects on water, sediment and agricultural chemical yield in large complex watersheds with varying soils, land use and management conditions over long periods of time. To satisfy this objective, the model

- is partly physically based and partly distributed
- uses readily available inputs
- is computationally efficient to operate on large basins in a reasonable time
- runs in continuous time (daily updating of the water balance, plant growth, nutrient and pesticide concentrations, etc.)
- is capable of simulating long periods for computing the effects of management changes.

The water quantity processes simulated by SWAT include precipitation, evapotranspiration, surface run-off and lateral, ground water and river flow. The water quality section includes the calculation of the wash-off of sediment, nutrients and pesticides and the percolation of the latter two. Nutrient transformations as well as crop growth and agricultural management practices are also incorporated. Figure III.3 shows the hydrological cycle in SWAT and figure II.4 the in-stream processes modelled by SWAT.

The simulator is integrated in a GIS by an ArcView or GRASS pre-processor. Subbasin delineation is automated by means of a Digital elevation map (DEM). Within the subbasins, HRU's (Hydrological Response Units) can be defined by combining land use and soil maps. The program calculates the fluxes of each- HRU (per surface unity e.g. m²). These outputs will be aggregated to sub-basin output, in accordance to the fractions of the HRU's. The subbasin outputs will then be routed through river reaches according to the river network.

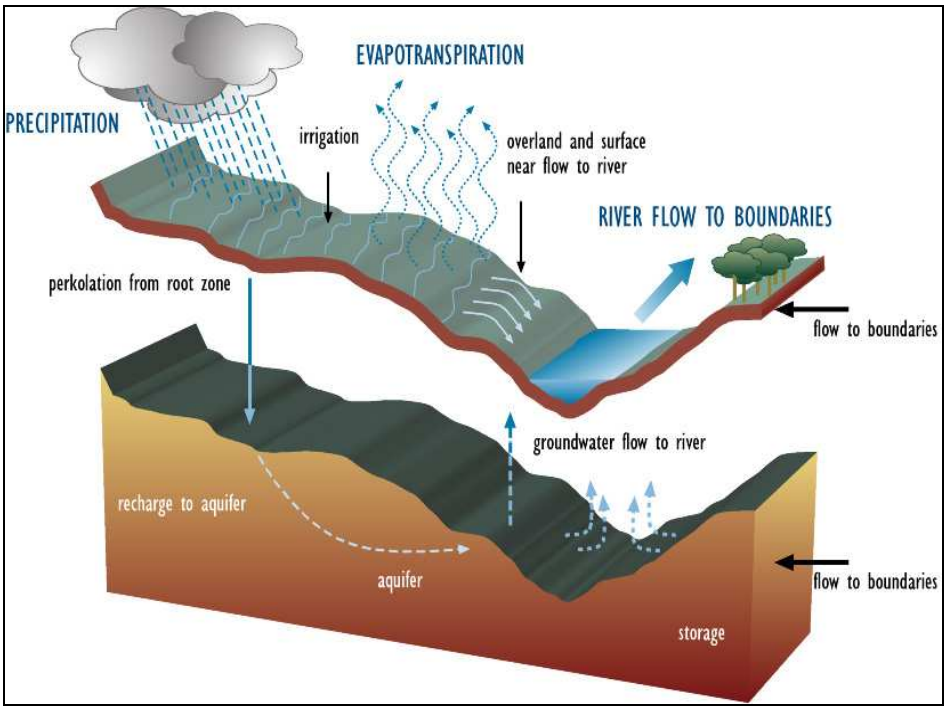


Figure III.3: Scheme of the hydrologic cycle in SWAT (Neitsch et al., 1999)

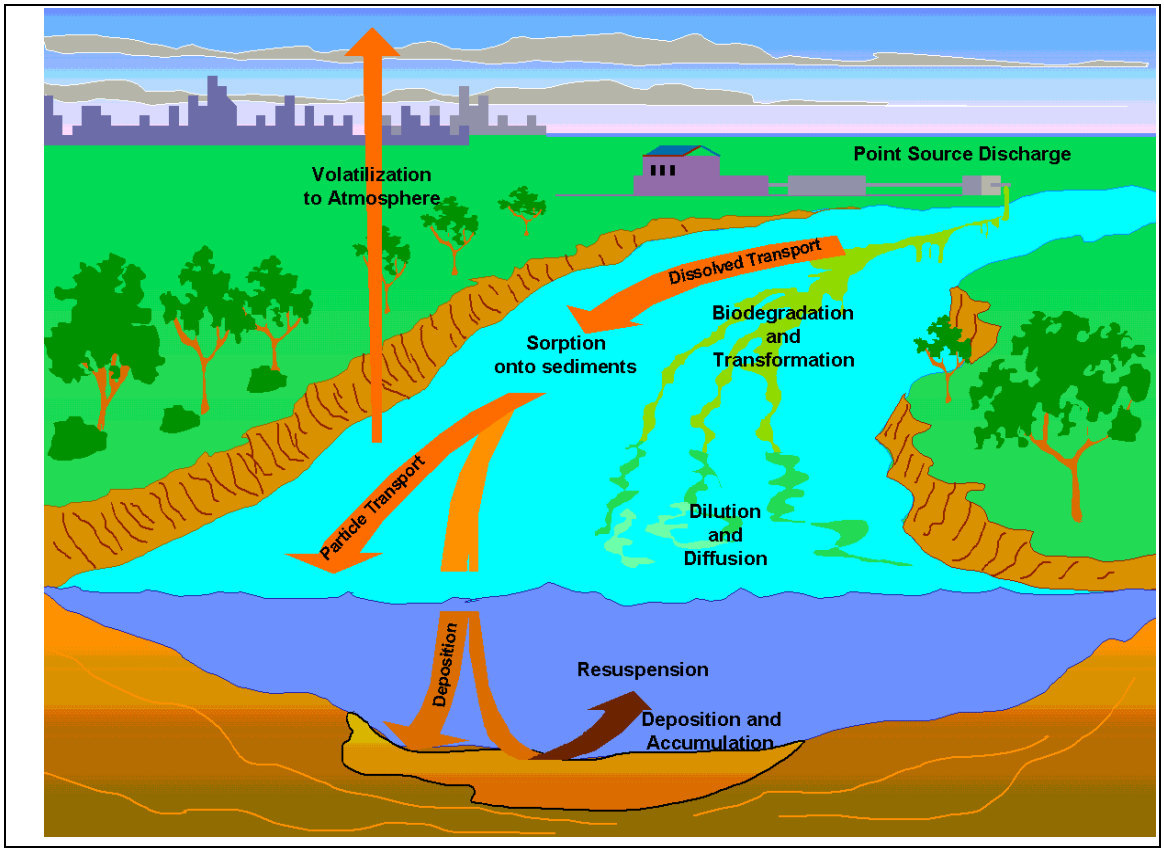


Figure III.4: In-stream processes modelled by SWAT (Neitsch et al., 1999)

The spatial variability of the terrain strongly affects the storm runoff and non-point source pollution processes. The use of GIS (Geographical Information System(s)) creates new

possibilities to account for the spatial variability. GIS can be used as a modelling tool itself or as a link between the heterogeneous terrain data and an existing non-GIS model. For SWAT, an interface was developed which links a GIS (Arcview) with the model (Di Luzio et al., 2000). The interface calculates some input parameters and creates all the input files for the model based on topographic, soil and landuse maps of the catchment. The SWAT Arcview interface was created as an Arcview extension rather than as a stand-alone program. The interface uses Arcview map themes and database files, which need to be prepared before running the interface.

2.1.2. Development of ESWAT

ESWAT is developed by van Griensven (2002) starting from SWAT98.1 (table III.2). The extension of SWAT focuses on the incorporation of a detailed river water quality module. Because sub-daily processes - such as algae respiration or combined sewer overflows- can determine the river water quality, the simulator was also modified to perform calculations on a sub-daily time step. An hourly time step is used for the simulation of water, nutrients, pesticides and river quality processes. The simulation of erosion processes is performed at a user-defined fraction of an hour and requires precipitation data with a sub-hourly time step.

Another important feature of ESWAT is the incorporation of modules to perform multi-objective auto-calibrations based on the SCE-UA method.

In this dissertation ESWAT is used because of several strong points:

- It is free available software.
- The extensions made it possible to work on a sub daily time scale, which was really needed because algal blooms are modelled.
- There are two possibilities for the water quality model: one based on QUAL2E and the other is the RWQM1 model including processes in the sediment. The availability of both models makes it possible to compare the results.
- Modelling the influence of structures and weirs was another important modification because the river Dender contains 12 sluices.
- A last and very important aspect of ESWAT is the easy manipulation of all input files. Model parameters and inputs for the model are all accessible. For SA and UA based on Monte Carlo methods this is necessary.

It should be mentioned that the USDA in the SWAT2000 version and the SWAT2003 version adopts several of the changes. In this paragraph, an overview will be given of the major new or modified modules of ESWAT.

Table III.2: New or modified modules of ESWAT

MODULES OF ESWAT	*changes to SWAT*	*DESCRIPTION*
CLIMATE	EXTENDED	sub-hourly rainfall data series
		Potential Evapotranspiration (PET): data series option
		radiation, wind speed, relative humidity: data series option
INFILTRATION/RUNOFF	EXTENDED	new hourly infiltration module
RIVER ROUTING	EXTENDED	new hourly river routing method instead of daily method
CANOPY STORAGE	EXTENDED	hourly option
REDISTRIBUTION	ORIGINAL	
EVAPOTRANSPIRATION	EXTENDED	PET data
LATERAL SUBSURFACE FLOW	ORIGINAL	
PONDS	ORIGINAL	
RETURN FLOW	EXTENDED	inclusion of initial value for the groundwater flow
EROSION	EXTENDED	sub-hourly peak runoff calculation
PLANT GROWTH	ORIGINAL	
NUTRIENT TRANSPORT	ORIGINAL	
PESTICIDES TRANSPORT	ORIGINAL	
CROP MANAGEMENT	ORIGINAL	
RIVER WATER QUALITY	NEW	Original QUAL2E processes
		extended QUAL2E processes based on BOD
		extended QUAL2E processes based on COD
		RWQM processes
REAERATION AT WEIRS	NEW	
SEDIMENT ROUTING	EXTENDED	hourly routing
AUTO-CALIBRATION	NEW	extended SCE-UA method

2.1.2.1 Hydrology

Sub-hourly Runoff/Infiltration Module

Runoff is calculated with a simplified infiltration model. Before saturation, the potential infiltration rate varies linearly between a maximal infiltration rate (F_0) and the saturation infiltration rate (F_E), as a function of soil water content. After saturation, the potential infiltration rate equals the saturation infiltration rate. The hourly runoff is then the result of the rain minus the infiltration. The soil water content will also change due to evapotranspiration and percolation to lower soil layers and the groundwater (Arnold et al., 1998).

The maximal and saturated infiltration rates are calculated using the saturated soil conductivity (K_s).

$F_E = f_1 * K_s$ (mm/hr) and $F_0 = f_2 * F_E$ (mm/hr)

where f1 and f2 are obtained by calibration, Ks is the saturated infiltration rate (mm/hr).

Hourly River routing

The continuity equation expresses the mass balance for a river reach over a time step dt. The storage at the beginning and at the end of the time step is represented by V_1 and V_2 respectively. The inflow rate "I" and outflow rate "Q" are considered constant over the time step "dt". Additional losses, such as evaporation (EVAP) and infiltration (INF) can also be taken into account.

$$Q\,dt = V_1 - V_2 + I\,dt - EVAP - INF$$

The routing method is based on the assessment of V_2, considering a constant flow velocity over the length of the reach. The latter velocity, v, is related to the inflow rate I by an empirical power function:

$$v = \frac{b}{W} * I^C$$

where W is the channel width and b and c are parameters. This relation can be assessed when using corresponding flow and river height observations or by literature.

According to this equation, the corresponding reach volume, V_{eq}, and residence time, γ, are:

$$V_{eq} = \frac{L*W}{b} * I^{1-c}$$

$$\gamma = \frac{V_{eq}}{I}$$

In case the residence time γ is smaller than the calculation time step dt (thus one hour), the reach volume at the end of the time step will be stabilised to V_{eq}:

$$V_2 = V_{eq}$$

However, when γ is larger than the time step, only part of V_1 will be replaced by V_{eq}:

$$V_2 = V_1 - \frac{dt}{\gamma}(V_1 - V_{eq})$$

Hourly time convolution module

All runoff variables undergo a time convolution before entering the river reach. This was done using the Nash Cascade algorithm (Nash, 1958), where three virtual reservoirs transform

the runoff variables. The following equations describe how the Nash Cascade algorithm was implemented:

$V' = V_1 + I^* (t_2-t_1)$

$Q = V' * r_{nash}$

$V_2 = V'-Q^*(t_2-t_1)$

where V = reservoir volume (m^3), I = reservoir inflow (m^3/hr), Q = reservoir outflow (m^3/hr), t_2-t_1= time step between time 2 and time 1 (hr), r_{nash} = coefficient ranging from 0-1($=1/k_{nash}$).

2.1.2.2 Water quality

The water quality modules of ESWAT represent different concepts.

One of them is based on the equations of QUAL2E (Brown and Barnwell, 1987) with the inclusion of denitrification and phosphate adsorption/desorption. The adsorption of dissolved P to sediments is simulated using the Freudlich equation (Parfitt and Rochester, 1983). It is this one that is used in this thesis work.

Considering the criticisms of Masliev et al. (1995) and Shanahan et al. (1998) , new modules were developed to close the mass balance. In the original QUAL2E equation, the sink and release of pollutants at the level of the river bed are dissociated. In order to close the mass balances, VUB-QUAL-BOD includes new state variables for the river bed. Also sessile macrophytes were added in the model in the form of plants, with processes similar to algae, but without settling and death. In VUB-QUAL-COD the biological oxygen demand (BOD) component is replaced by fast and slow chemical oxygen demand (COD) components.

The VUB-RWQM module is based on the equations of RWQM as presented by Reichert et al. (2001b). This model is also used in this thesis for a comparison of the applicability of different model concepts (see chapter Sensitivity Analysis). The RWQM model was not directly applicable in an integrated modelling context and the following modifications were needed:

- Splitting up of the organic components (organic N, organic P and organic C)
- Separate rates of hydrolysis for these components

The RWQM model defines processes and variables for the water column and the river bed, but does not specify the exchange between those phases. Following processes are proposed:

- Diffusion processes of the soluble components at the sediment/water column interface
- Deposition/resuspension of the solids

2.2. WEST

WEST (World-wide Engine for Simulation, Training and automation) is a multi-platform modelling and experimentation system (Vanhooren et al., 2003). It allows one to construct models and conduct virtual experiments on any kind of system that can be represented by differential algebraic equations. The WEST simulator was originally used to simulate wastewater treatment plants and an extensive WWTP model base is available (Vanhooren et al., 2003). The model base plays a central role in WEST. In this model base, models are described in a high level object-oriented declarative language specifically developed to incorporate models. The model base is aimed at maximal reuse of existing knowledge and is therefore structured hierarchically. This indicates that WEST has an open structure in that the user is allowed to change existing models and define new ones as needed. Next to the ASM-WWTP models, a runoff/sewer model based on Kosim (itwh, 1995; Paulsen, 1986) and the RWQM1 (Reichert et al., 2001b) a river water quality model are now implemented in this package and can run in simultaneous simulations mode e.g. for integrated RTC investigations (Meirlaen et al., 2001).

In order to formulate and run a new model for a specific application in the WEST simulator, three main steps must be followed hierarchically:

- Writing a MSL-USER model
- Use the modelling environment to make the particular configuration
- Use the experimentation environment to perform model evaluations

In the first step, the user-defined model is described or written using the Model Specification language (MSL code). Once the model is described and documented with the appropriate syntax, it will be loaded in the modelling environment, also called the configuration builder. In the second step, which occurs in the modelling environment, the user represents the set up of the system graphically using annotated icons. Each icon is linked with an appropriate model implemented in the first step. The compiler of the modelling environment translates the MSL code into so called MSL-EXEC (c++code), which is then used by a standard C++ compiler to create executable code. In the WEST compiler, the MSL-EXEC is prepared for experimentation. In the third step, done in the experimentation environment, the compiled model is used to simulate the system, plot the output, make sensitivity analysis and do parameter estimation or optimisation.

2.2.1. The simplified RWQM1 river model in WEST

In the model base different river models are available. First of all, the complex RWQM1 that was developed for data rich conditions. However, in many cases not enough data is available or the problem of the river under consideration can be tackled with a simpler model. Therefore a simplified RWQM1 was implemented in the WEST model base by Deksissa (2004).

The complex hydrodynamic river model, which is based on the St. Venant equations (De St. Venant, 1871), was simplified to a typical Continuously Stirred Tank Reactor in Series (CSTRS) modelling approach in which the river is represented as a series of river compartments (tanks), each of which is assumed completely mixed (Beck and Reda, 1994; Whitehead et al., 1997). This relatively simple hydraulic model can then be extended quite easily to include the water quality submodel.

The complex RWQM1 contains pH and zooplankton (primary consumer) calculation, which requires large sets of specific monitoring data and high computational power. Selecting and modifying the most important sub-model components derive a simplified version of RWQM1. The procedure for sub-model selection is presented in Vanrolleghem (2001). The state variables and process descriptions in the simplified version of the model are given in tables III.3 and III.4 respectively.

Table III.3: State variables in the simplified river quality model and relation to RWQM1 formulation (Reichert et al., 2001a)

	State variables	Description
1	S_I	Inert soluble COD
2	S_S	Readily degradable COD
3	S_O	Dissolved oxygen
4	S_NH(S_{NH4}+S_{NH3})	Ammonia nitrogen
5	S_NO(S_{NO2}+S_{NO3})	Nitrite+nitrate nitrogen
6	S_PO(S_{HPO4}+S_{H2PO4})	Phosphate phosphorus
7	X_H	Heterotrophic biomass
8	X_N(X_{N1}+X_{N2})	Nitrifying biomass
9	X_P	P adsorbed to particles
10	X_I	Particulate inert COD
11	X_S	Particulate organic matter

Table III.4: Processes used in the simplified river water quality model and relation to RWQM1 formulation (Reichert et al., 2001a)

	Processes
1	Aerobic growth of Heterotrophs with ammonia
2	Aerobic growth of Heterotrophs with nitrate
3	Aerobic respiration of Heterotrophs
4	Anoxic growth of Heterotrophs with nitrate
5	Anoxic respiration of heterotrophs
6	Growth of nitrifiers
7	Aerobic respiration of Nitrifiers
8	Hydrolysis of particulate organic materials
9	Adsorption of Phosphate
10	Desorption of Phosphate

For other applications the model base was further extended with other river water quality models, all derived from the complex RWQM1 and then adapted and simplified according to the problem at hand. As such there was another simplified model made which contains the processes as implemented by Deksissa (2004) with an addition of a temperature model and the processes for algae growth and death. It is the latter that is used in section 9 of chapter V.

CHAPTER IV
DESCRIPTION OF THE CASE STUDIES

Parts of this chapter were published as:

- Vandenberghe, V., van Griensven, A. and Bauwens, W. (2001). Sensitivity analysis and calibration of the parameters of ESWAT: Application to the river Dender. Water Science and Technology, 43(7), 295-301
- Vandenberghe, V. , van Griensven A. and Bauwens W. (2002). Detection of the most optimal measuring points for water quality variables: application to the river water quality model of the river Dender in ESWAT, Water Science and Technology, 46(3), 1-7
- Vandenberghe, V., Bauwens, W. and Vanrolleghem, P.A. (2004). The Evaluation of Uncertainty Propagation into River Water Quality Predictions to Guide Future Monitoring Campaigns. Environmental Monitoring and Software, 22, 275-232.
- Vandenberghe V., van Griensven A., Bauwens W. and Vanrolleghem P.A. (2006). Effect of different river water quality model concepts used for river basin management decisions Water Science & Technology, 53(10), 277-284.

CHAPTER IV: DESCRIPTION OF THE CASE STUDIES

1. Introduction

In this chapter extended descriptions are given of two case studies used to illustrate and perform the different aspects of sensitivity and uncertainty analysis and optimal experimental design. The first one is the Dender, which was chosen for the considerable amount of data that was already available for this river thanks to previous studies (Manache, 2001; VMM, 1992) and because a model was already made in ESWAT for the year 1994 in the context of a PhD research by van Griensven (van Griensven, 2002). The second case study, the Grote Nete, was chosen for the different characteristics that made this river suitable for a study about shading and its effect on river water quality (Ghermandi, 2004).

2. The Dender catchment

The Dender is an example of a river system that is highly characterised by human activities with impacts on both the river morphology and the water quality. High pollution loads and long residence times in summer are translated in very bad water quality indices. The pollution originates from manure applications in agriculture (up to 80 % of the area), industrial activities and households (the inhabitant density is more than 500 inhabitants per km². In 1994; less than 10% of the wastewater was treated) (Demuynck et al., 1997).

2.1. Description of the basin

2.1.1. Geography

The Dender river, a tributary of the Schelde river in Belgium (figure IV.1), drains a total area of about 1384 km^2, 707 km^2 of which is situated in the Flemish Region. The Dender rises in the Wallonian Region of Belgium by the confluence at Ath of the Eastern and Western Dender and the channel Ath-Blaton. The Western Dender rises in the Barry Region at a height of between 60 and 70 m above sea level. The confluence at Ath is situated at a height of about 40 m above sea level. The mouth of the Dender River is situated in Dendermonde at a height of less than 10 m above sea level. The Dender model used in this dissertation only covers the Flemish part of the basin. The following descriptions are thus only regarding this part. The main tributaries of the Dender River in the Flemish region are shown in table IV.1 and figure IV.2.

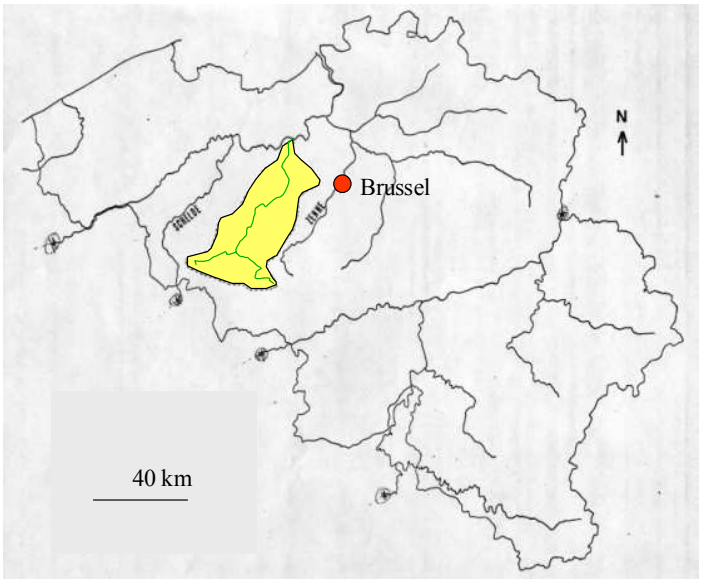


Figure IV.1: The Dender river in Belgium

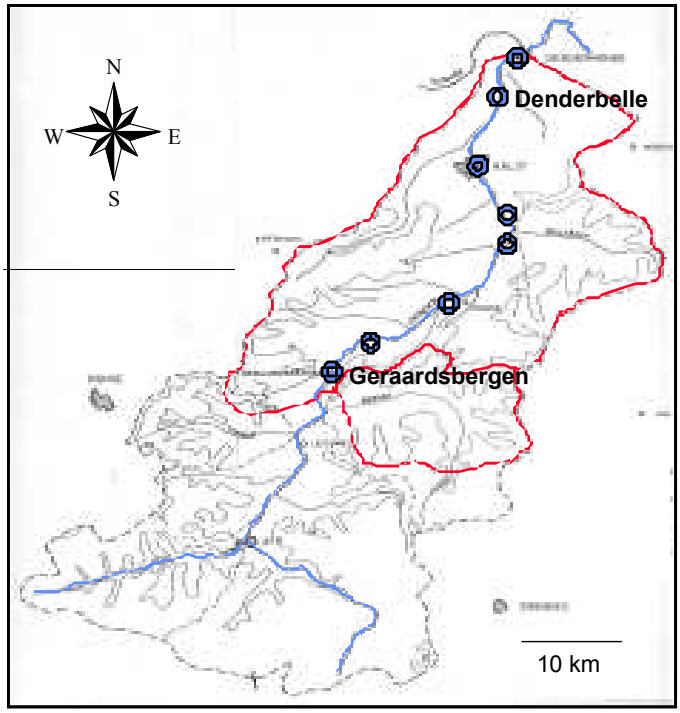


Figure IV.2: Delineation of the Flemish part of the Dender basin and the location of the weirs

Table IV.1: The main tributaries of the Dender in Flanders (VMM, 1992)

Tributary	Length (km)	Area (km^2)	Mouth at:
Molenbeek	21.5	55	Geraardsbergen
Wolfputbeek	15	49	Ninove
Bellebeek	22.5	103	Teralfene
Molenbeek	12	28	Aalst
Molenbeek	24	83	Mespelare
Mark	25	170	Deux-Acren

2.1.2. The topography

A digital elevation model (DEM) of the Dender basin is shown on figure IV.3. The map was constructed by the National Geographic Institute of Belgium by scanning, vectorising and identifying the altitude lines of a 1/50:000 map. Heights are given in meters, referring to the Belgian zero-level, spread according to a raster (50 m). The accuracy of the elevation is around 8 m with a confidence level of 90%. While the basin is very flat in the northern part, steep slopes – of up to 20% - can be observed in the southern part.

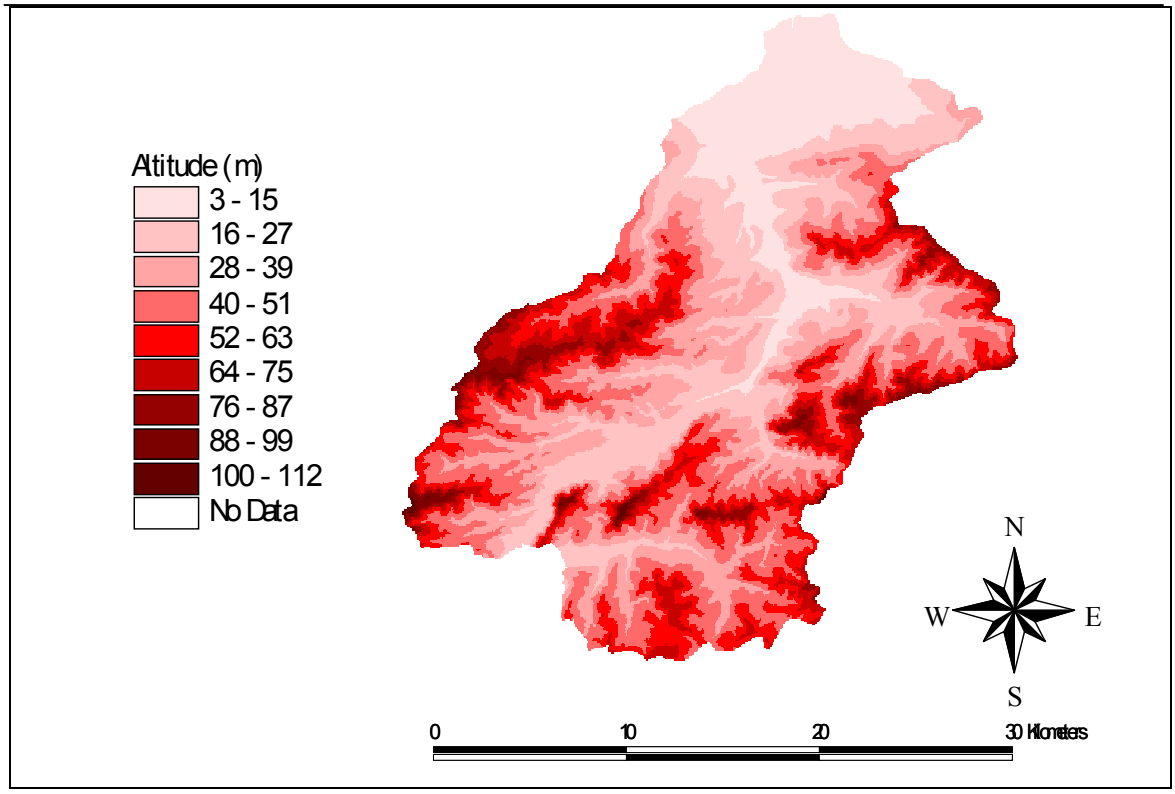


Figure IV.3: DEM of the Dender catchment

Table IV.2: Conversion table for soils

Texture class	Percentage (%)	Class	SWAT name
X, O, Z	1.03	Sand	Sand
S	2.24	Loamy-sand	Loamsand
L	22.	Sandy-loam	Sandyloam
P	1.5	Silty Loam	Siltyloam
A	60	Loam	Loam
E	2	Clay Loam	Clayloam
U	0.27	Clay	Clay
OB	10	Buildings	Impervious
7V	0.011	Unknown	Impervious
B	0.04	Unknown	Impervious
Other O	0.001	Unknown	Impervious

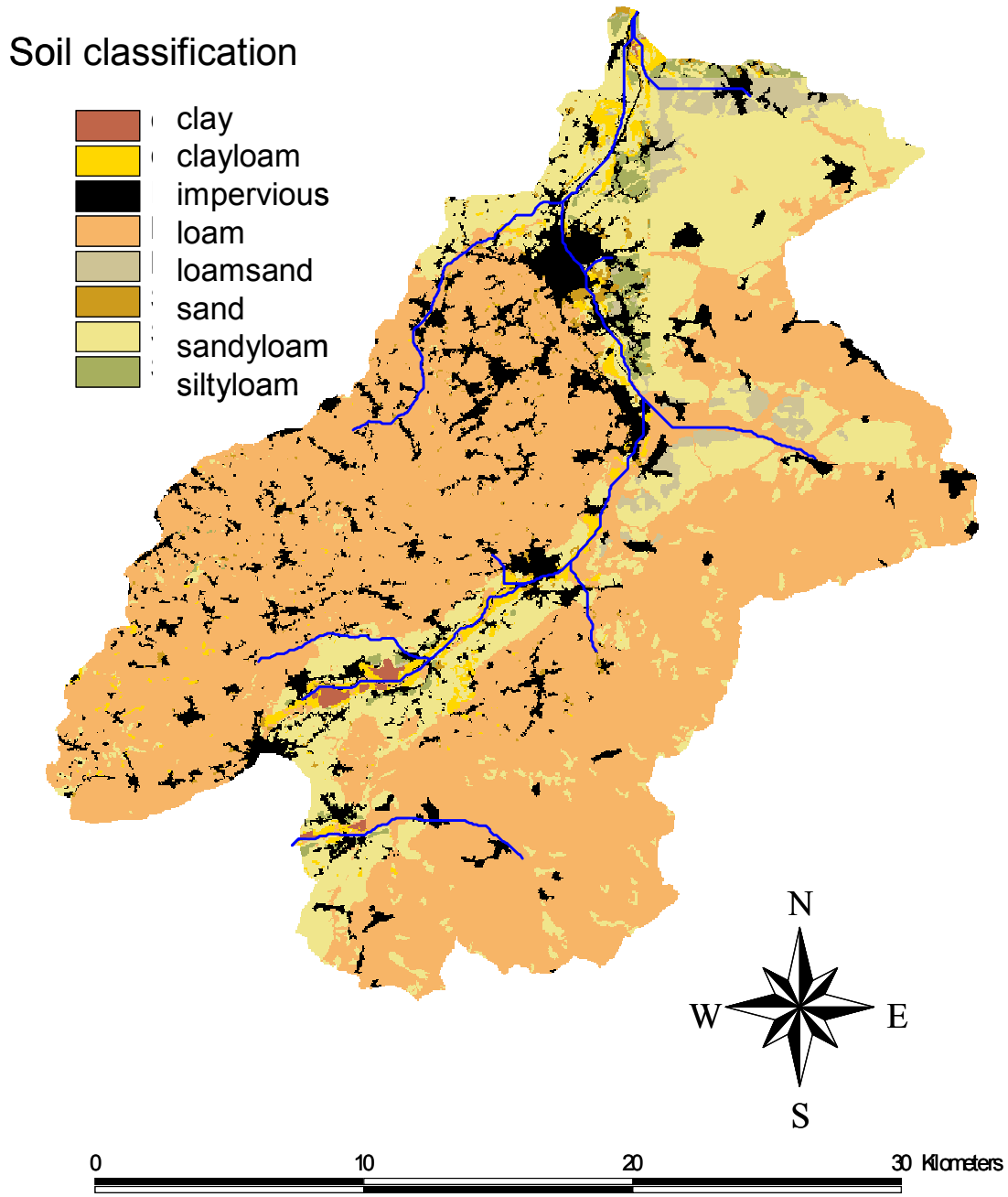


Figure IV.4: Soil map for the Dender basin

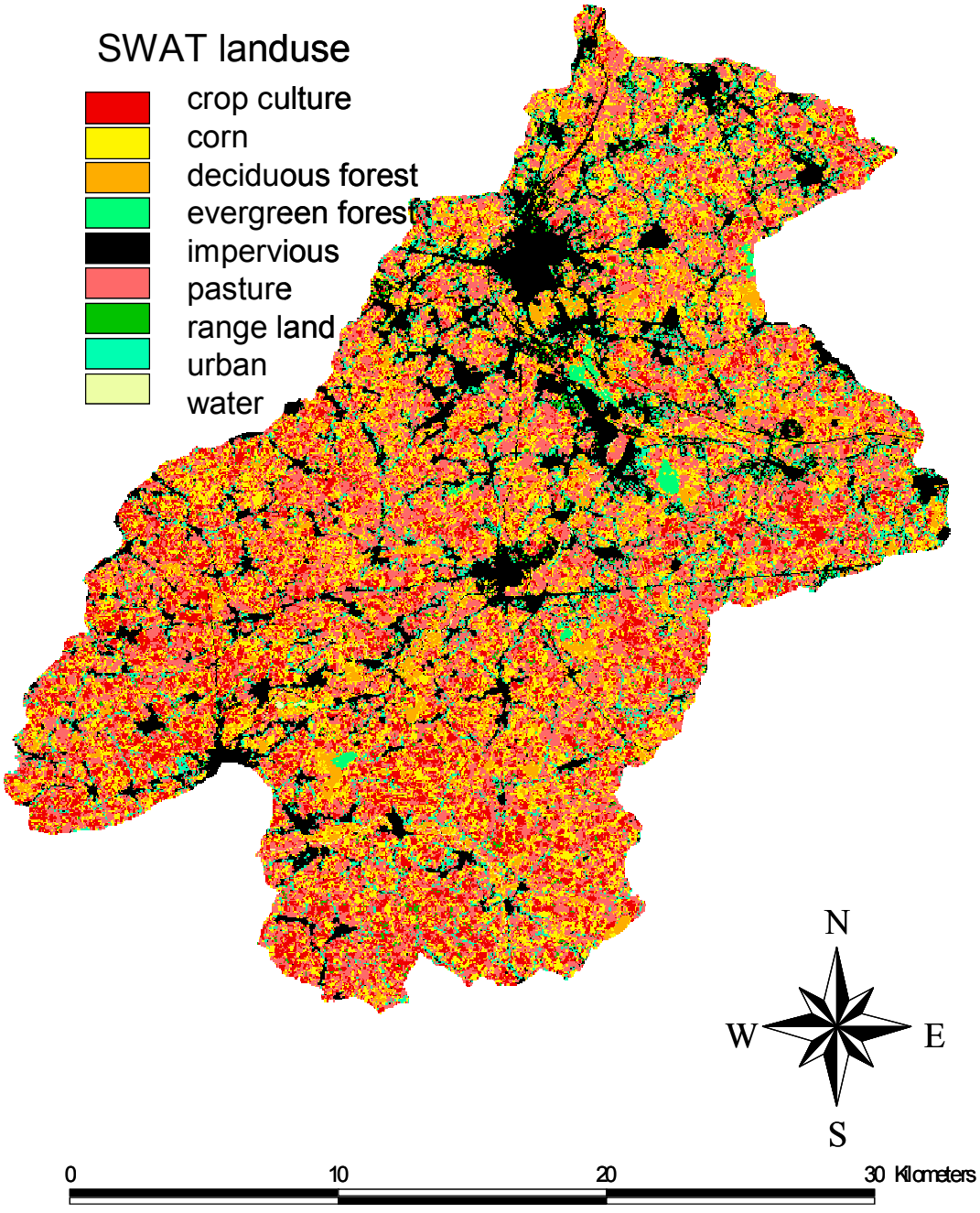


Figure IV.5: Land use map for the Dender basin

2.1.3. Soil characteristics

The soil map, based on data from the Soil Map of Belgium and the Fysische Systeemkaart Vlaanderen, originates form the Geographical Institute of Belgium (figure IV.4.). The dominant soil type is loam (table IV.2). Sandyloam and loam cover 83 % of the area. The soil type Sandyloam occurs mainly in the north of the basin and near the rivers. It is assumed that the texture class OB can be classified as IMP (impervious) that means that there will be no infiltration in those areas.

2.1.4. The land use

The land use map (figure IV.5) is originating from the Bodembedekkingskaart of GIS Vlaanderen. This map was created using a LANDSAT image of August 1995. The original map has a grid cell size of 20 x 20 meter. Table IV.3 provides an overview of the land use distribution within the basin.

Table IV.3: Land uses in the Dender basin

SWAT class	*% in Dender Basin*	*Description*
AGRL	17.91	Crop culture (not corn)
CORN	21.88	Corn culture
FRSD	8.50	Deciduous forest
FRSE	0.64	Evergreen forest
IMP	9.92	Impervious area
PAST	29.96	Pasture
RNGB	2.39	Range land
URBN	8.46	Urbanised area
WATR	0.33	Water

The land use map was derived by classification from 3 LANDSAT TM images by combining the reference classification (numeric product) and the CORINE Land Cover data (manual interpretation) for Flanders. The final dataset comprises the following classes: continuous urban fabric, discontinuous urban fabric, urban fringe/green urban area, industry/commercial, infrastructure, harbour, airport, mineral extraction sites, highway, regional way, arable land, grassland, maize/tuberous plants, alluvial grassland, orchard, deciduous forest, coniferous forest, mixed forest, parks/gardens, heathland/bare soil, beach/dunes, mud flat, navigable waterway, unnavigable waterway, estuaria, sea.

In the Dender basin, it is observed that the main urban centres are located in the valley of the main river. About 30% of the landuse is pasture, while crop farming represents ca. 50% of the landuse.

2.2. The river

The river was canalised to guarantee ship-traffic. Ship locks and weirs, which maintain a constant water level during low flows, are situated at: Dendermonde, Denderbelle, Aalst, Teralfene, Denderleeuw, Pollare, Idegem, Geraardsbergen (figure IV.2). The longitudinal profile in figure IV.6 shows the water level and the bottom level at different places along the main stream.

The canal has a typical width of 20 to 30 m and a depth of 3 m between Geraardsbergen and Aalst; downstream of Aalst, the canal widens to 45 to 55 m and deepens to 3.7m.

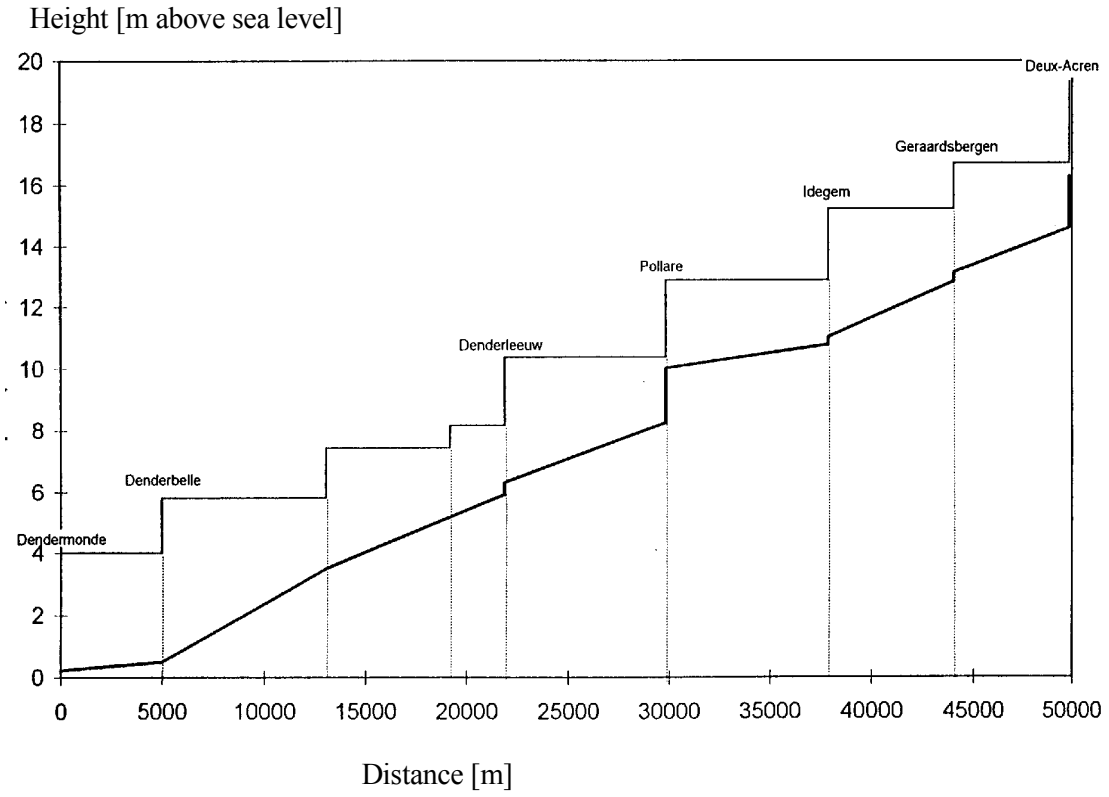


Figure IV.6: Longitudinal profile of the Dender between Deux-Acren and Geraardsbergen

2.3. Hydro-meteorological and water quality data

2.3.1. Meteorological data

Daily records of the Royal Meteorologic Institute were used for the study. Table IV.4 shows the meteorological datasets. Although Ukkel is not situated in the Dender basin, the datasets of these stations are assumed to be representative for the climate in the Dender basin. The available rainfall data at Dendermonde, Pollare and Geraardsbergen, located inside the basin allow a

representation of the spatial variability of the rainfall. The minimum and maximum temperatures after 1978 are generated using the average daily temperatures and rainfall data (Olivié, 1999).

Table IV.4: Meteorological data for the Dender Basin

Variable	Station	Available years
Average daily temperature	Ukkel	1968-2000
Min. & max. daily temperature	Ukkel	1968-1978
Sub-hourly precipitation	Ukkel	1970-1994
Daily precipitation	Pollare	1970-2000
Daily precipitation	Dendermonde	1970-2000
Daily precipitation	Geraardsbergen	1970-2000
Daily solar radiation	Ukkel	1970-1998

2.3.2. Hydrological data

Measured discharges of the Dender and some of the tributaries (table IV.5) were obtained from the Hydrologic Information Center of the Ministry of the Flemish Region. The flow at Denderbelle is measured at a weir, near a lock, based on a stage-discharge relation. The relation is believed not to be very reliable, especially at low flows (due to leakage losses at the lock). Therefore, a lower limit of 1 m^3/s was applied (VMM, 1992). This explains why in some periods, mainly in summer, a constant daily flow of 1 m^3/s is measured for a period of time. The flow at the mouth of the river has an average value of 10 m^3/s and covers a range of more than 100 m^3/s to less than 1 m^3/s.

Table IV.5: Available hydrological data

River/Tributary	Station	Draining area [km^2]	Available years	Years
Dender	Denderbelle	1244	1970-1994	25
Bellebeek	Essene	92	1972-1981	6
Molenbeek	Hofstade	57	1969-1977	7
Molenbeek	Aalst	28	1969-1977	6
Molenbeek	Geraardsbergen	19	1972-1991	15
Mark	Viane	171	1977-1991	7

2.3.3. In-stream water quality data

The river water quality is monitored by the Flemish Region, by analysing a number of samples (+/- 12/year) during the year (VMM, 2000). This study uses 4-hourly water quality data from continuous measurement campaigns conducted during the second part of 1994 (Anonymous, 1995). The data consist of measurements of BOD, DO, NH_3, NO_3 and PO_4 at three locations along the Flemish part of the river (figure IV.7).

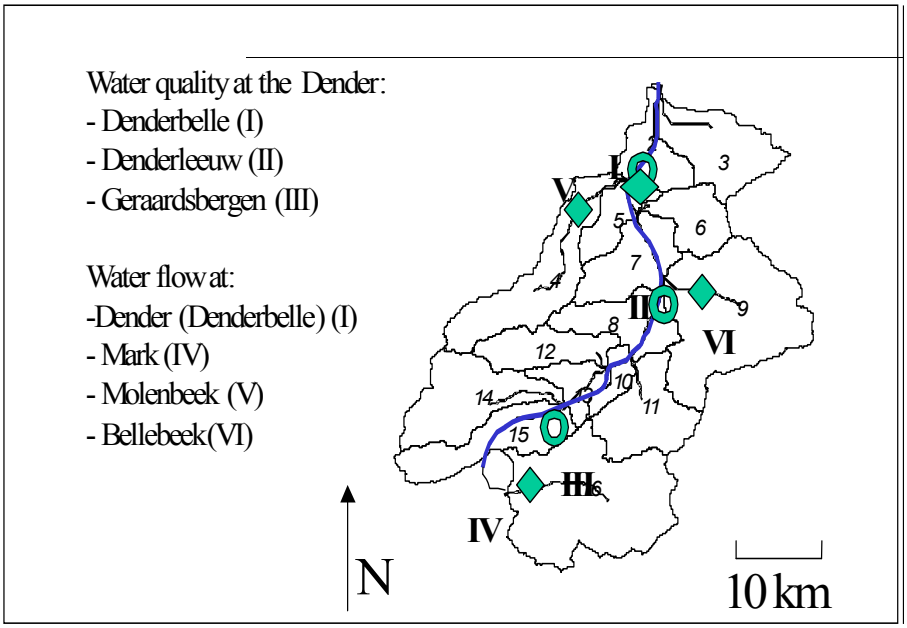


Figure IV.7: Scheme of the modelled basin with the locations of the measuring points

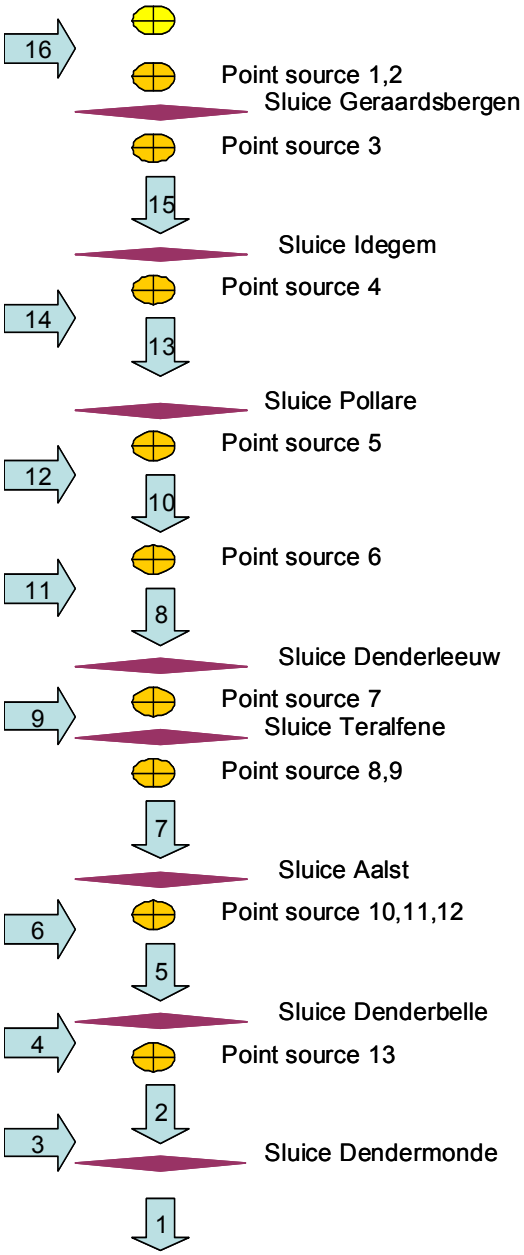


Figure IV.8: The scheme of the Dender river

2.3.4. Point source emissions

The situation in 1994

In table IV.6 overall emissions of point sources are shown for the different pollution sources (see also figure IV.8). The domestic pollution is assessed by using Inhabitant Equivalents and by applying removal efficiencies when the wastewater is treated. Measuring campaigns assesses the industrial pollution. The border-crossing pollution is the pollution coming from neighbouring catchments. This pollution includes the pollution coming from the Walloon part of the Dender catchment but also the Mark River is included (Demuynck et al., 1997).

Table IV.7 gives an overview of the domestic pollution from different sources in the Dender basin as for 1994. Sixteen % of the population is not connected to any sewer system or WWTP and directly pollutes the Dender. However, the biggest part of the domestic pollution comes from the sewer systems connected to the Dender. In 1994 less than 10 % of the domestic pollution was treated before it reached the Dender.

Table IV.6: Emission of point sources – situation 1994 (VMM, 1994; VMM, 2000)

Parameter	Domestic	Industry	Border crossing	Agriculture	**Total**
BOD (kg/day)	17 000	1 700	2 300	NA	21 000
COD (kg/day)	34 354	5 153	25 978	NA	65 485
Total N (kg/day)	2 690	420	4 450	2050	10 650
Total P (kg/day)	525	140	500	110	1 275

Table IV.7: Overview of sources of domestic pollution in the Dender basin (VMM, 1994)

Source	Inhabitants	BOD (kg/d)	COD (kg/d)	Tot. N (kg/d)	Tot. P (kg/d)
Via sewer system	239000	12900	21000	2390	477
Via WWTP	39400	166	881	210	29
Diffuse	54000	3700	2400	272	54
Total	332000	16700	25000	2870	560

The AWP scenario

In 1994, the Flemish environmental agency proposed the AWPII plan (VMM, 1994). Hereby more than 90 % of the domestic and industial pollution should be treated by 2010 (figure IV.9).

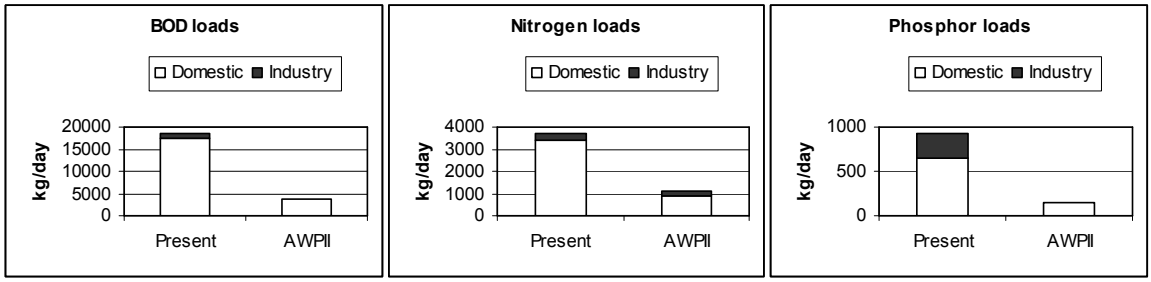


Figure IV.9: Domestic and industrial loads in 1994 and after AWP II

Table IV.8: Yearly nitrogen and phosphorus application rates for each municipality

Name	area [ha]	Nitrogen [kg]	Phosphates [kg]	Nitrogen [kg N /ha]	Phosphates [kg P_2O_5 /ha]
Aalst	7856	613927	242037	78	31
Affligem	1799	112033	43676	62	24
Asse	5023	561484	232488	112	46
Bever	1923	352947	138869	184	72
Brakel	5705	1028669	379500	180	67
Buggenhout	2563	356163	138813	139	54
Denderleeuw	1389	111364	44878	80	32
Dendermonde	5645	697199	290034	124	51
Dilbeek	4148	244395	104099	59	25
Erpe Mere	3434	419734	170078	122	50
Galmaarden	3525	510698	194836	145	55
Geraardsbergen	8008	965973	388680	121	49
Gooik	4028	767006	285851	190	71
Haaltert	3055	356276	140182	117	46
Herne	4471	862507	350028	193	78
Herzele	4786	932657	383194	195	80
Lebbeke	2738	350048	140638	128	51
Lede	2992	280036	113002	94	38
Lennik	3116	429599	169642	138	54
Liedekerke	1009	39553	20380	39	20
Lierde	2639	532687	210072	202	80
Merchtem	3691	619614	260385	168	71
Ninove	7306	1022820	398640	140	55
Opwijk	1995	290559	117458	146	59
Pepingen	3597	783463	315511	218	88
Roosdaal	2191	232243	95160	106	43
Ternat	2470	229971	90325	93	37
Zottegem	5745	862906	328804	150	57

2.3.5. *Diffuse pollution sources*

Data on fertiliser and manure use were provided by the VLM (Vlaamse Landmaatschappij), as data on the nutrient use and production for each commune in Flanders. Manure transports in and out of the villages are hereby not considered. The data are divided into three groups: animal production, chemical fertilisers and other fertilisers.

The data collected for the municipalities within the Dender basin for the years 1992 and 1993 are summarised in table IV.8.

3. The Nete catchment

The Nete is another tributary of the Scheldt River. The basin is part of the Flanders Region in Belgium. Approximately 600.000 inhabitants live in the basin and 4.121 companies are situated inside the region. There is a big variation of the concentrations of the different pollutants but most often the quality standards are not met and still a lot of measures are needed to improve the water quality.

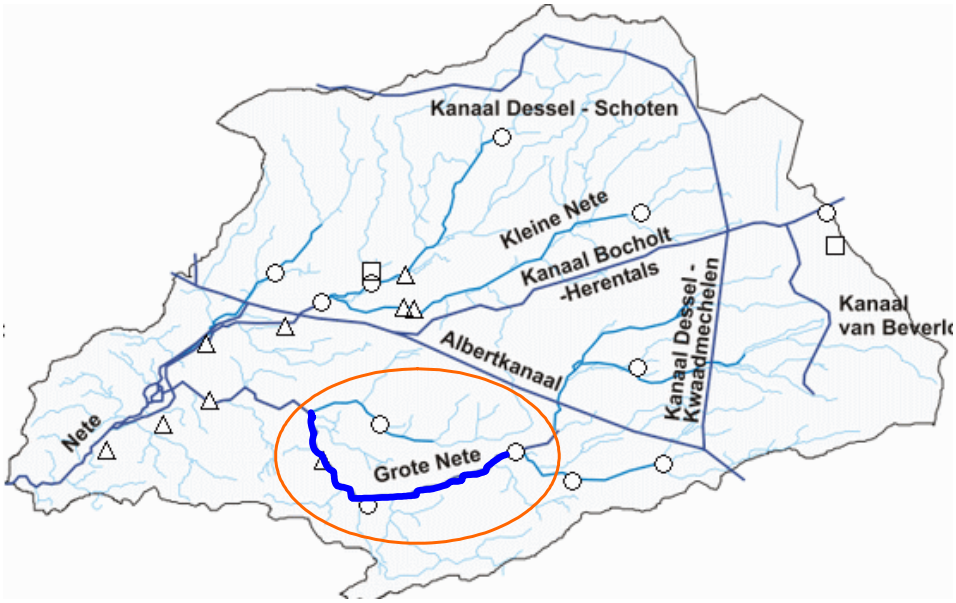


Figure IV.10. The Nete catchment basin and the selected reach

The studied reach in this dissertation is the one of the Grote Nete, 19.5 km between the most upstream and the most downstream water quality measuring station. Figure IV.10 shows the whole Nete catchment basin and, highlighted, the river stretch selected for the case study.

Most of the information about the Nete catchment has been taken from the general water quality plan (AWPII) of the Nete basin published by the Flemish Environmental Agency (VMM, 2000).

3.1. Description of the basin

3.1.1. *Geography*

The Nete river basin district is located entirely within the Flanders region in Belgium (see figure IV.11) and covers a surface of 1673 km² and a total length of watercourses of 2224km.

Figure IV.11: Geographical position of the Nete basin in Flanders

The basin is administratively subdivided into three provinces (Antwerp, Limburg and Flemish Brabant) and 54 municipalities, 27 entirely and 27 partially located in the basin (see figure IV.12). Almost the whole catchment is situated within the borders of the province of Antwerp, but the source of the Grote Nete and the most Southern parts of the watercourse network are located respectively in the provinces Limburg and Flemish Brabant.

The main rivers within the river basin district are the Grote Nete and the Kleine Nete. The total length of Grote and Kleine Nete amount to 151 km, while the total length of all watercourses in the water basin district amounts to 2224 km. In Lier the Kleine and the Grote Nete together form the Beneden-Nete, which drains into the Scheldt via the Rupel.

The boundaries of the river basin district are the river basin of the Maas in the North, the Dutch border and the river basin of the Maas in the East, the basins of the Demer and the Dijle-Zenne in the South, and the basin of the Beneden-Schelde in the West.

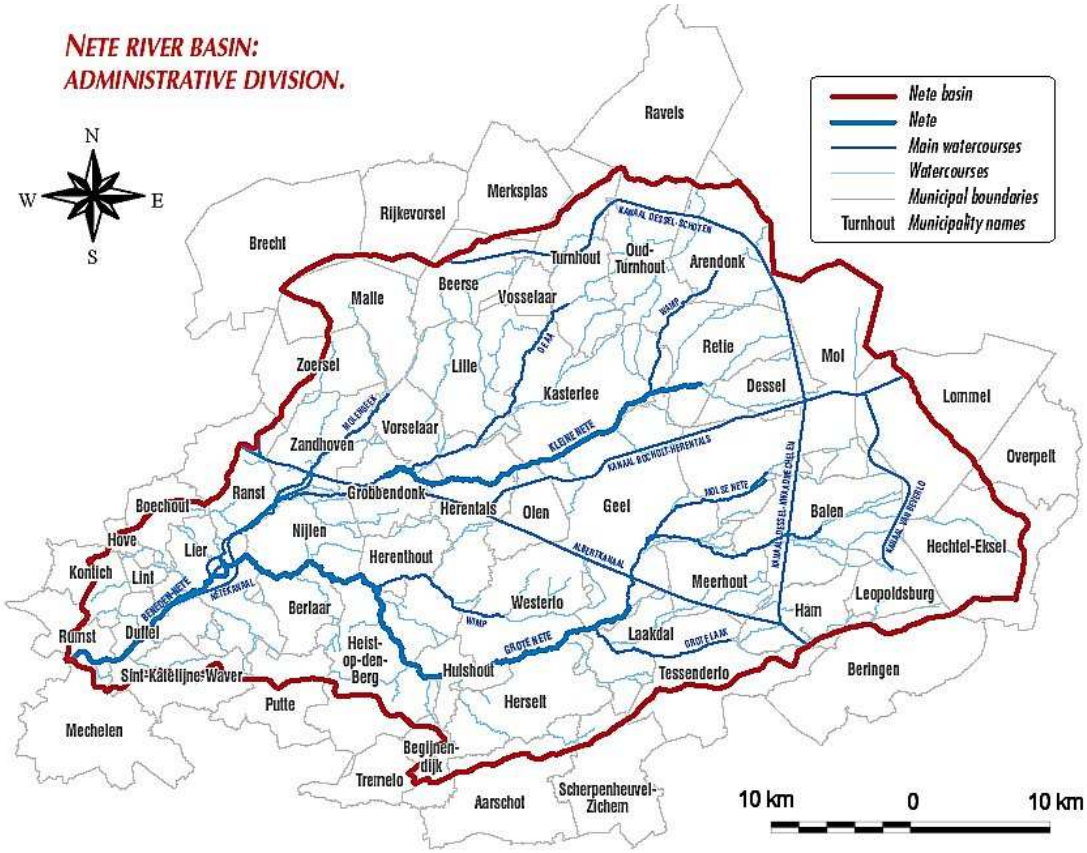


Figure IV.12: Administrative organisation of the Nete river basin (VMM, 1992)

3.2. Pressures in the basin

The principal users of water can be divided into three groups: agriculture, industry and households. Through their use of water, these three groups produce wastewater or other waste products that, released into the environment, pollute surface and groundwater and have in general a negative impact on the quality of water dependent ecosystems.

3.2.1. The households

The number of inhabitants of a river basin district and the percentage of households connected to the sewage infrastructure are two of the aspects that mainly determine the contribution of households to surface water pollution.

The AWPII reports a population of 600.000 people in the Nete catchment basin at the end of year 1997. The principal residential areas are Turnhout, Lier, Geel, Herentals, Beerse and Vosselaar. Figure IV.13 illustrates the main residential areas in the Nete catchment basin.

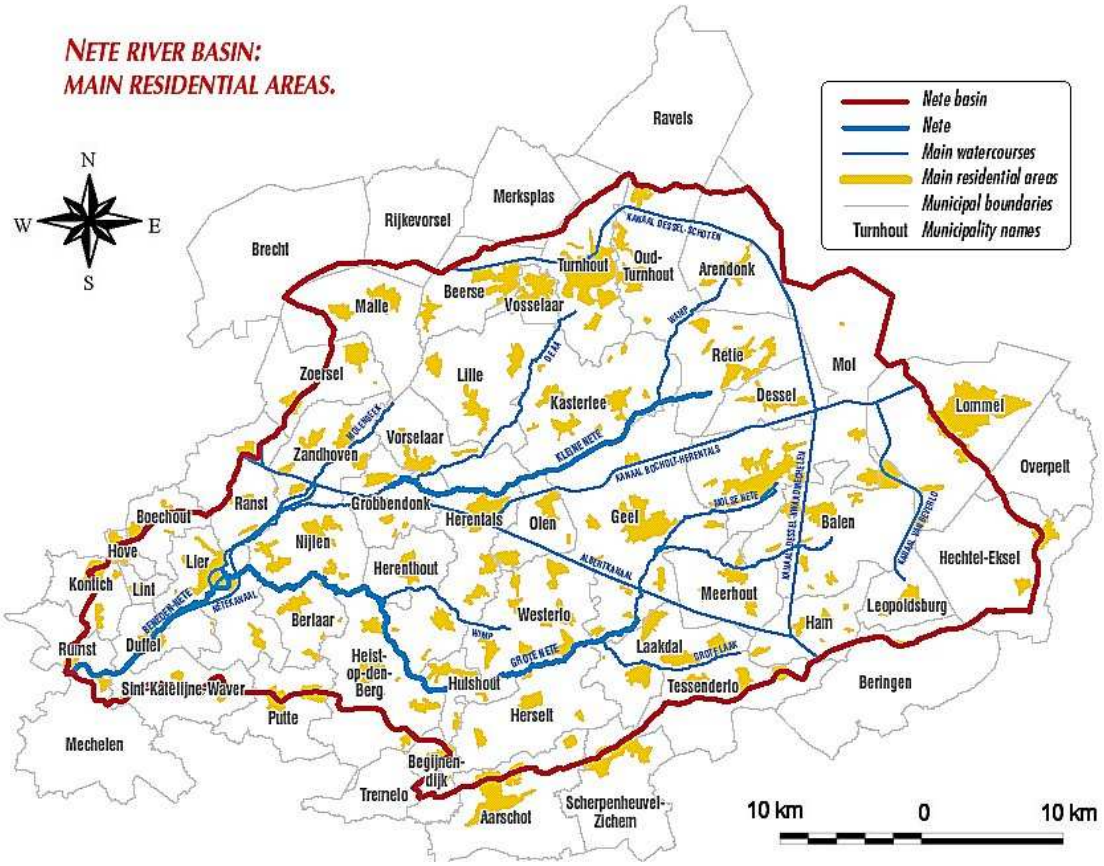


Figure IV.13: Main residential areas in the Nete catchment basin (VMM, 1992)

At the end of 1997, only 58% of the population was connected to sewerage with treatment. Since then, the situation has significantly improved thanks to the investment programmes of the Flemish Region that resulted in an expansion of the regional collector system on the one hand and of the municipal sewage systems on the other. In spite of these improvements, however, households are still expected to be one of the most significant sources of oxygen binding substances (BOD, COD), suspended solids, nutrients and zinc.

3.2.2. Industry

The biggest industrial areas in the catchment basin of the Nete are concentrated around the Albert Channel (in the municipalities of Herentals, Olen and Geel) and in the municipality of Lommel. Important industrial sites also exist in the municipality Tessenderlo. The heavy salt pollution released by these installations is responsible for the serious degradation of the ecological status of the Grote Laak, a tributary of the Grote Nete. Figure IV.14 illustrates the main industrial areas in the Nete basin.

Like the households, industries can be connected to public sewerage and hence their wastewater can be treated in WWTP together with wastewater coming from households. In the last years, however, the trend has been to disconnect the largest companies from public WWTP and to provide them with an own treatment installation and a direct discharge into surface water.

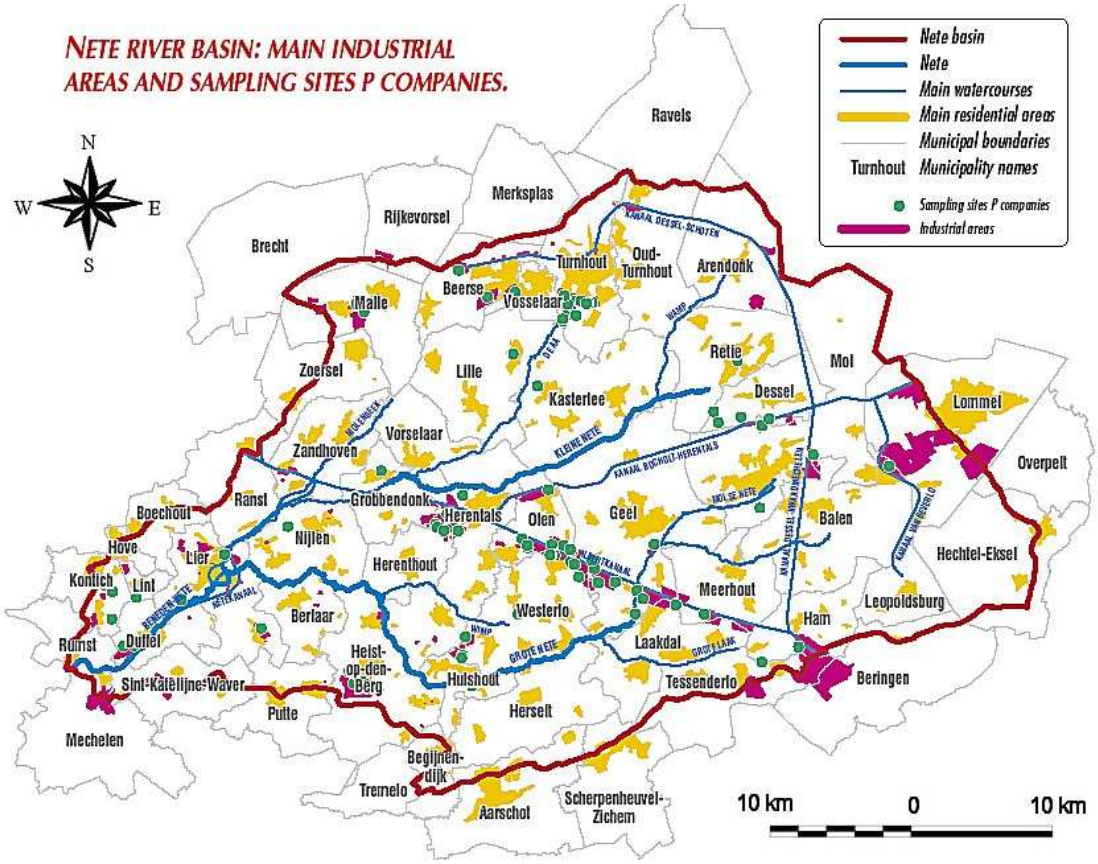


Figure IV.14. Main industrial areas in the Nete catchment basin (VMM, 1992)

3.2.3. Agriculture

The principal contribution of agriculture to the pollution of surface water bodies consists in the release of nutrients like nitrogen and phosphorus via diffuse pollution from arable land. In comparison to it, the direct point pollution of a farm is relatively slight.

The quantification of diffuse pollution is a complex task. To examine the impact of diffuse nutrient pollution from agricultural land-use, a series of processes must be taken into account that determine the fate of the nutrients after being released on the field as fertilisers or manure. Among the different fate determining processes absorption by plants, dispersion and formation of gas, which escapes into the atmosphere, leaching into the ground- and surface water and binding of nutrients to the soil and water bottom, are probably the most important ones. The quantification of these processes requires the use of mathematical models.

Several different model approaches are reported in the literature. The most simplified approaches suggest the use of export coefficients that take into account only the land-use type. Other authors suggest slightly more complex approaches that also take into account some of the release processes mentioned previously, generally in a statistical and not physical based way. The second General Water Quality Plan (GWQP2) suggests the use of the SENTWA model (VMM, 2002), which estimates the partial losses through atmospheric deposition, losses into groundwater, direct impact of mineral and organic fertilisers, effect of natural drainage, of erosion and or run-off, and excessive organic pressure (VMM, 1992).

It must be stressed that a correct estimation of the nutrient load from agriculture is of particular importance in the Nete basin since agriculture represents the principal land-use in the area. Besides, phosphorus and nitrogen concentrations are, together with light and temperature, the main factors affecting for eutrophication in water bodies.

3.3. Water quality

3.3.1. Biological water quality

The AWPII reports a description of the biological water quality in the Nete basin based on the Belgian Biotic Index (BBI) (VMM, 1992). This index is based on the presence of freshwater macro-invertebrates in the water, including worms, leeches, snails, crustaceans, shellfish and insects. As the pollution of a watercourse increases (in terms of reduction of dissolved oxygen or increase in toxic substances), the number and species of macro-invertebrates decrease significantly. The BBI can therefore be considered as a standard for the general status of a watercourse over a period of time of weeks/months.

Figure IV.15 illustrates the biological water quality of the watercourses in the Nete catchment basin district according to the BBI classification.

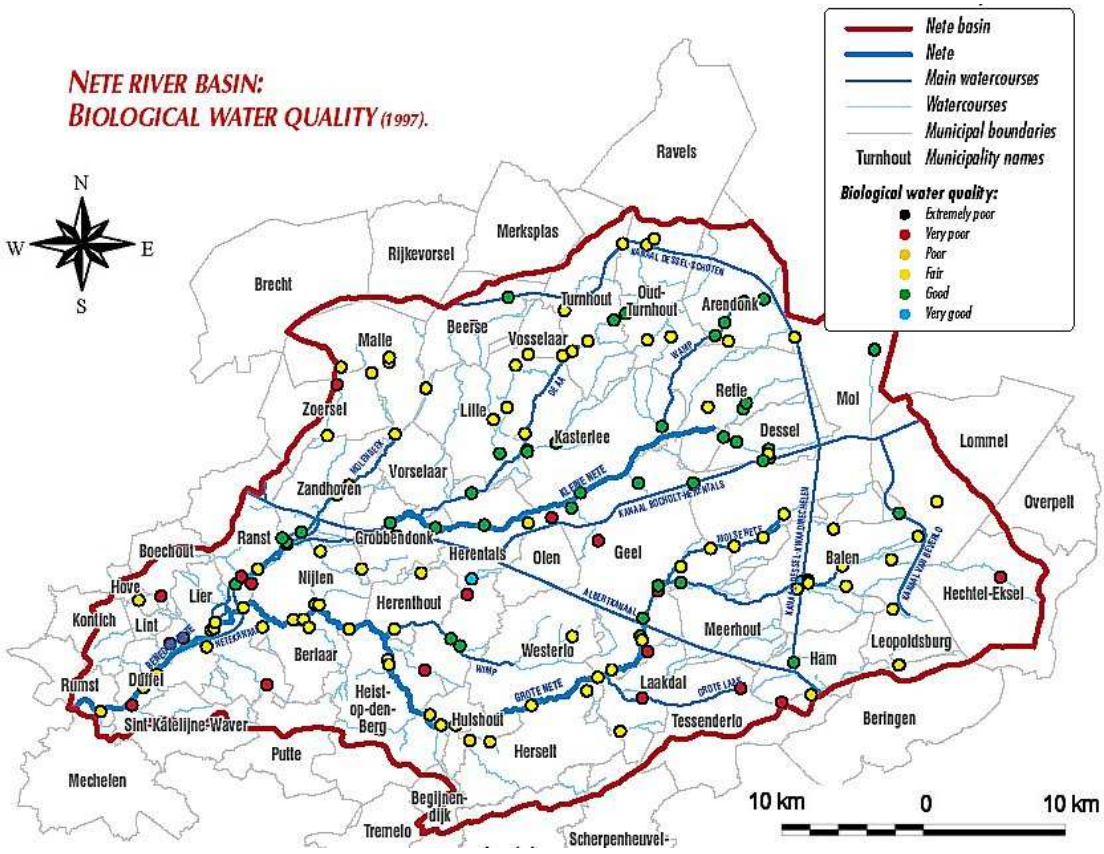


Figure IV.15: Biological water quality in the Nete catchment based on BBI (VMM, 1992)

Figure IV.15 shows that the biological water quality in the Nete catchment basin is generally quite low. The studied reach has an overall ppor water quality. Table IV.9 shows the BBI classification of the biological water quality in the Nete as reported in the AWPII (VMM, 1992).

Table IV.9: Classification of biological measuring sites in the Nete catchment based on the BBI (VMM, 1992)

BBI class	Percentage of measuring sites (%)
Extremely poor	0
Very poor	12
Poor	16
Fair	40
Good	29
Very good	3

3.3.2. Physico-chemical water quality

The description of the physico-chemical water quality in the AWPII is made by means of the oxygen-Prati Index (PI_O), which is based on measurements of dissolved oxygen. The lower the Prati-Index, the better is the water quality. Figure IV.16 shows the results of 12 monthly measurements of PI_O during 1997.

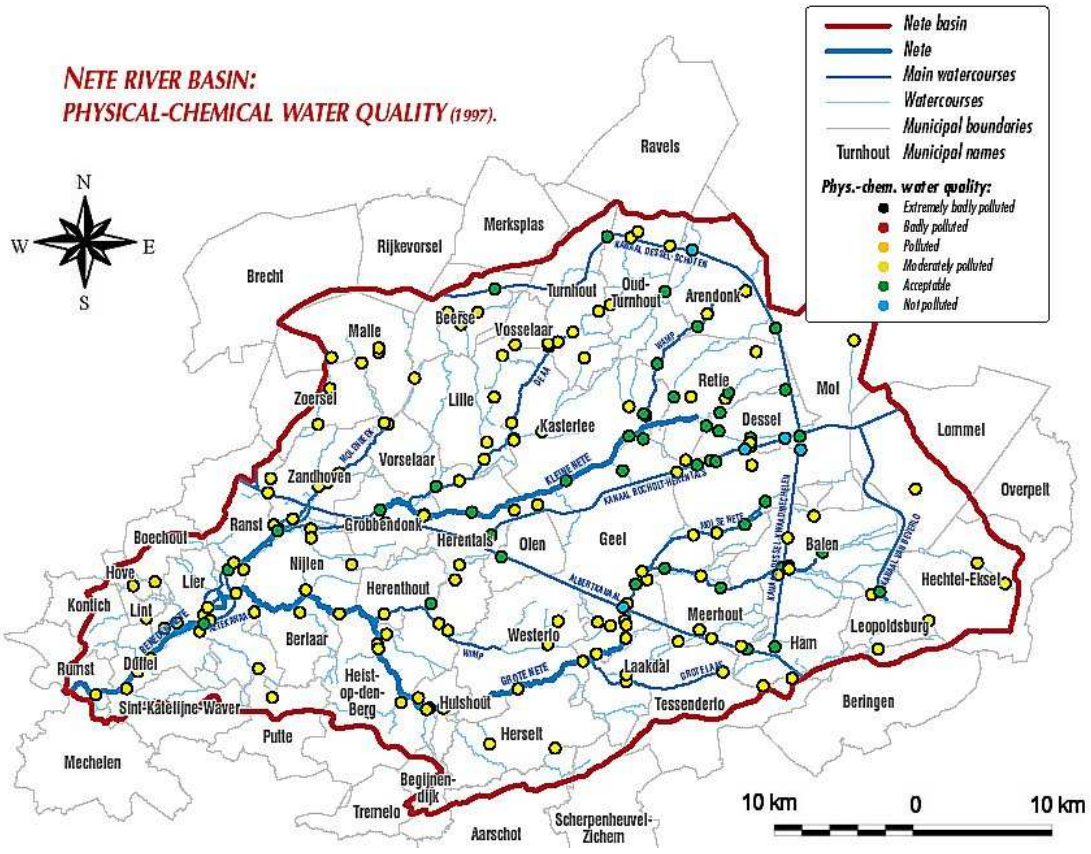


Figure IV.16: Physico-chemical water quality in the Nete catchment based on the PI (VMM, 1992)

The physico-chemical water quality in the Nete catchment is generally higher than in the rest of Flanders. Nevertheless the average value of the Prati Index is 2.8, below the accepted standard value. The studied stretch of the Grote Nete has a moderately polluted status. Table IV.10 shows the classification of the physico-chemical water quality in the Nete based on the PI_O as reported in the AWPII.

Table IV.10: Physico-chemical water quality in the Nete basin based on the PI_O

PI_o class	Percentage of measuring sites (%)
Extremely polluted	0
polluted	16
Moderately polluted	56
acceptable	25
Non polluted	3

An exhaustive description of the chemical status of the watercourses in the Nete basin must also take into account the presence of other specific chemical pollutants like heavy metals and pesticides.

These specific pollutants can be highly toxic for aquatic organisms. Furthermore, given their characteristics of bioaccumulation and, in some cases, bio-magnification along the food chain, they can provide a serious ecological as well as sanitary problem. Pesticides can be virtually non-biodegradable and can therefore accumulate in the environment.

The sources of heavy metal pollution in surface water bodies are generally industry discharges and run-off from urban areas or roads. Pesticides can enter the watercourses via run-off from agricultural land or by direct entrance into the water body (spray drift during application of pesticides).

The presence of seven heavy metals is reported in the Nete catchment basin see table IV.11. Among these seven elements, cadmium appears to represent the most serious danger, while the concentration of the other six is below the water quality standard required by the VMM. The average concentration of arsenic, cadmium, nickel and zinc in the Nete catchment is, however, higher than in the Flemish region. Some areas, like the upper course of the Grote Nete, show high concentrations of both cadmium and zinc due to a historical contamination by these pollutants.

Table IV.11: Heavy metals and pesticides present in the catchment and their main sources

	Pollutant	**Source**
Heavy metals	arsenic, cadmium, chrome, copper, nickel, lead and zinc	industry, traffic, agriculture ad households
Pesticides	isodrine, alpha-endosulfan, atrazine, isoproturone and diazonine	agriculture

Pesticide investigation is extremely complex due to the huge number of different components actually available on the market and their rapid and far-reaching contamination of the environment. Five pesticides are reported in the Nete catchment (see table IV.11).

The river stretch selected as case study in this thesis is the reach of the Grote Nete located between the confluence with the Grote Laak (upstream) and with the Wimp (downstream).

CHAPTER V
CALCULATION AND REDUCTION OF OUTPUT UNCERTAINTY

Parts of this chapter were published as:

- Vandenberghe, V., van Griensven, A. and Bauwens, W. (2001). Sensitivity analysis and calibration of the parameters of ESWAT: Application to the river Dender. Water Science and Technology, 43(7), 295-301.
- Vandenberghe, V. , van Griensven A. and Bauwens W. (2002). Detection of the most optimal measuring points for water quality variables: application to the river water quality model of the river Dender in ESWAT, Water Science and Technology, 46(3), 1-7.
- Vandenberghe, V., Bauwens, W. and Vanrolleghem, P.A. (2004). The Evaluation of Uncertainty Propagation into River Water Quality Predictions to Guide Future Monitoring Campaigns. Environmental Monitoring and Software, 22, 275-232.
- Vandenberghe V., van Griensven A., Bauwens W. and Vanrolleghem P.A. (2006). Effect of different river water quality model concepts used for river basin management decisions Water Science & Technology, 53(10), 277-284.
- Vandenberghe V., van Griensven A., Bauwens W. and Vanrolleghem P.A. (2006). Effect of different river water quality model concepts used for river basin management decisions Water Science & Technology,53 (10), 277-284.
- Vandenberghe V. and Vanrolleghem P.A. (2005) Cost-effectiveness of in-stream aeration to improve river water quality. In: *Proceedings 10th International Conference on Urban Drainage*. Copenhagen, Denmark, August 21-26, 2005.

CHAPTER V: CALCULATION AND REDUCTION OF OUTPUT UNCERTAINTY

1. Introduction

In the literature chapter (section 3.3), the modelling process is presented in figure II.2. For every step of this modelling process, a lot of issues and questions can be put forward by modellers, water managers and stakeholders to attain the most reliable model results. In this chapter it is the aim to discuss and apply methodologies to answer these questions and problems. Figure II.2 is brought again in this chapter to visualise the modelling process together with the different sections of the research part of this dissertation work, as figure V.1 to make it easier to follow through the different sections of this chapter.

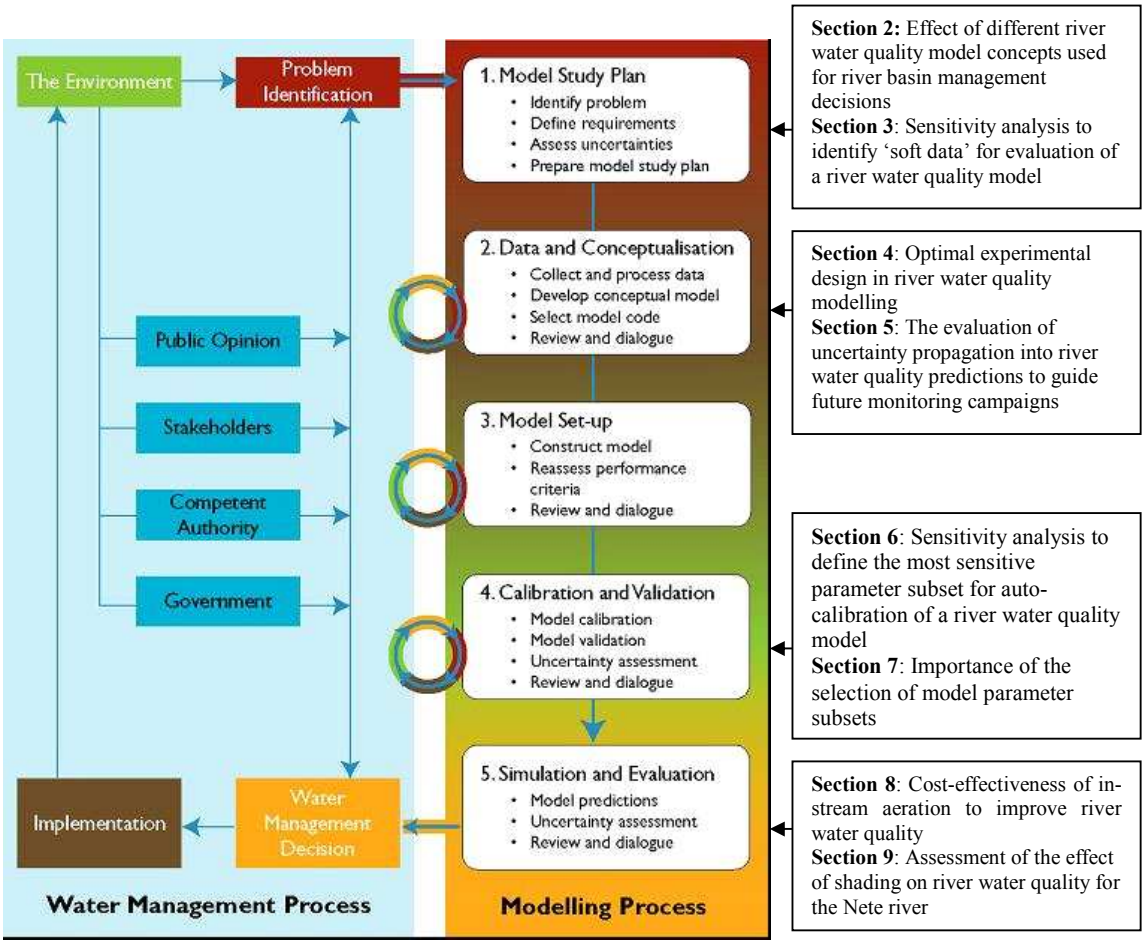


Figure V.1: The modelling process refsgaard et al. (2004) with related sections of this chapter

Step 1. The model study plan and the decision of the most adequate model for the problem under consideration.

The water manager needs to describe the problem for which he/she needs modelling and its context as well as the available data. A very important task is then to analyse and determine what are the various requirements of the modelling study in terms of the expected accuracy of modelling results. The acceptable level of accuracy will vary from case to case and must be seen in a socio-economic context. It should, therefore, be defined through a dialogue between the modeller, water manager and stakeholders/public. In this respect an analysis of the key sources of uncertainty is crucial in order to focus the study on the elements that produce most information of relevance to the problem at hand. This is achieved with a sensitivity analysis.

It is not only necessary to decide for a model that can model well the current state of the river, but there comes an additional question: What model concept should be used, in view of evaluating the probable changes in the system when the model is used for scenario analysis? To find answers about what are the most influencing parameters and processes, not only for evaluation of the current state of the water but also with regard to scenarios, in section 2 of this chapter, a sensitivity analysis is performed for two different water quality concepts with regard their use in management decisions.

Sometimes one needs to make a model of a basin with few or no data available. Often extra data will be necessary but due to time restrictions or budget limitations decisions have to made regarding priorities for data collection. In such situation it is also difficult to decide what processes are important and needs to be in the model. The only data that are easily obtained are data which can be gathered by direct observation like hilly region, algae bloom in summer, high summer temperatures. In this work a study for model application in ungauged basins is performed in which the most important parameters in different circumstances are identified with a kind of sensitivity analysis of a sensitivity analysis (section 3).

Step 2. Data gathering and measurement campaigns

In this step the modeller should gather all the relevant knowledge. Consideration must be given to the spatial and temporal detail required of a model, to the system dynamics, to the boundary conditions and to how the model parameters can be determined from the available data. It is obvious that it is important to know what input data is needed and what kind of measurement data (frequency, location, amount, …) for calibration is best suited. To minimise the uncertainty of the output results, in section 4, a method of iterative optimal experimental design is proposed to minimise uncertainty of parameter estimates during calibration. When extra measurement campaigns are possible it is best to do previous investigation about what measurements are best to get more reliable results. In section 5 an uncertainty analysis to guide measurement campaigns for the collection of input data is presented.

The need to model certain processes in alternative ways or to different levels of detail in order to enable assessments of model structure uncertainty should also be evaluated. Like this it is

possible to make the uncertainty on the model results in some cases much smaller. This is not discussed in this work.

Step 3. The set-up of the model

Model set-up implies transforming the conceptual model into a site-specific model that can be run in the selected model code. A major task in Model set-up is the processing of data. A profound check that all the input files are error free is for sure needed to avoid errors. To avoid mistakes it is always good to check the mass balances.

No items are discussed for this step in this dissertation.

Step 4. Calibration and validation of the model

This step is concerned with the process of tuning and analysing the model that was constructed during the previous step, first by calibrating the model, and then by validating its performance against independent field data.

Two problems arise during the calibration. First of all not all the parameters can be estimated because of correlation and dependencies. In section 6 a sensitivity analysis is applied to detect the most important parameters related to a modelling problem. A validation is then performed for the model calibrated with these most important parameters but for a different year than the calibration period. Secondly, the problem of fixing wrong parameter subsets on literature values should be dealt with. Section 7 shows in a practical example the consequences of using the wrong parameter subset for the calibration of the model.

Step 5. Simulation and evaluation of the model results with an uncertainty analysis (UA) to evaluate the trustworthiness of the model outcomes

In this step the modeller uses the calibrated and validated model to make simulations to meet the objectives and requirements of the model study. Depending on the objectives of the study, these simulations may result in specific results that can be used in subsequent decision making (e.g. for planning or design purposes) or to improve understanding (e.g. of the hydrological/ecological regime of the study area). It is important to carry out suitable uncertainty assessments of the model predictions in order to arrive at a robust decision. It can be that the uncertainty on the results are too high to see difference between the results of two scenarios. Two practical examples, the evaluation of the cost-effectiveness of in-stream aeration for the Dender river (section 8) and the assessment of the effect of shading (section 9) along the Nete river are presented. In these part it is the aim to show the role of uncertainty bounds around the results in the evaluation and to answer the question whether the difference between the scenarios is significantly different from 0 or not.

All methods and procedures in section 2 till 8 are applied on a real case study: the river Dender in Flanders, Belgium. The model of the river Dender is made in ESWAT, an extension of SWAT (van Griensven and Bauwens, 2001), the Soil and Water Assessment Tool developed by the USDA (Arnold et al., 1996). More information about the ESWAT modelling environment can be found in the chapter III “Materials and methods”. For section 9 the case study is the Nete river. A model for the Nete river was implemented in the WEST®

software (MOSTforWATER NV) (Vanhooren et al., 2003) which is explained in chapter III 3 “Materials and Methods”. The description of these two case studies can be found in chapter IV.

1.1. Modelling approach for the river Dender in ESWAT

The ESWAT model for the Dender covers the Flemish part of the basin. The upstream Walloon part of the basin is added to the river as a dynamic upstream point source. A basic SWAT model for the basin was implemented using the Arcvieuw interface. Then the SWAT model was subsequently adapted manually to build an ESWAT model, by adding data as manuring scheme and point source pollution.

1.1.1. The subbasins

Based on the DEM of the catchment, the Dender was divided into 16 subbasins and reaches, from which 7 form the main channel (figure IV.7). Each of the major tributaries of the Dender River is also represented by one subbasin. The subbasins get precipitation data of the nearest rain gauge observations. The daily precipitation records are transformed to minute rainfall by combining it to the 10 minute rainfall of Ukkel using the rainfall converter. The subbasins are further partitioned into a total of 80 HRU's, as defined by land use (impervious, agriculture, corn culture, forest, pasture) and soil type.

1.1.2. The land use

Table V.1 shows how the original land use classes are converted to the classification used by ESWAT. To assure a better match between the "impervious" areas in the soil map and the impervious areas in the land use map, all impervious areas in the soil map were also defined as impervious in the land use map.

Table V.1: Land uses in ESWAT

Land Use Class	% in Dender basin	ESWAT code	Description
City Centre	0.672	IMP	Impervious
Urban area	4.761	IMP	Impervious
Industrial zone	0.605	IMP	Impervious
Infrastructure	3.286	IMP	Impervious
Airport	0.001	IMP	Impervious
Green Urban zone	8.476	URBN	Urban grass
Farming land	17.931	AGRL	Agricultural land generic
Pasture	28.171	PAST	Pasture
Amiss	21.904	CORN	Corn
Wet pasture	1.828	PAST	Pasture
Leaf forest	8.510	FRSD	Deciduous forest
Needle forest	0.248	FRSE	Evergreen forest
Mixture of leaf and needle forest	0.396	FRSE	Evergreen forest
Heath land	2.394	RNGB	Range
Salt marsh, mud	0.004	RNGB	Range
River (Boats)	0.184	WATR	Water
Lakes	0.021	WATR	Water
Estuary	0.000	WATR	Water
River (Small boats)	0.129	WATR	Water
Highway	0.073	IMP	Impervious
Road	0.406	IMP	Impervious

1.1.3. The soils

A simple soil classification system was used. A detailed soil and land use classification is indeed not useful in SWAT because only the most common combinations appear in the HRU's and thus the less common soil types disappear. Main soil classes are sand, loamsand, silty loam and impervious areas. For land use, 5 classes are important: impervious areas, forests, pasture, corn (maize and corn) and land for common agricultural use (crop culture, not corn). About 30% of the land use is pasture, while crop farming represents ca. 50% of the land use.

The soil classes used and their parameters (taken from Arnold et al. (1996) and Dingman (1994)) are shown in table V.2.

Table V.2: The soil data in SWAT

SWAT name	Bulk. Density (g/cm3)	Avail Water Capacity	Hydraulic Conductivity (mm/hr)	Clay (fraction)	Silt (fraction)	Sand (fraction)	Rock (fraction)	USLE Soil factor
Sand	1.6	0.13	720	0.05	0.05	0.9	0	0.08
Loamsand	1.6	0.14	2880	0.1	0.15	0.75	0	0.13
Sandyloam	1.6	0.14	115.2	0.1	0.4	0.5	0	0.37
Siltyloam	1.5	0.2	46.8	0.1	0.5	0.4	0	0.24
Loam	1.6	0.15	22.7	0.15	0.8	0.05	0	0.62
Clayloam	1.6	0.13	7.9	0.3	0.35	0.35	0	0.21
Clay	1.4	0.11	2.9	0.6	0.2	0.2	0	0.08

1.1.4. HRU's

To build the model, the total catchment was subdivided into 16 subbasins. Input information for each subbasin is grouped into categories of unique areas of land cover, soil and management within the subbasins called hydrological response units (HRU's). HRU's were defined using a lower bound percentage of 10% for soil and land use within a subbasin. In total 80 HRU's were defined with 5 different crops and 6 different soil for the 16 subbasins. Tab. VI-11 provides a summary of the land use in the river basin, after application of the HRU's. The distribution shown in table V.3 differs from the distribution of the land uses of the original map (table V.1). The land use classes FRSE (evergreen forest), RNGB (range), URBN (Urban Grass Land) and WATR (Water) cannot be found anymore in the new land use distribution; AGRL, CORN, IMP and PAST have become more important while FRSD becomes less important. This is because in most of the subbasins, the fraction of FRSD is too small to be a HRU, so it is neglected. The other land uses get bigger parts of the total area because of the disappearance of some land uses.

Table V.3: Calculated distribution of land uses (percentages)

land use\soil	IMP	Clayloam	Loam	Loam sand	Sand	Sandy loam	Silty loam	Total
IMP	16.	0.000	0.0	0.000	0.000	0.0	0.000	16.
AGRL	0.0	0.005	18.	0.003	0.000	1.7	0.000	20.
CORN	0.0	0.007	21.	0.009	0.000	4.8	0.000	26.
FRSD	0.0	0.129	0.9	0.000	0.000	0.67	0.000	2.
PAST	0.0	0.007	30.	0.000	0.005	6.2	0.005	36.
Total	16.	0.148	70.168	0.012	0.005	13.3	0.005	100.

The original SWAT land use classification does not contain a land use class accounting for bare soil or impervious areas. The latter classes are however very important when runoff or sediment losses are modelled. To overcome this drawback, an additional 'crop' was created in the crop database by putting all crop parameters equal to zero. In addition, a specific crop management option had to be defined.

1.1.5. The river

The SWAT Arcview Interface automatically calculates for each subbasin, the average main channel width, depth and length. Since the Dender River is not a natural river, the channel depths of the main river are hereby underestimated. Table V.4 shows the river characteristics, set in SWAT. Also, the channel length of some of the subbasins was underestimated by the SWAT Arcview interface. The channel length of these subbasins was corrected using the cross section plans for the Dender river.

Table V.4: Channel characteristics for the Dender river **(Bold = main channel)**

Subbasin	Channel Width [m]	Channel Depth [m]	Channel Length [km]
1	**57.**	**3.7**	**0.27**
2	**54.**	**3.7**	**8.2**
3	13.	0.6	6.6
4	15.	0.7	24.
5	**48.**	**3.6**	**3.**
6	9.	0.48	12.
7	**45.**	**3.0**	**5.7**
8	**34.**	**3.0**	**7.3**
9	21.	0.84	22.5
10	**27.**	**2.5**	**2.1**
11	12.	0.59	15.
12	10.	0.51	2.1
13	**22.**	**3.3**	**5.1**
14	14.	0.64	21.5
15	**12.**	**2.72**	**5.5**
16	22.	0.85	25.

1.1.6. Pollution

For each subbasin, the domestic pollution was assessed by considering the inhabitant densities and inhabitant equivalents (IE's). Domestic and industrial pollution were added as constant point sources in the model.

For the diffuse pollution sources first application of nutrients needs to be simulated. Although there is an unmistakable relation between intensive agricultural activity and the occurrence of high nutrient concentrations in the environment, few precise data are available about the contribution of agricultural activity to the total nutrient concentrations. The data needed for the model implemented in ESWAT were also very sparse and on municipal level and so conversions had to be made to make the data useful for the model (Smets, 1999). An Avenue script for ArcView was developed to transform the data for the villages to data at sub-basin scale (Table V.5). The amounts of fertiliser are distributed over pasture, corn land and generic agricultural land according to the typical manuring periods for these land uses.

Table V.5: Fertiliser application rates for every subbasin

Subbasin	Nitrogen [kg N /ha]	Phosphorus [kg P / ha]
1	184	33
2	128	23
3	162	29
4	174	31
5	193	33
6	99	17
7	201	34
8	136	24
9	107	19
10	225	39
11	158	27
12	186	33
13	198	34
14	194	34
15	165	28
16	166	28

The following assumptions are hereby made:

- The application of fertilisers is assumed to be homogeneously spread over the commune.
- The application rates for the different crops are assumed to be the same. Fertilisers are applied to AGRL, CORN and PAST. While this assumption may be crude, the objective was to apply the correct total amount of fertilisers to the Dender basin, rather than applying the correct amount of fertiliser to each crop.

- The composition of animal manure and chemical fertilisers are assumed to be the same. Table V.6 shows the assumptions that were made about the composition.
- The mechanism by which animal manure and chemical fertilisers are spread in nature and the losses occurring from that, are assumed to be the same.
- It is assumed that the fertiliser application rate remains constant during the simulation period.

Table V.6: Composition of the manure as input in SWAT

Chemical	Percentage of total fertiliser (100*kg/kg)
HNO3	28.5%
Mineral P	7.5 %
Organic N	28%
Organic P	7.5%
Ammonia	28.5 %

Next to the application of nutrients, additional management information needs to be provided in SWAT concerning planting and harvesting dates, dates on which tillage is applied,…. Limited information was available with regard to these activities. Originally, the data of table V.7 have been used:

Table V.7: Agricultural management practices dates (day.month)

	AGRL Generic agriculture	CORN Corn Maize	FRSD Deciduous Forest	PAST Pasture	IMP Impervious
Planting	1.03	1.04	NA	NA	1.01
Harvesting	1.10	1.10	NA	NA	2.01
Fertilising	01.03, 01.04, 01.05	01.03, 01.04, 01.05	No	01.03, 01.04, 01.05	no
Tillage	No	No	No	no	no

In this way, for IMP, a crop is planted but is already harvested the next day. Although the land use IMP does not have a planting and harvesting date, SWAT requires those data.

As the application of fertiliser was concentrated to one day in the month, this could cause enormous nutrient loads at the first rainy day following the manuring. To avoid these unrealistic peaks, fertilisation has been spread over 10 days for each the month in stead of manuring at the first day of the month.

1.1.7. Boundary conditions

To account for the water flow coming from the Wallonian part of the Dender catchment, a point source was added as an upstream boundary of the catchment. The water flows used for this boundary are based on measured values of Bilhee, which were corrected to account for the full draining area of the Wallonian part of the Dender catchment (without Mark).

1.2. Modelling approach for the river Nete in West

1.2.1. The water quantity model

The hydraulic behaviour of the river Nete in the selected stretch is approximated in this study with a cascade of tanks. A number of 10 tanks-in-series with different lengths and variable volumes was chosen as an acceptable compromise between calibration results and computation time. It was assumed that the rating curve for all tanks was the same as in the flow measurement station, since topography and morphology are uniform in the river stretch. The limits in the applicability of the tanks-in-series approach, including the difficulty to take into account backwater effects (Solvi et al., 2005), were of little limitation in the present study.

The developed model does not include a hydrologic model. The flow rate from the upstream section of the stretch is taken as input of the model. The contribution due to the base flow has been accounted for by estimating the groundwater inflow as 10% of the water flowing in each tank.

1.2.2. The biochemical model

The biochemical model used for the present study is a sub-model of the River Water Quality Model Nr.1 (RWQM1) (Reichert et al., 2001a; Vanrolleghem et al., 2001). This sub-model does not include processes and state variables that are not relevant for the problem at hand such as chemical pH-dependent reactions and the state variable “consumers” (and connected processes). Neglecting the pH-dependent reactions is justified by the fact that the measurements of pH show that in the whole simulation period and in all measuring stations the pH is relatively constant, in the range between 6.8 and 7.8. The same RWQM1 sub-model has been successfully tested on a South African basin (Deksissa et al., 2004) and on an Italian basin (Benedetti et al., 2004). A heat balance model was included in the model in order to account for the effect of changes in solar radiation on water temperature. Based on Talati and Stenstrom (1990) the heat balance model includes the effects of solar radiation, atmospheric radiation, surface evaporation and surface convection as a function of radiation intensity, air temperature, wind speed, relative humidity and water surface of the river (for each of the 10 tanks-in-series). In addition, the heat balance contribution due to the base flow has been accounted for by assuming the groundwater temperature equal to 11°C. This temperature represents the yearly average in the region as reported in the measurement database in Flanders (DOV, 2005).

The reduction of light intensity induced by the shading of tree species that are commonly found on the banks of the Nete River (*Alnus glutinosa*, *Salix spp*. and *Populus nigra*) was

evaluated by means of field measurements. The measurements showed that in the full shade of a tree the incident solar radiation can decrease by 95%, which is in agreement with what indicated by Hill et al. (1995) and Hill (1996).

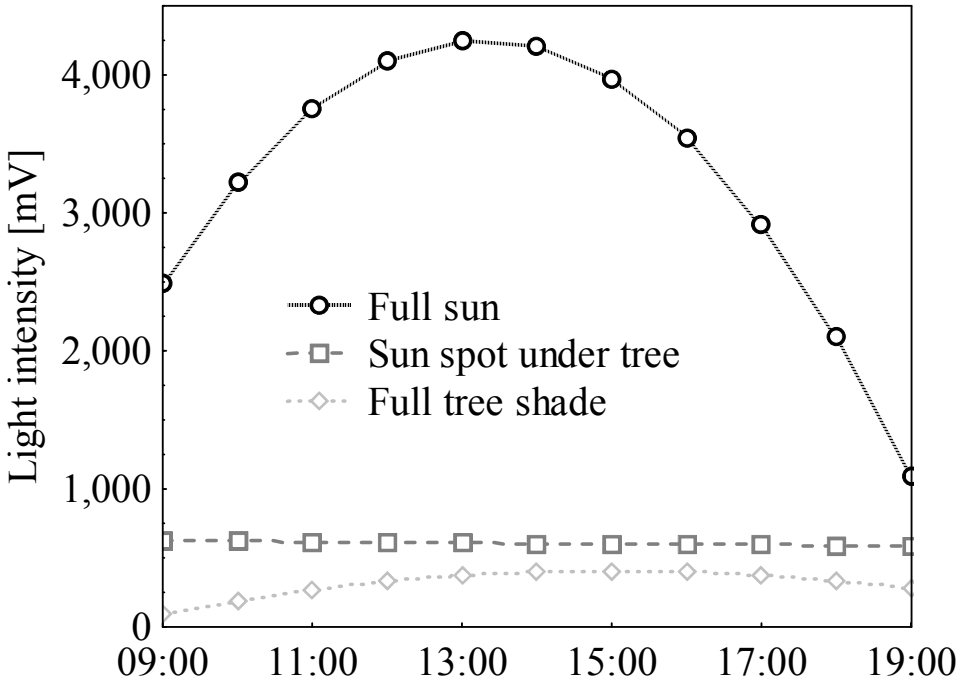


Figure V.2: Pattern of solar radiation during daytime in three different conditions of shading

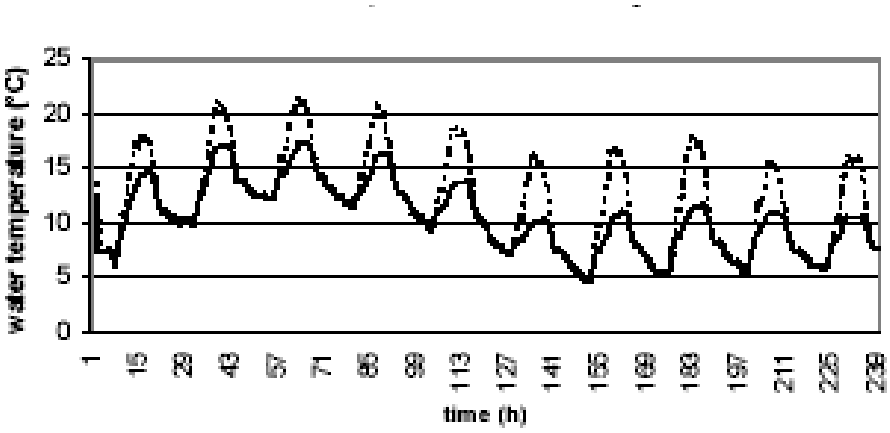


Figure V.3: Modelled temperature profile along the river with (black) and without shading (dashed)

Figure V.2 shows an example of the intensity of solar radiation during daytime as estimated through measurements in three different conditions: full sun, sunspot under a tree and full tree shade. For introduction of shading into the model, conditions analogous to those of "sun spot under a tree" are assumed, as a conservative hypothesis, in the scenarios.

The effect of shading on the water temperature obtained with the temperature model, was compared with the indications found in literature. The reduction in the daily maximum temperatures was of about 7°C, and of about 3°C for the daily average temperature, consistent with the 4-10°C difference in peak temperature reported in literature for watercourses in New Zealand (Quinn et al., 1992), and with the daily fluctuations of water temperature for Australian catchments reported by Lovett and Price (1999). Figure V.3 is an extraction of some days of the temperature profile along the river, with and without shading.

1.2.3. The simulation period

Since the present study mainly focuses on the effects of shading on water quality and in particular on algal blooms, the summer period of 2002 (from April 1st to October 31st) is taken as simulation period. Because of the absence of algal blooms and reduced foliage density, other seasons are of little importance for the objectives of this study.

1.2.4. The input data

The flow rate from the upstream section of the stretch is available from an automated measurement station. To calibrate the model, the flow in a section 12.2 km downstream the initial section as well as water quality measurements collected by VMM at seven measurement locations along the stretch were used.

Four sources of pollution are considered in the model: agriculture, untreated industrial effluents, untreated households effluents and effluents of WWTPs. The impact of diffuse nutrient pollution from agricultural land-use has been estimated by VMM by means of the SENTWA model (System for the Evaluation of Nutrient Transport to Water), which takes into account the partial losses through atmospheric deposition, the losses into groundwater, the direct impact of mineral and organic fertilisers, the effect of natural drainage, erosion and run-off (VMM, 2004). VMM also provided statistics concerning the number of households not connected to any WWTP for each of the hydrographic zones of the Nete basin. The pollutant loads entering the stream from untreated municipal sewage were estimated on the basis of typical loads per inhabitant per day (60 g/d of BOD; 110 g/d of COD; 90 g/d of suspended solids; 12 g/d of total nitrogen; 2 g/d of total phosphorus). Data concerning industrial effluents and effluents from WWTPs were provided respectively by VMM and by Aquafin NV, the latter being responsible for the construction and operation of sewage treatment plants in the whole of Flanders.

The frequency with which data for the various model input were available ranged between hourly (flow, water level, temperature and solar radiation), daily (WWTP effluent), twice-weekly (water quality parameters in the WWTP effluents) to monthly (nutrient loads from agriculture and water quality parameters in the upstream section). For untreated households and industrial effluents a steady state value was assumed for the whole simulation. The input file for the model was created with hourly time-steps. The loads of pollutants were assumed to remain constant between two measurements.

2. Effect of different river water quality model concepts used for river basin management decisions

2.1. Introduction

For integrated water quality management, a holistic approach is necessary at river basin scale. As diffuse pollution sources are increasingly responsible for water quality problems, water quality modelling entered the field of catchment modelling. Upscaling of agricultural field-scale modelling tools or the inclusion of erosion and nutrient equations in catchment hydrological models has led to a number of tools that enable the calculation of the contributions of water, nutrients and sediments from drained areas. In integrated river water quality modelling, the in-stream processes play a key role, as it is here that the pollution of different origins are added and are transformed to what finally determines the water quality.

Within the Soil and Water Assessment Tool (SWAT) (Arnold et al., 1996), the original water quality module – based on QUAL2E (Brown and Barnwell, 1987) - appeared to be erroneously implemented. Time steps of only 1 day were possible that cannot be used in evaluating river water quality processes that change on a subdaily time base. Therefore, two alternative formulations using hourly time steps based on the QUAL2E and the more elaborated River Water Quality Model nr. 1 (RWQM1) (Reichert et al., 2001b) were incorporated in the SWAT model codes and applied on the highly polluted Dender river basin (Belgium) (van Griensven and Bauwens, 2001). Since these concepts represent different processes or different formulations of the processes (see table V.8), they may give rise to different results. This is revealed when the two models are applied for pollution abatement scenarios. When using water quality models for management purposes it is important to have knowledge of the key processes in the river system. To this end a sensitivity analysis (SA) on the parameters of both concepts was performed. With the results of this SA, one is able to define the restrictions of use of a certain river water quality model, for instance, when the model results are not sensitive towards parameters of sediment processes, this model cannot be used for the evaluation of anti-erosion measures.

Table V.8: Comparison between QUAL2E and RWQM1 based water quality models

QUAL2E	RWQM1
	Based on activated sludge modelling concept
Effect focused	Cause focused
No microbial masses modelled	Microbial masses modelled
Simple	Complex
Few parameters and variables	Many parameters and variables
Not closed mass balances	Closed mass balances

To show the effects on management decision, a specific scenario is evaluated in which the pollution load to the river Dender originating from agricultural fertilizer use, is to be

diminished. Both river water quality concepts were used to evaluate the decrease in diffuse pollution input and a comparison is made in this study.

2.2. Methodology

The capabilities of the two different concepts of river water quality modelling to predict and assess the effects of future scenarios for pollution abatement are explored by studying a reduction in diffuse pollution load towards the river Dender. The ESWAT model was calibrated for the two water quality model concepts with two weekly measurements taken in 1994. The calibration was done with the multi-objective calibration method described in van Griensven and Bauwens (2003). The calibration of the flow was also done by multi-objective calibration, the parameters calibrated were the hydraulic conductivity of the soils, the canopy index, the infiltration runoff time lagging, the groundwater parameters and the routing parameters. The calibration led to a Nash-Sutcliffe efficiency of 0,9 for the hourly flow. For both concepts, the results are given for the time series of NO_3 and DO. Sensitivity analysis (SA) on the models is performed on the model results for 1994 as well as the model results obtained after decreasing the diffuse pollution input. This SA is performed with a global sensitivity analysis to see the most influential parameters of the water quality model. The method used is a regression and correlation technique (Saltelli et al. 2000) with Latin Hypercube Monte Carlo sampling (McKay 1995). Regression is done between the parameters and the output. This output is chosen depending on the problem. Because one of the problems in the river Dender is oxygen shortage during some periods of the year, due to eutrophication, and the diffuse pollution is influencing the nitrate content of the river, the critical output considered here is the amount of hours that the oxygen concentration drops below 5 mg/l and the nitrate concentration is higher than 3 mg/l.

Table V.9: Parameters and initial conditions used in the sensitivity analyses for the QUAL2E model in ESWAT. (*Arnolds et al, 1996; **Bowie et al, 1985; ***calibrated)

variable	Description	Units	Range	Nominal value
aio	Ratio of chlorophyll to algae biomass	µg-chl a/mg-algae	10-100*	10***
ai1	Fraction of algae biomass that is nitrogen	mgN/mg algae	0.07-0.09*	0.09***
ai2	Fraction of algae biomass that is phosphorus	mgP/mg algae	0.01-0.02*	0.02***
ai3	O_2 production per unit algae growth	mg O_2/mg algae	1.4-2.6**	2.3**
ai4	O_2 uptake per unit of algae respiration	mg O_2/mg algae	1.6-2.3*	2.0*
ai5	O_2 uptake per unit of NH3 oxidation	mg O_2/mg NH_3-N	3.0-4.0*	3.5*
ai6	O_2 uptake per unit of HNO2 oxidation	mg O_2/mg HNO_2-N	1.00-1.14*	1.07*
µmax	Maximum algae growth rate	1/day	1.0-3.0*	2.2*
rhoq	Algae respiration rate	1/day	0.05-0.5*	0.2*
Kl	Michaelis-Menten half-saturation constant for light	langley/hour	0.72-6.16**	5.226***
Kn	Michaelis-Menten half-saturation constant for Nitrogen	mgN/l	0-10*	0.1*
Kp	Michaelis-Mentn half-saturation constant for Phosphorus	mgP/l	0-10*	0.014*
Λ0	Minimum light intensity for algae bloom	J/m^2	1.5-7.5***	5.0***
Λ1	Algae light self-shading coefficient	g algae biomass/m²	0.01-2.0***	0.3***
Λ2	Sediment shading coefficient	mg/l	10-200***	100***
Pn	Algae preference factor for ammonia	mg/l	0-1*	0.3***
kdd	Algae die-off rate	1/day	0.01-0.8***	0.2****
rs1	Local algae settling rate in the reach	m/day	0.01-1.85*	0.15*
rs2	Benthic (sediment) source rate for dissolved phosphorus in the reach)	mg dissolved $P/(m^2 \cdot day)$	0.01-0.03**	0.01**
rs3	Benthic source rate for NH_4-N in the reach	mg NH_4-$N/(m^2 \cdot day)$.	0.0004-1.8**	1.0**
rs4	Rate coefficient for organic N settling in the reach	m/day	0.001-3.0***	0.05*
rs5	Organic phosphorus settling rate in the reach	m/day	0.001-0.1*	0.03*
rk1	Carbonaceous biological oxygen demand deoxygenation rate coefficient in the reach	1/day	0.02-3.4*	0.87*
rk2	Oxygen reaeration rate in accordance with Fickian diffusion in the reach	m/day	0-100*	0.3***
rk3	Rate of loss of carbonaceous biological oxygen demand due to settling in the reach	m/day	0.1-3.0***	0.2***
rk4	Benthic oxygen demand rate in the reach. If no value for rk4 is entered, the model sets rk4 = 2.0	m²/day	0.02-12.8**	5**
rk5	Rate constant for denitrification	day^{-1}	0.05-4.0*	0.9*
Rk6	Decay rate for arbitrary non-conservative constituent in the reach.	day^{-1}	0-10***	1***
bc1	Rate constant for biological oxidation of NH_4 to NO_2 in the reach	day^{-1}	0.1-1*	0.1***
bc2	Rate constant for biological oxidation of NO_2 to NO_3 in the reach	day^{-1}	0.2-2*	1.0*
bc3	Rate constant for hydrolysis of organic N to NH_4 in the reach	day^{-1}	0.2-0.4*	0.4***
bc4	Rate constant for mineralization of organic P to dissolved P in the reach	day^{-1}	0.01-0.7*	0.1*
rktemp	Rate constant for heat exchange	$m*day^{-1}$	0.1-1***	0.35***

Table V.10: Parameters and initial conditions used in the sensitivity analyses for the RWQM1 model in ESWAT, see also appendix B

Parameter	Units	Minimum	Maximum	Nominal value
water column				
k,death, alg	T^{-1}	0.0500	0.2000	0.14
k,death,con	T^{-1}	0.0250	0.0750	1.05
k,gro,alg	T^{-1}	4.0000	7.0000	4.292
k,gro,con	$L^3M^{-1}T^{-1}$	0.000016	0.000024	0.00002
k,gro,h,aer	T^{-1}	1.0000	3.0000	2.758
k,gro,h,anox	T^{-1}	1.0000	3.0000	2.021
k,gro,N1	T^{-1}	0.5000	2.0000	1.042
k,gro,N2	T^{-1}	0.1000	2.0000	0.96
k,hyd, orgC	T^{-1}	0.0100	0.5000	0.213
k,resp,,alg	T^{-1}	0.0500	0.5000	0.5
k,resp,con	T^{-1}	0.0500	0.5000	1.05
k,resp,H,aer	T^{-1}	0.0500	0.5000	0.35
k,resp,H,anox	T^{-1}	0.0500	0.5000	0.13
k,resp,N1	T^{-1}	0.0500	0.5000	0.463
k,resp,N2	T^{-1}	0.0500	0.5000	0.206
k,eq,1	T^{-1}	fixed value	fixed value	100000
k,eq,2	T^{-1}	fixed value	fixed value	10000
k,eq,w	$L^3M^{-1}T^{-1}$	fixed value	fixed value	10000
k,eq,N	T^{-1}	fixed value	fixed value	10000
k,eq,P	T^{-1}	fixed value	fixed value	10000
k,eq,so	$L^3M^{-1}T^{-1}$	fixed value	fixed value	2
k,ads	T^{-1}	0.0500	1.5000	1.2
k,set,org	T^{-1}	0.1000	10.0000	0.761
k,set,eros	T^{-1}	0.0000	30.0000	0.1
k,res,sed	T^{-1}	0.0000	10.0000	1.3
kcon,set,xii	T^{-1}	0.0000	10.0000	0.5
kexp,set	T^{-1}	0.6000	1.0000	0.8
Kreaer	T^{-1}	0.5000	10.0000	2.187
kCO_2	T^{-1}	0.2550	0.3450	0.3
diff O_2	T^{-1}	0.0014	0.0018	0.0016
diff SS	T^{-1}	0.00081	0.00109	0.000952
diff HPO_4	T^{-1}	0.00102	0.00138	0.0012
diff NH_4	T^{-1}	0.00102	0.00138	0.0012
diff NO_2	T^{-1}	0.00102	0.00138	0.0012
diff NO_3	T^{-1}	0.00102	0.00138	0.0012
diff CO_2	T^{-1}	0.00102	0.00138	0.0012
k,hyd, orgN	T^{-1}	0.0100	0.5000	0.1
k,hyd, orgP	T^{-1}	0.0100	0.5000	0.1
Rktemp	T^{-1}	0.0010	0.0014	0.0012
Boundlayer	L	0.0010	0.3000	0.006
k,death,alg,sed	T^{-1}	0.0085	0.0115	0.01
k,death,sed	T^{-1}	0.0425	0.0575	0.05
k,gro,alg,sed	T^{-1}	1.7000	2.3000	2
k,gro,con,sed	$L^3M^{-1}T^{-1}$	0.0002	0.0002	0.0002
k,gro,h,aer,sed	T^{-1}	1.7000	2.3000	2
k,gro,h,anox,sed	T^{-1}	1.3600	1.8400	1.6
k,gro,N1,sed	T^{-1}	1.2750	1.7250	1.5
k,gro,N2,sed	T^{-1}	1.2750	1.7250	1.5
k,hyd,sed	T^{-1}	0.0255	0.0345	0.03
k,resp,alg,sed	T^{-1}	0.0850	0.1150	0.1
k,resp,con,sed	T^{-1}	0.0425	0.0575	0.05
k,resp,H,aer,sed	T^{-1}	0.1700	0.2300	0.2
k,resp,H,anx,sed	T^{-1}	0.0850	0.1150	0.1
k,resp,N1,sed	T^{-1}	0.0425	0.0575	0.05

k,resp,N2,sed	T^{-1}	0.0425	0.0575	0.05
k,eq,1	T^{-1}	fixed value	fixed value	100000
k,eq,2	T^{-1}	fixed value	fixed value	10000
k,eq,w	$L^3M^{-1}T^{-1}$	fixed value	fixed value	10000
k,eq,N	T^{-1}	fixed value	fixed value	10000
k,eq,P	T^{-1}	fixed value	fixed value	10000
k,eq,so	T^{-1}	1.7000	2.3000	2
k,ads,sed	T^{-1}	0.2000	0.8000	1
M,HPO_4,alg	ML^{-3}	0.0170	0.0230	0.02
M,HPO4,h,aer	ML^{-3}	0.0170	0.0230	0.02
M,HPO_4,H,anox	ML^{-3}	0.0170	0.0230	0.02
M,HPO_4,N1	ML^{-3}	0.0170	0.0230	0.02
M,HPO_4,n2	ML^{-3}	0.0170	0.0230	0.02
M,N,alg	ML^{-3}	0.0850	0.1150	0.1
M,N,H,aer	ML^{-3}	0.1700	0.2300	0.2
M,NH_4,n1	ML^{-3}	0.4250	0.5750	0.5
M,NO_3,H,anox	ML^{-3}	0.0850	0.1150	0.1
M,NO_2,H,anox	ML^{-3}	0.0850	0.1150	0.1
M,NO_2,n2	ML^{-3}	0.4250	0.5750	0.5
M,O_2,alg	ML^{-3}	0.1700	0.2300	0.2
M,O_2,con	ML^{-3}	0.4250	0.5750	0.5
M,O_2,H,aer	ML^{-3}	0.8500	1.1500	1
M,O_2,N1	ML^{-3}	0.0850	0.1150	0.1
M,O_2,n2	ML^{-3}	0.0850	0.1150	0.1
M,S,H,aer	ML^{-3}	1.7000	2.3000	2
M,S,H,anox	ML^{-3}	1.7000	2.3000	2
Ki	EL^{-2}	3.4000	4.6000	4
M,NH_4,alg	ML^{-3}	0.0850	0.1150	0.1
M,alg,alg	ML^{-3}	0.0850	0.1150	0.1
M,algbed,alg	ML^{-3}	0.0850	0.1150	0.1
depth sed layer	L	0.0850	0.1150	0.1

The sensitivity analysis presented here focuses on the parameters of the in-stream QUAL2E based water quality model only, which includes 33 parameters and the parameters of the RWQM1 model which includes 86 parameters. In table V.9 and V.10 all water quality parameters with nominal default values and boundaries are given for resp. the parameters of the QUAL2E and the RWQM1 model. Those values come from literature, the SWAT manual and from own experience with the model.

Various statistical methods can be employed to quantify the sensitivity and uncertainty contribution of the sources to the model outputs. Widely used are those based on linear regression analysis and correlation analysis between the inputs and the simulated model outputs and whereby the parameters with significant correlation are determined to be important.

A linear relation is assumed between the model parameters $x_1,...,x_p$ and the model output Y :

$Y(k) = \beta_0 + \beta_1 x_1(k) + ... + \beta_p x_p(k) + e(k)$ with k = 1,...,N where N is the number of model-outcomes.

The quantities β_0 ,β_1,....,β_p denote the ordinary regression coefficients (ORC), obtained by minimizing the criterion $\sum_{k=1}^{N}\left[Y(k)-\beta_0-\sum_{i=1}^{p}\left(\beta_i x_i(k)\right)\right]^2$ and e(k) represents the error due to a non-perfect matching of the linear approximation.

The goodness of the linear approximation can be assessed by considering the coefficient of determination (R^2) of the regression:

$$R^2 = S_{\hat{y}}^2 \Big/ S_y^2$$

with $S_{\hat{y}}^2, S_y^2$ resp. the variation on the model results and the variation explained by the linear regression on the approximated value.

The confidence in the ordering of importance of the input factors based on that statistic is as good as the associated model coefficient of determination R^2 of the whole multi-linear regression. The closer R^2 is to 1, the better the results.

Because an extension of the set of regressors with additional variables will invariably lead to an increase of R^2, independent of the significance of the added variable, an alternative measure can be introduced: the adjusted coefficient of determination R^2_{adj}: $R_{adj}^2 = 1-\left(1-R^2\right).\left[(N-1)/(N-(1+p))\right]$

The closer the value of this coefficient is to 1, the better the regression. It is recommended to use the rank transformed values to calculate the sensitivity when the value of R^2 or R_{adj}^2 is smaller than 0.7 (Saltelli et al., 2000).

When the input variables are linearly related, the application of a linear regression can lead to an accuracy problem, the collinearity problem (Hocking, 1983). The Variation Inflation Facor (VIF) is a measure of collinearity and is defined as:

$$VIF_i = [C_x]_{ii} = \left(1-R_i^2\right)^{-1}$$

where $[C_x]_{ii}$ represent the diagonal elements of the covariance matrix relating y versus x and R_i^2 = the R^2 value that results from regressing y on only x_i.

A linear regression can be applied as long as the VIF is smaller than 5 (Janssen et al., 1992) .

In this study, the standardized regression coefficients (SRC) are used as sensitivity measures.

$$\mathrm{SRC_i} = \frac{\Delta y / S_y}{\Delta x_i / S_{x_i}}$$

with $\Delta y / \Delta x_i$ the change in output due to a change in an input factor and S_y , S_{x_i} the standard deviation of respectively the output and the input. The input standard deviation S_{x_i} is specified by the user and based on literature values or own experience with the model.

Only the parameters contributing significantly in this linear regression (90% level) are presented.

The sensitivity analysis on the base scenario reveals which processes will typically be taken into account when the abatement scenarios are evaluated. The sensitivity analysis on the reduced diffuse pollution scenario shows the importance of the changed input on the modelled processes. It helps to decide which processes have to be measured and evaluated in view of attaining more reliable results of the model when using it to evaluate a future scenario.

2.3. Results

2.3.1. Time series

The base scenario with real input of the year 1994 and the scenario with 90% fertiliser use reduction are presented in figures V.4 to V.7. In figures V.4 and V.5 the DO and NO_3 time series with a QUAL2E model concept are given at Denderbelle, a river stretch close to the mouth of the river. Figures V.6 and V.7 give the time series at the same location as a result of simulations with the RWQM1 model.

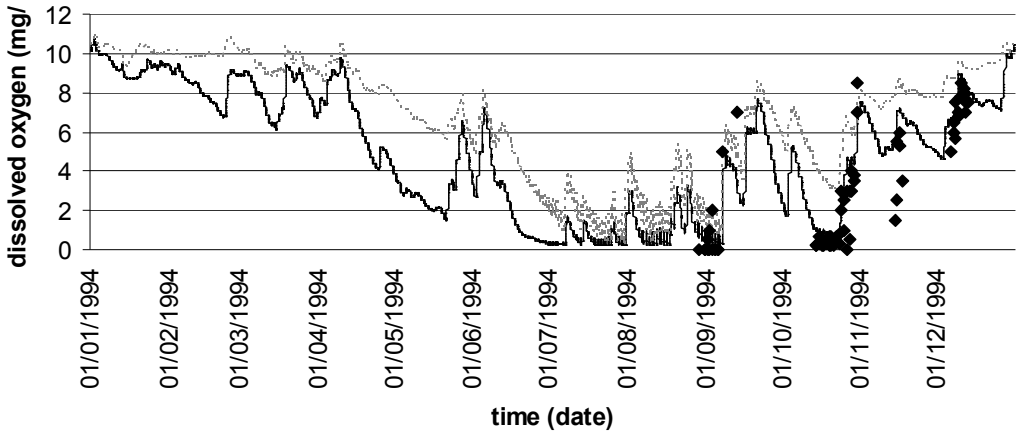


Figure V.4: Time series 1994 (base (full line) and scenario reduction diffuse pollution (dashed line)) with measurements (symbols) in 1994 for DO at Denderbelle, simulated with the QUAL2E-based model

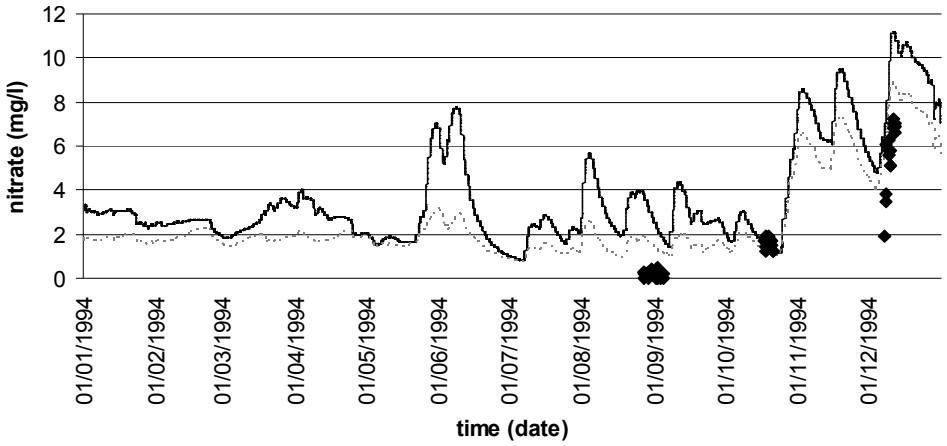


Figure V.5: Time series 1994 (base (full line) and scenario reduction diffuse pollution (dashed line)) with measurements (symbols) in 1994 for NO_3 at Denderbelle, simulated with QUAL2E based model

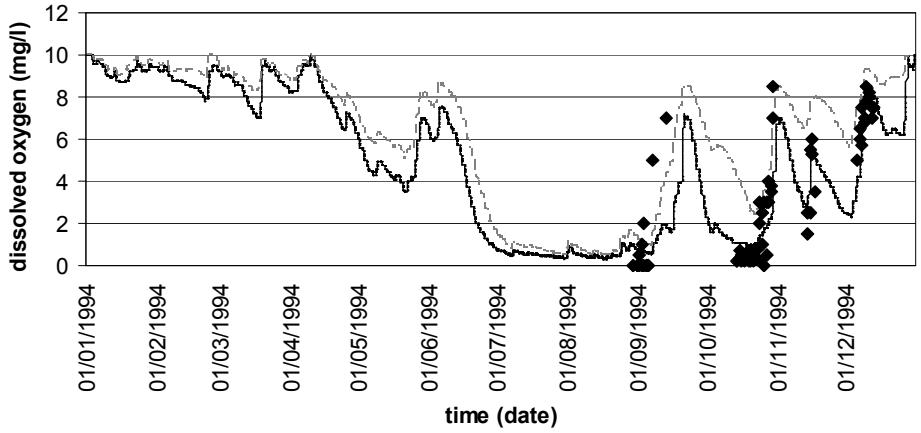


Figure V.6: Time series 1994 (base (full line) and scenario reduction diffuse pollution (dashed line)) with measurements (symbols) in 1994 for DO at Denderbelle, simulated with RWQM1 based model

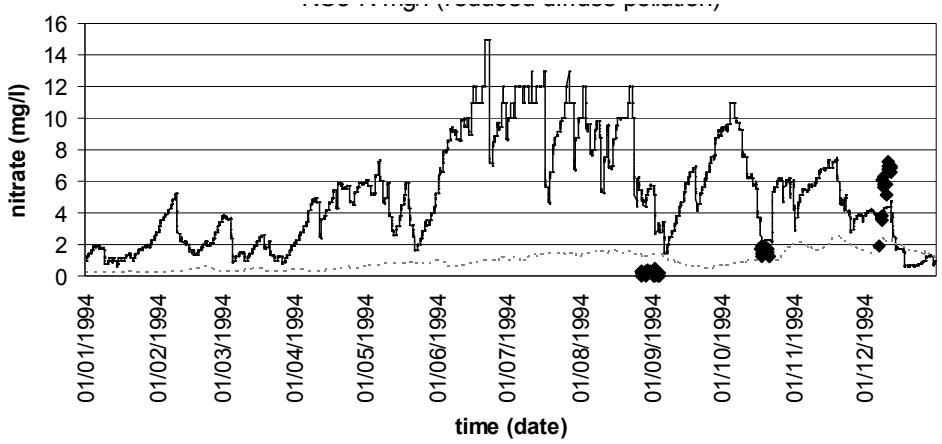


Figure V.7: Time series 1994 (base (full line) and scenario reduction diffuse pollution (dashed line)) with measurements (symbols) in 1994 for NO_3 at Denderbelle, simulated with RWQM1 model

From the comparison of the simulations with the two water quality concepts, it can be concluded that the dissolved oxygen profiles of the base and the reduction scenario are approximately the same for both model concepts, but for the nitrate concentration in the river, the profiles are different, although calibrated in the same way. As a possible explanation for this difference it should be mentioned that the RWQM1 model was difficult to calibrate for nitrates. The mass balance is closed here and by calibrating with data on DO, BOD, NO_3, NO_2, NH_4 and PO_4 it was apparently not possible to find a good fit for all of them. More and more accurate data are needed to obtain better results. It can be concluded that the QUAL2E model with its lumping of processes of different microbial communities is easier to calibrate with less data.

Comparing the results of the scenarios, the same conclusions would be drawn from both model results on dissolved oxygen. Lowering the diffuse pollution towards the river is not a solution in itself as the nutrients coming from households are still high and still lead to algae growth during summer, with extremely low oxygen concentrations. For nitrates the conclusions with RWQM1 are more optimistic, showing that nitrates are much lower in the river during the whole year. Due to the importance of sediment processes by this model, nitrates are lowered. In the reduction scenario, the sensitivity analysis for RWQM1 (table V.12) shows that sedimentation and diffusion processes become even more important in this reduced diffuse pollution scenario. So, to attain more accurate results with more reliability, special attention will be needed towards the calibration and validation of those processes if a RWQM1 model is used. For the QUAL2E model too the settling processes come more into the picture (compare also table V.13 to table V.11 further on) showing the importance of the sediments when the input of nitrates and phosphates decrease.

When looking at diffuse pollution abatement scenarios, algae play an important role as the amount of nutrients used by algae for growth (P and N) originate mainly from agricultural fertilizer use. In this study, the difference between the modeling approach towards algae

growth only becomes relevant when in the future scenario point pollution loads are diminished as well. In the Dender case it appears that the nutrients never become limiting, and algae growth continues with increased temperature and solar radiation. Consequently, the differences in dissolved oxygen profiles between base and reduction scenarios are not really significant. Processes that are of importance are denitrification in the water and in the sediments.

2.3.2. Sensitivity analysis

Tables V.11 to V.14 gives the result of the sensitivity analysis on the base case and the scenario of reduced diffuse pollution. The results of the base case are similar to the results found in (van Griensven and Vanrolleghem, 2005) with a one factor-at-the-time method for the sensitivity analysis. There is an indication that QUAL2E is suited for evaluations related to algae while RWQM1 is better representing the settling and river bed interactions, and the microbial dynamics/limiting factors, as can be seen in the SA in which these process related parameters are ranked as highly important. The results of the SA for the reduction scenarios indicate that due to the decreased load of nutrients to the river some processes become more or less important. For the QUAL2E model for the base case, nitrification/denitrification is important, but for the reduction scenario the benthic oxygen demand, organic N settling and cBOD deoxygenation become also important. In the SA for RWQM1 the results show a shift in importance of processes towards sediment processes and diffusion in the river water and stresses processes performed separately by different microbial communities. As the microbial masses change between scenarios, and this is explicitly considered in the RWQM1, this can give better results. However, this only holds if sufficient measurement data are available for calibration and validation. If one needs to work with a restricted amount of data, the QUAL2E-based modelling will perform better.

Table V.11: Ranking of parameters of QUAL2E model based on the standardized regression coefficient for the output time of NO_3 >3 mg/l and time of DO < 5 mg/l (base case)

NO_3 >3 mg/l		DO < 5 mg/l	
Parameter	SRC	Parameter	SRC
O_2 uptake/NH_4 oxidation	-0.704	O_2 uptake/NH_4 oxidation	0.521
Denitrification rate	-0.342	Rate biological oxidation of NH_4 to HNO_2	0.354
Reaeration rate	0.321	O_2 uptake/algae respiration	0.279
O_2 uptake/HNO_2 oxidation	-0.211	cBOD deoxygenation rate	0.268
Rate biological oxidation of HNO_2 to HNO_3	-0.268	O_2 production/algae growth	-0.240
cBOD loss due to settling	0.173	Algae resp rate	0.159
O_2 uptake/algae respiration	0.121	O_2 uptake/HNO_2 oxidation	0.159
		Max algae growth rate	-0.159
		cBOD loss due to settling	-0.149

Table V.12: Ranking of parameters of RWQM1 model based on the standardized regression coefficient for the output time of NO_3 >3 mg/l and time of DO < 5 mg/l (base case)

NO_3 >3 mg/l		DO < 5 mg/l	
Parameter	SRC	Parameter	SRC
Growth rate first stage Nitrifiers	-0.662	Growth rate heterotrophs, aerobic	0.482
Respiration rate first stage Nitrifiers	0.341	Respiration rate algae	0.394
Respiration rate heterotrophs, aerobic	0.150	Respiration rate first stage Nitrifiers	0.319
Respiration rate heterotrophs, anoxic	-0.145	Growth rate algae	-0.313
Growth rate consumers in sediment	-0.123	Growth rate second stage Nitrifiers	-0.260
Hydrolysis rate in sediment	0.111	Growth rate heterotrophs, aerobic in sediments	-0.073
Diffusion suspended solids	-0.101	Reaeration rate	-0.072
Growth rate heterotrophs, aerobic in sediments	- 0.097		
Respiration rate algae	0.088		
Reaeration rate	0.086		

Table V.13: Ranking of parameters of QUAL2E model based on the standardized regression coefficient for the output time of NO_3 >3 mg/l and time of DO < 5 mg/l (reduced diffuse pollution)

NO_3 >3 mg/l		DO < 5 mg/l	
Parameter	SRC	Parameter	SRC
Reaeration rate	-0.728	Reaeration rate	-0.728
Benthic oxygen demand	0.360	Rate biological oxidation of NH_4 to HNO_2	0.360
CBOD loss due to settling	0.229	Benthic source rate NH_4	0.229
Rate biological oxidation of NH_4 to HNO_2	0.185	Benthic oxygen demand	0.185
Algae preference factor for ammonia	0.122	O_2 uptake/NH_4 oxidation	0.122
Rate org N settling	-1.00	Rate org N settling	-1.00
Half saturation constant for nitrogen	-0.083	Algae respiration rate	-0.087
cBOD deoxygenation rate	0.078	Halfsaturation constant for phosphorus	-0.083
O_2 uptake/NH_4 oxidation	0.12		

Table V.14: Ranking of parameters of RWQM1 model based on the standardized regression coefficient for the output time of NO_3 >3 mg/l and time of DO < 5 mg/l (reduced diffuse pollution)

NO_3 >3 mg/l		DO < 5 mg/l	
Parameter	SRC	Parameter	SRC
Growth rate first stage Nitrifiers	-0.853	Growth rate heterotrophs, aerobic	0.416
Respiration rate first stage nitrifiers	0.331	Growth rate first stage nitrifiers	-0.376
Respiration rate heterotrophs, aerobic	0.100	Respiration rate algae	0.373
Respiration rate heterotrophs, anoxic	-0.099	Respiration rate first stage Nitrifiers	0.328
Diffusion ammonium	0.065	Growth rate algae	-0.265
Respiration rate heterotrophs, anoxic in sediments	-0.060	Growth rate second stage nitrifiers	-0.237
Growth rate consumers in sediment	0.059	Growth rate heterotrophs, anoxic	0.101
Growth rate algae	0.048	Respiration rate heterotrophs, aerobic	-0.093
Hydrolysis rate in sediment	0.043	Sediment boundary layer	-0.085
Diffusion nitrite	0.08		

2.4. Conclusions

The two main concepts in river water quality modelling in use today, QUAL2E and RWQM1 were compared in view of their role in management decision-making. It is shown that the focuses for the two concepts are somewhat different. For this case study on the Dender River, the output of the QUAL2E-based water quality models is mainly influenced by the algae processes where as in the RWQM1 different microbial communities perform processes separately and also sedimentation is taking into account.

When a RWQM1 model can be used that is well calibrated, it should be preferred over a QUAL2E-based model for evaluation of a scenario of reduced diffuse pollution, because as it was shown that the sediment processes then become more important.

The sensitivity of the model results with respect to the processes is not the same for the 2 river water quality modelling concepts and the different models are not always able to properly answer the same management problem. This clearly shows that managers should be aware of the possibilities and limitation of the model they use and choose a model that fits their problem and expectations. Also, knowing which processes will become important after execution of a scenario can make that extra attention is paid towards those processes during model set up in order to get more reliable results. Here expert knowledge also plays an important role. In the Dender river case study, the sediment and diffusion processes become more important.

3. Sensitivity analysis to identify 'soft data' for the evaluation of a river water quality model

3.1. Introduction

The results of a sensitivity analysis can provide guidelines about how parameter uncertainty will affect the model output, but these are always related to the specific circumstances under which the model was built and calibrated. If the model has to be applied on a river with different characteristics, again an extended dataset is needed to identify the important parameters of the model and the associated uncertainty levels. If it were possible to link uncertainty and characteristics of the river basin in advance, this could open perspectives for model applications in ungauged basins. Research on this topic is also performed in other studies. One of the methods proposed in Belgium is the method by Hundecha (2002). They linked the catchment properties, i.e. the model parameters, with a transfer function. That way similar catchments could be linked with similar parameter values. They calibrated these transfer functions with the runoff data of gauged catchments.

The aim of this research was to examine the link between catchment properties and sensitivity of parameters of a river water quality model by testing the local sensitivity of a river water quality model to the a priori assumption of parameter values. In non-linear models, the propagation of uncertainty of a particular parameter depends on several factors, such as the values of the other model parameters and the specific conditions. The values of parameters also can differ according to specific circumstances. For example, a river with important algae blooms during summer periods will have its parameters of the algae growth model adapted to the growing species when calibrated.

The presented analysis can reveal important information about the uncertainty propagation for situations in which no or poor data are available. Indeed, if general clusters can be found of cases in which some parameters are more sensitive than others, then this information can be used as 'soft data' to identify when certain parameters become more important than others and this can for example be used to divide the parameters in uncertainty classes or to get an idea of the values of those parameters. Another aspect is that once the important parameters are detected, optimal experimental design techniques can be used to determine the optimal measurement strategy that allows a better identification of the parameter values before calibrating the model.

3.2. Methodology

The method used here is based on the one described in Weijers and Vanrolleghem (Weijers and Vanrolleghem, 1997). It is like a kind a kind of sensitivity analysis of the sensitivity analysis. It starts with a Latin Hypercube Monte Carlo sampling (McKay et al., 1979) of all the parameters over the whole parameter space, 100 samples are taken (method is the same as

described in section 2 of this chapter). The parameter space is delineated based on literature, mostly out of Jorgensen et al. (1991). For each set of sampled parameters, a regional sensitivity analysis is done in which the values are changed 10 % around their nominal value, again with a Latin Hypercube Monte Carlo using 100 samples. This procedure is visualised in figure V.8.

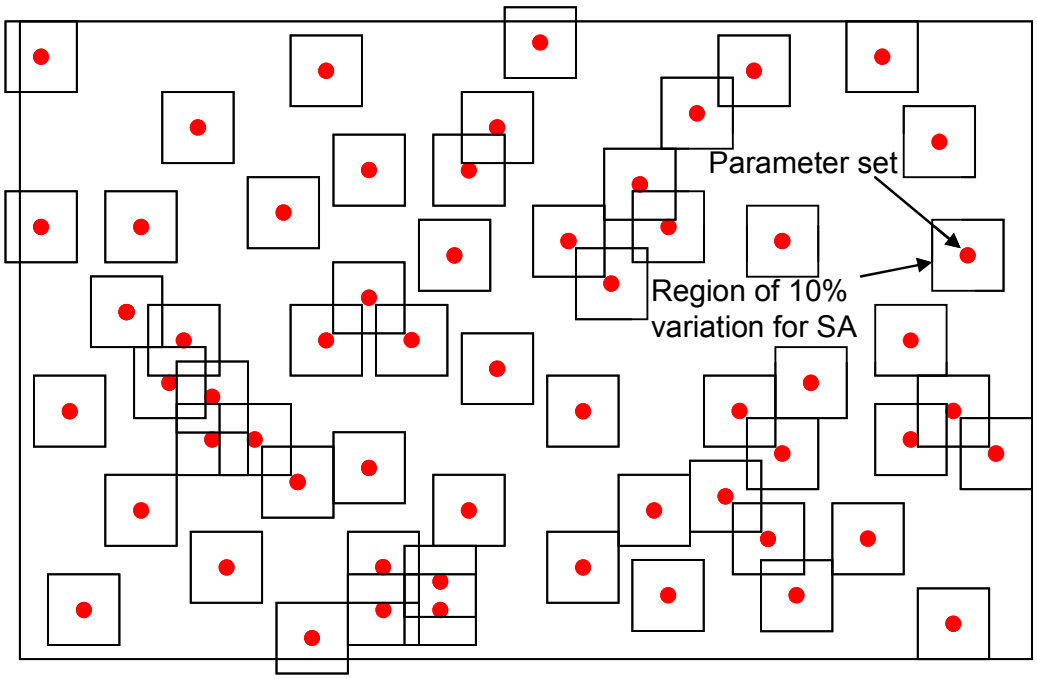


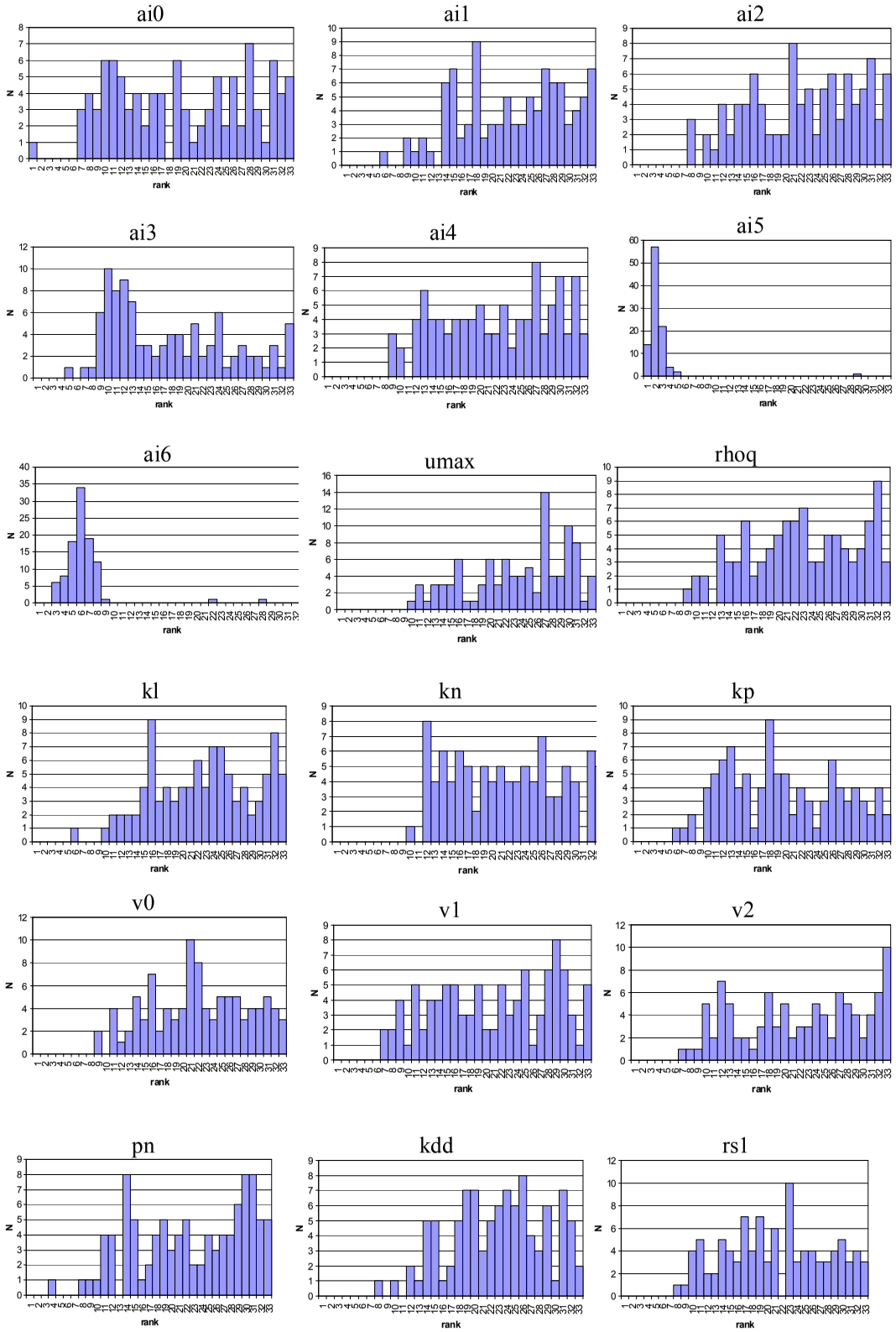
Figure V.8: Sampled parameter sets and their 10% variation region around them.

In this way for each sampled set of parameters the most sensitive parameters can be detected by ranking them. Given the model's non-linearity it is obvious that these most important parameters will not be the same for all sampled sets. The ranking will be related to the nominal values of the parameters. From this analysis the parameters can be identified that are sensitive in all cases, in some cases or never. For those that sometimes appear to be the most sensitive ones, we can try to see under which circumstances they become more important and what kind of parameter set they are linked with. That way a link is created between parameter sensitivity, value and external circumstances.

One must realise an assumption is made, namely that the model is general and complete in the description of all the processes so that 10000 Monte Carlo-runs cover all possible situations for the river Dender. Different situations in the watershed are corresponding to different parameter values which lead to different sensitivities. These situations can be called the "soft data". An example of soft data can be: temperature of the water, colour of the water, residence time, important diffuse pollution, …

3.3. Results and discussion

The results are shown in figure V.9. The figure presents for each parameter the frequency of the different rankings it had in the regional sensitivity analysis.



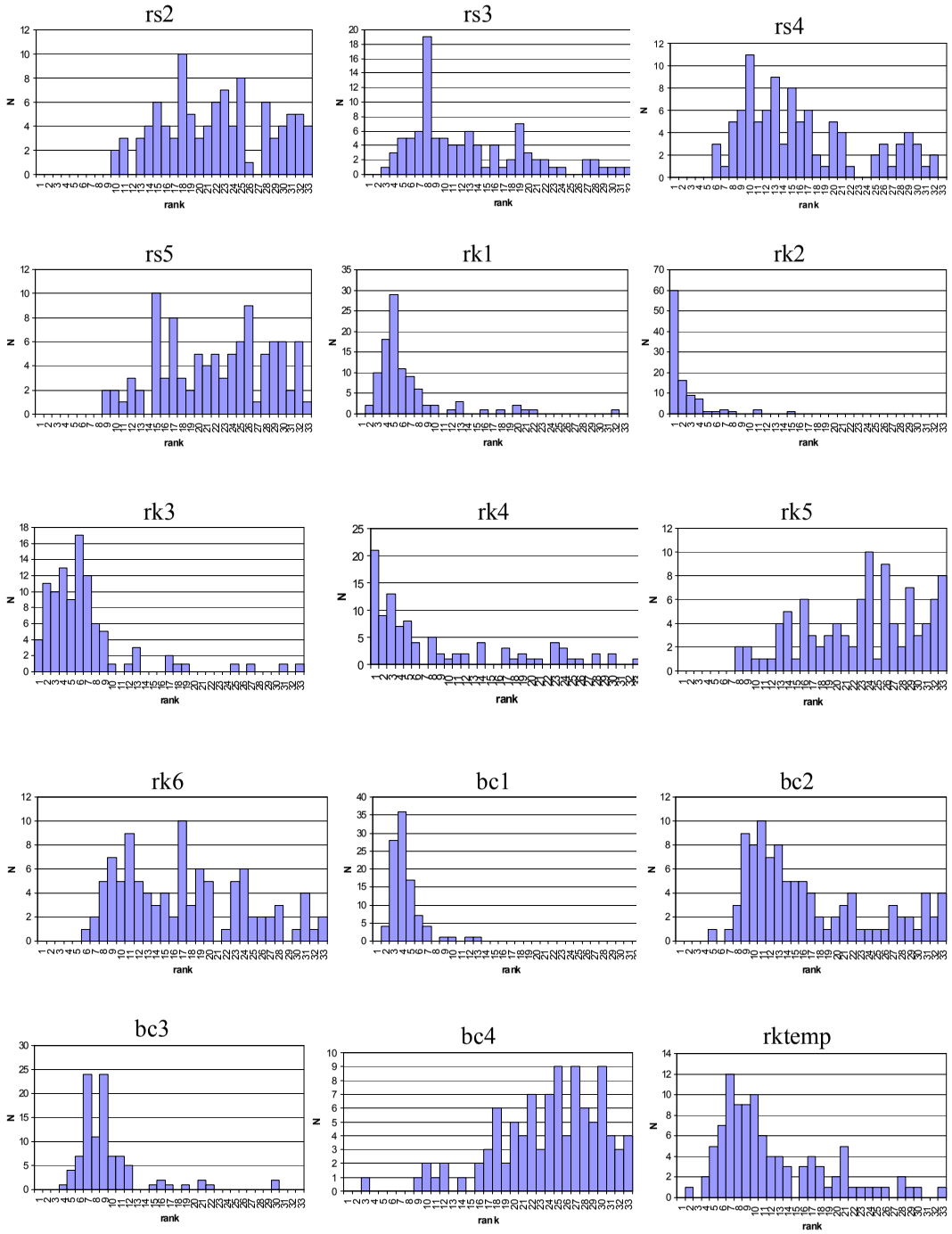


Figure V.9: Ranking results of the regional sensitivity analysis of the 100 different parameter sets

The parameters that appear to be influential in almost every run are clearly: ai5, ai6, bc1, bc3, rk1, rk2, rk3, rk4, rktem. The other 30 parameters appear to come on all the other possible places. Out of these we can see when some of the parameters become important. This is done first visually by looking what parameters are sometimes important, then find the parameter set for the corresponding Monte Carlo simulation and see the major differences between the

results and the corresponding characteristics of the river. Figure V.10 gives an example of two such different runs, with or without algae growth.

No algae growth

- Most important parameters: rk2, ai5, ai6, bc1, rk1, rk3, rk4, bc3, rktem, bc2

(O_2 reaeration rate, O_2 uptake per unit of NH_3, rate constant for biological oxidation of NH_4 to NO_2, O_2 uptake per unit of HNO_2, cBOD oxygenation rate, cBOD loss rate due to settling, rate constant for hydrolysis of organic N to NH_4, rate constant for heat exchange, rate constant for biological oxidation of NO_2 to NO_3)

With algae growth

- Most important parameters: ai5, bc1, ai4, rk1, ai3, rhoq, ai6, pn, rk3, rk5

(O_2 uptake per unit of NH_3, Rate constant for biological oxidation of NH_4 to NO_2 in the reach, O_2 uptake per unit of algae respiration, cBOD oxygenation rate , O_2 production per unit of algae growth, algae respiration rate, O_2 uptake per unit of HNO2 oxidation, algae preference factor for ammonia , cBOD loss rate due to settling, rate constant for denitrification)

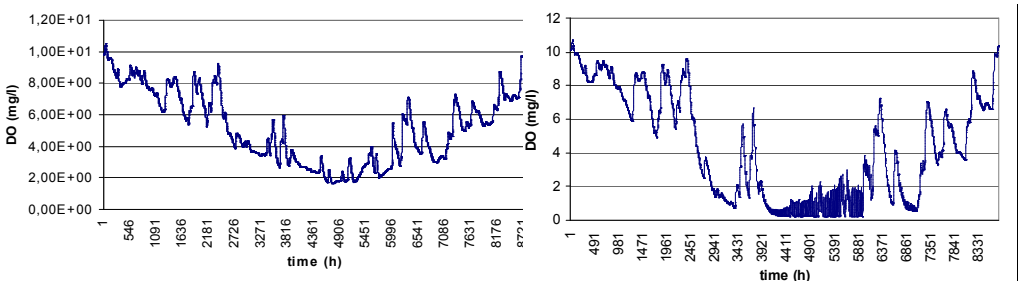


Figure V.10: Simulations of DO in the Dender simulated with two different parameter sets

With the analysis it was detected that if the river has a low ammonium concentration the parameter rs3 becomes also important, and if the river has a high ammonium content rs4 becomes more important. A river with high phosphates gives bc4 as important parameter in addition to the parameters related to benthic processes.

The analysis of all the different runs is very time consuming and it was therefore decided to only consider the most obvious cases. Table V.15 summarizes some of the findings of this limited study. Not only the importance of the parameters under different circumstances can be detected but also linking of the parameter values to the "soft data" is possible. As an example two different parameter sets are given, one with and one without algae growth (table V.16). These values give an idea of the magnitude of the parameters to start a calibration with when a particular situation is to be modelled, but it's obvious that much more analysis is needed to also identify other parameter sets which give similar outputs, but for which other aspects are different. This may be the subject of different research.

Table V.15: Some observed relations between soft data and sensitive parameters

Soft data	Sensitive parameters
No algae growth (no green colouring of water)	rk2,ai5,ai6,bc1,rk1,rk3,rk4,bc3,rktemp,bc2
Algae growth (green colouring of water)	ai5, bc1, ai4, rk1, ai3, rhoq, ai6, pn, rk3, rk5
Low ammonium content	+ rs3
High ammonium content	+ rs4
High phosphate	+ bc4 + rs2

Table V.16: Values for two different parameter sets with as main difference with and without algae growth

variable	Description	units	Without algae growth	With algae growth in summer
aio	Ratio of chlorophyll to algae biomass	µg-chl a/mg-algae	10	10
ai1	Fraction of algae biomass that is nitrogen	mgN/mg algae	0.09	0.09
ai2	Fraction of algae biomass that is phosphorus	mgP/mg algae	0.02	0.02
ai3	O_2 production per unit algae growth	mg O_2/mg algae	2.3	2.3
ai4	O_2 uptake per unit of algae respiration	mg O_2/mg algae	2.0	2.0
ai5	O_2 uptake per unit of NH3 oxidation	mg O_2/mg NH_3-N	3.35	3.35
ai6	O_2 uptake per unit of HNO2 oxidation	mg O_2/mg HNO_2-N	1.065	1.065
µmax	Maximum algae growth rate	1/day	2.1	2.1
rhoq	Algae respiration rate	1/day	0.3	0.3
Kl	Michaelis-Menten half-saturation constant for light	langley/hour	4.4	1.4
Kn	Michaelis-Menten half-saturation constant for Nitrogen	mgN/l	0.1	0.1
Kp	Michaelis-Mentn half-saturation constant for Phosphorus	mgP/l	1.1	1.2
Λ0	Minimum light intensity for algae bloom	J/m^2	4.3	4.3
Λ1	Algae light self-shading coefficient	g algae biomass/m²	100	1
Λ2	Sediment shading coefficient	mg/l	1	50
Pn	Algae preference factor for ammonia	mg/l	0.3	0.3
kdd	Algae die-off rate	1/day	0.02	0.02
rs1	Local algae settling rate in the reach	m/day	0.1	0.01
rs2	Benthic (sediment) source rate for dissolved phosphorus in the reach)	mg dissolved $P/(m^2 \cdot day)$	0.01	0.01
rs3	Benthic source rate for NH_4-N in the reach	mg NH_4-$N/(m^2 \cdot day)$.	1.0	1.0
rs4	Rate coefficient for organic N settling in the reach	m/day	1	2.8
rs5	Organic phosphorus settling rate in the reach	m/day	0.05	0.03
rk1	Carbonaceous biological oxygen demand deoxygenation rate coefficient in the reach	1/day	0.15	1.01
rk2	Oxygen reaeration rate in accordance with Fickian diffusion in the reach	m/day	0.01	2.6
rk3	Rate of loss of carbonaceous biological oxygen demand due to settling in the reach	m/day	1	2.15
rk4	Benthic oxygen demand rate in the reach. If no value for rk4 is entered, the model sets rk4 = 2.0	m²/day	0.05	0.046
rk5	Rate constant for denitrification	day^{-1}	0.05	0.9
Rk6	Decay rate for arbitrary non-conservative constituent in the reach.	day^{-1}	1	1
bc1	Rate constant for biological oxidation of NH_4 to NO_2 in the reach	day^{-1}	0.15	0.48
bc2	Rate constant for biological oxidation of NO_2 to NO_3 in the reach	day^{-1}	1.0	1.0
bc3	Rate constant for hydrolysis of organic N to NH_4 in the reach	day^{-1}	0.4	0.4
bc4	Rate constant for mineralization of organic P to dissolved P in the reach	day^{-1}	0.1	0.1
rktemp	Rate constant for heat exchange	$m*day^{-1}$	0.35	0.35

3.4. Conclusions

With a sensitivity analysis of the sensitivity analysis it is found that the model has different sensitivities of the parameters in different external circumstances. A table in which external circumstances, here called soft data, are related to the sensitivity of the parameters could be established. This table with soft data, e.g. occurrence of algae growth, plants in the water, high summer temperatures, a lot of agriculture with fertiliser use in the region, is 'not case specific', because it is assumed that all possible situations are presented by the different parameter subsets. It is a first indicator of which parameters/processes one should focus on in a particular catchment characterised by the soft data. Knowing the most influential set of parameters is important for calibration of a model, optimal experimental design, uncertainty estimations and scenario analysis where other processes can become important compared to the base case. The latter aspect will be illustrated in section 1 of the next chapter dealing with scenario analysis.

This study reporting soft data is here only done for water quality parameters. It should be extended to other parts of a catchment model like the parameters of the rainfall/runoff module or the diffuse pollution processes. In this research the analysis of the different subsets was done visually and manually, to show the usefulness. It would be better and more complete to use a cluster method. Such a method can make use of clustering techniques in which the parameter sets that give more or less identical results for one variable are clustered. Within these sets of parameters again other results, for other variables, can be considered for further clustering.

4. Optimal experimental design in river water quality modelling

4.1. Introduction

Parameters of a river water quality model are not always practically identifiable because there is an insufficient amount of data or data taken in periods or in places that are not suitable for calibration of the model. Optimal experimental design (OED) techniques are a useful tool to construct experiments to obtain information needed for calibration of a model of the system under consideration. OED has been applied in many disciplines like modelling of waste water treatment plants (De Pauw, 2006; Vanrolleghem and Coen, 1993), fermentation processes (Versyck et al., 1997; Zelic et al., 2004) soil processes (Catania et al., 2004), systems biology (Faller et al., 2003), food technology (Foubert, 2003; Nahor et al., 2001), pharmacology (Fedorov and Leonov, 2001), electrical engineering (Ko et al., 2004) and chemical engineering (Atkinson and Hunter, 1968). A common thing in all those researches is that the experimental conditions are 'controllable': temperature, time, pH, measurement frequency, initial concentration,… In OED for a natural river system, things become more complicated as a combination of different factors like temperature, flow and concentration is not occurring on the desired moments and as such, a method has to be found which maximises the content of information of experiments, without knowing the exact situations under which those

measurements will occur. Further, external conditions like weather, discharges in the river or diffuse pollution into the river can change year after year, so measurements that are likely to be optimal for a particular year can appear to be sub-optimal the next year. All those reasons make that a normal straightforward optimal experimental design cannot be used for river water quality modelling and extensions of those designs are needed to find a good measurement set-up.

In this section it is the aim to find a good set-up for measurements to reduce the uncertainty of a river water quality model, based on a set of previous measurements and a model calibrated with those measurements. It is assumed that the calibrated model gives good results but that the uncertainty bounds related to the model outcomes are too wide to draw reliable conclusions for management decisions. It is further the aim to find a cost-effective solution, so that the obtained amelioration with more or better measurements can be linked and compared to costs and practical considerations. The methods are applied on a practical case study, the river Dender in Flanders, Belgium.

4.2. Methodology

The purpose is to maximize the practical identifiability by defining an optimal experimental design to increase the information content of the data. Different experiments (sampling schemes) will reveal more or less information and more or less reliability, e.g. schemes that lack dynamics will provide less information than schemes with more variation in time. Optimal sampling design techniques aim at the identification of sampling schemes to improve different facets of the mathematical modelling process, according to explicitly stated objectives. The objective considered here is to increase the precision of the parameters for the water quality module of ESWAT.

According to the experimental design theory, described in more detail in the literature study, chapter “Optimal Experimental Design”, the method used here is the D-optimal experimental design (Goodwin and Payne, 1977; Walter and Pronzato, 1999), because this method is the most general method for minimising the overall error on the estimated parameters.

For the ‘traditional’ use of optimal experimental design in river water quality modelling, three problems arise:

- The experimental circumstances cannot be imposed and data cannot be collected for any preferred circumstance.
- The behaviour of the system varies randomly according to the natural variability of external circumstances.
- The model used for the OED contains itself a lot of uncertainty: the parameters can be under or overestimated.

Therefore, it is not possible to find one exclusive best experimental design but the experimental design can help in giving information about how, where and when the

measurements are best taken, because there exist periods and circumstances under which the model is more sensitive to parameter changes than others.

(Wald, 1974) has demonstrated that when experiments are carried out in sequence, a smaller number of them are required, on the average, than when they are performed simultaneously. This is true even where no use is made of information gained in one experiment for planning the next one. The gain in this case accrues entirely from the ability to terminate the experimentation precisely at the point at which one's goal has been met. If, in addition, one is able to design each experiment in the light of the results of the previous ones, the gain in efficiency can be even more impressive. This can be generalised when considering an experiment as a collection of data.

In a D-optimal experimental design, considering the determinant of the inverse of the covariance matrix of the parameter estimates (C) or Fisher Information Matrix (FIM) (Godfrey and Distefano, 1985) assesses the precision of the parameters:

$$C(b) = \left(S^T Q S\right)^{-1} \qquad FIM(b) = C^{-1}(b)$$

with b representing the model parameter vector, Q a diagonal matrix, the elements being the squares of the observation weights (these are the a priori probability of the observations) and S the sensitivity matrix of the outputs to the parameters in comparison to the observations. Calculation of the covariance matrix based on the Jacobian matrix instead of the Hessian is acceptable when assuming linearity and assuming observations with constant standard deviations (Bard 1974). The determinant of the FIM, Det(FIM) is inversely proportional to the volume of the confidence region. Thus, by maximizing Det(FIM), the volume of the confidence ellipsoids, and, correspondingly, the geometric average of the parameter errors is minimized. D-optimal experiments also have the advantage of being invariant with respect to any scaling of the parameters (Petersen, 2000). An extra aspect to be considered here is that for non-linear models, the FIM is dependent on the particular set of parameter values at hand.

The OED technique requires an initial data set to calibrate the model. Non-accurate parameter estimates may therefore lead to an inefficient experimental layout. This means that for the processes related to the non-accurate parameters better measurements could be identified. The design can only be approached by an iterative process of data collection and design refinement, known as a "sequential design" (Casman et al., 1988). Experiment after experiment the model parameters can be updated and finally will converge to one best parameter set. Figure V.11 shows the iterative scheme that is used to find the optimal measurements starting with a model that is calibrated with the currently available data. Next the different steps are explained in more detail.

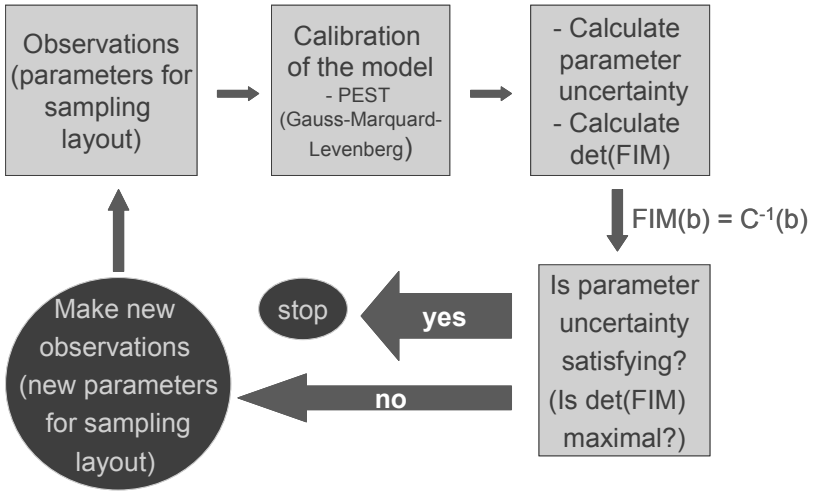


Figure V.11. Optimal experimental design for river water quality modelling (PEST = Parameter ESTimation model (Pest Manual, 1994))

Generating synthetic data series

The evaluation of different sampling schemes requires the availability of a long time series of high frequency water quality data at different places along the river. Because such historical series were not available, a simulation generated synthetic "observation" series with the Dender model using ESWAT. For realism, the output series were subsequently altered by addition of pseudo-random noise. The noise terms were generated, considering a normal distribution and variations that are consistent with the accuracy of the measuring devices used to measure the variables (Bols, 1999): 3% for Dissolved Oxygen (DO); 10% for Biological Oxygen Demand (BOD) and 5% for NO_3 and NH_4. Then the parameters for the sampling layout are defined. Examples of such parameters are (i) the sampling frequency e.g. every two hours,(ii) location of the measurements, e.g. at the mouth + 6 km more upstream the mouth and (iii) measured variables e.g. DO + NH_3.

Calibration of the model

With each set of data selected from the synthetic time series on the basis of a certain sample layout, the model can be calibrated. To be sure that the calibration process does not end in a local optimum, the initial parameter guesses are taken in the neighbourhood of the parameter values obtained during the calibration with the available data. Indeed, the purpose of this step is not to find the parameter values, but rather to obtain the covariance matrix from the optimisation method, because the inverse of the covariance matrix is the FIM (See literature chapter on OED and the chapter "Materials and methods". Here the PEST (Parameter ESTimation) program (Doherty, 2000) is used. The parameter estimation in the PEST program is done by a minimisation of the following objective function (J) by finding the optimal choice of the parameters θ.

$$J(\theta) = [y - y(\theta)]^T * Q * [y - y(\theta)]$$

with y being the output of the model and Q a weighing factor for the model outputs.

Calculating the determinant of the FIM

The PEST program also calculates the covariance matrix of the parameters at their best estimates, given the relation $FIM(b) = C^{-1}(b)$, this means that also the FIM and from this the Det(FIM) can be determined.

Maximization of the Det(FIM) by changing the sampling layout

In a loop, different observations related to a different sampling layout can be selected. The Shuffled Complex Method (SCE-UA) (Duan et al., 1992) is used here to find the sampling layout that maximises the Det(FIM) in order to optimize the parameters of the sampling layout. A description of this method is given in the chapter "Materials and Methods". After several evaluations of the Det(FIM), the shuffled complex method finds the optimum very fast because the method searches the whole parameter space in an efficient and effective manner. In this research the loop will end once the observation set that maximises the det(FIM) is found.

4.3. Results

The methodology has been applied for an OED at the Dender river. As an illustration of the applicability of the method, a simple case, whereby only DO is considered at one specific location is presented first. The synthetic "observation" series consists of 1 year of hourly data. The optimization is limited to (i) the measuring frequency, (ii) the number of samples and (iii) the period of the year for sampling. The sampling time step was allowed to vary between one hour and two days; the minimum number of samples is 1 and the maximum number is 8760 (365*24). Samples could be taken during winter, summer or a mixed summer–winter period, depending on the start of the period and the total number of samples that are taken.

In figure V.12, the optimisation process is shown. SCE-UA used 136 runs to find the layout for which the Det(FIM) is the largest. As could be expected, the results show that the uncertainty in the parameters became minimal for the smallest sampling interval (figure V.13 left), a very large number of samples (figure V.13 right) and a large period, mainly spring and summer months (data not shown). A sample every hour, starting in February and ending on August 30th, representing a total of 5804 samples appears to provide the best results.

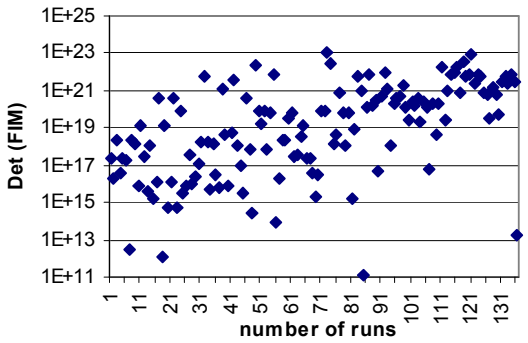


Figure V.12: Optimization of the Det(FIM) (3 parameters of sampling layout) (see text)

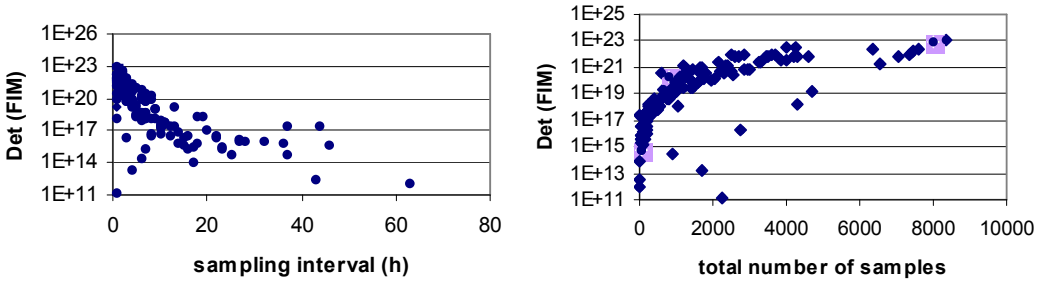


Figure V.13: The Det(FIM) as a function of the sampling interval (left) and total number of samples (right)

A second example supports a more complex planning, whereby in addition the measured variables (only DO or combined DO-NO_3, DO-NO_3-BOD or DO-NO_3-BOD-NH_4) and sample locations (4 possible combinations of 3 possible locations: upstream, halfway, downstream) are considered as parameters for the sampling layout.

A substantial increase in the number of iterations for the optimization is observed (figure V.14). The best way to take samples is on an hourly time basis (figure V.15 left), over nearly the whole year (8730 samples) (figure V.15 right), on two locations (data not shown) and with measurement of the four variables (data not shown). This is again a very logical result. However, looking at figure V.15 it can be deduced that other sampling schemes could be defined that provide a quasi-similar accuracy, with fewer samples or a lower frequency. The determinant of the FIM is not changing significantly between 5,000 to 8,000 samples that mean that the confidence regions around the parameters do not differ very much in that range. This is explained by other factors that influence the accuracy, such as the period of the year during which the sampling takes place.

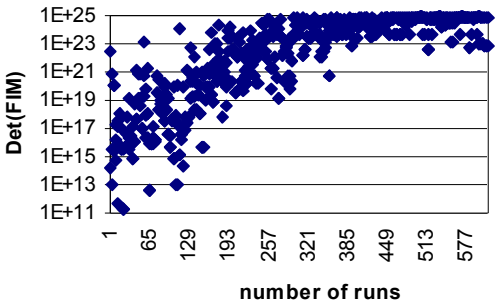


Figure V.14: The optimization of the Det(FIM) with variation of 5 parameters (see text)

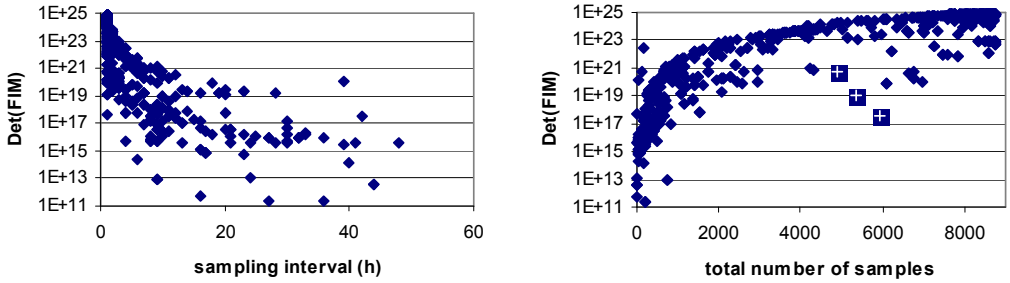


Figure V.15: The Det(FIM) as a function of the sampling interval (left) and the total number of samples (right) (points marked with ⊞are further investigated, see text)

Alternatively, some sampling schemes clearly appear as non-optimal (such schemes are indicated by squares in figure V.15): these schemes require a lot of samples, but due to the wrong choice of other factors, the information content of these schemes is poor. More details on these schemes are given in table V.17. The reason for the bad performance of these schemes is related to the sampling place (upstream) and to the fact that the sampling period does not include the spring period, which seems to be important for the calibration process.

A few points with high det(FIM) although with only a few sampling points can be seen on the graph. After checking these it was seen that these are high by miscalculation and coincidence because of too few samples.

Table V.17: Non-optimal sampling designs

Sampling interval (h)	Number of samples	Period	Location	Observed variables	Det(FIM)
1	5972	16 Apr.-31 Dec.	Geraardsbergen	DO-NO_3	4,08E+17
1	5340	22 May-15 Nov.	Geraardsbergen	DO-NO_3-BOD	1,19E+19
1	4902	11 May-31 Dec.	Geraardsbergen	DO-NO_3-BOD	5,92E+20

4.3.1. Optimal experimental design including practical considerations

In itself the value of the Det(FIM) has no physical meaning. A further analysis is needed to check the improvement of the calibration with the optimal set of measurements in contrast

with a - for calibration purposes - less good measurement set, which is however characterized by lower costs and efforts or that is more practically feasible.

The performance of the calibration is evaluated by looking at the final uncertainty on the model results taking into account the variances and correlation between the parameters after calibration. This is because finally, in practice, one may only be interested in the uncertainty of the model results and not in the parameters themselves. This uncertainty on the results is then evaluated in view of acceptability towards the purpose of the model.

To illustrate the procedure, three sampling schemes (table V.18) from the first test case are considered (indicated by squares in figure V.13). More details about the schemes are given in table V.18. The model outputs and the 95% confidence intervals for the considered schemes for a day (22 February), chosen because of the low oxygen content that increases during the day, are given in figure V.16. The results of the uncertainty analysis show that the average width of the confidence interval in the model output is reduced by 45% for scheme 2 when compared to scheme 1 and by 60% if scheme 3 is compared to scheme 1. The results illustrate the possibilities of the method to define a dedicated sampling strategy, in view of a given modelling accuracy.

Table V.18: Selected sampling schemes for evaluation of resulting uncertainty in model output

Sampling interval (h)	Number of samples	Period	Det(FIM)
37	42	26 Oct.-31 Dec.	4,93E+14
2	818	23 Oct.-31 Dec.	1,69E+20
1	8008	2 Feb.-30 Aug.	9,62E+22

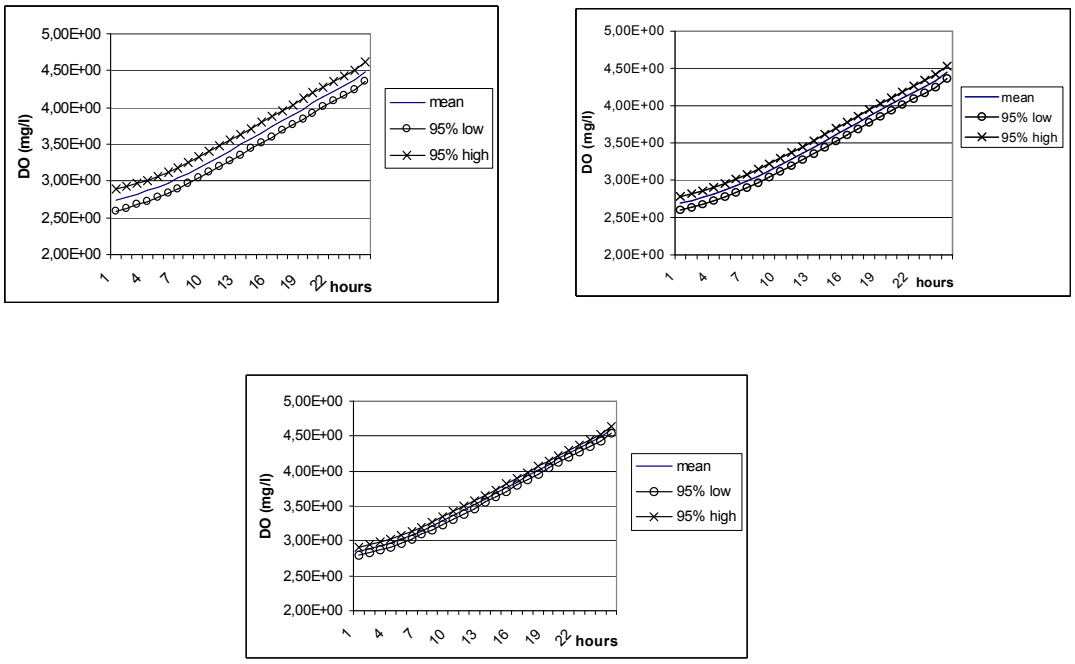


Figure V.16: DO with confidence bounds on 22 February, sampling scheme 1 (left), 2 (right) and 3 (under)

Based on the results of OED it is possible to find out to what extent some more expensive measurements can be substituted with less expensive ones. Therefore, a comparison is made of the Det(FIM) for different measured water quality variables (figure V.17).

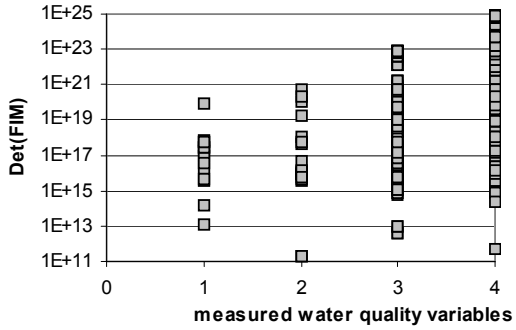


Figure V.17: Det(FIM) as a function of the measured water quality variables. (1= DO; 2 = DO + NO_3; 3 = DO + NO_3 + BOD; 4 = DO + NO_3 + BOD + NH_4)

As can be seen in figure V.20, the highest Det(FIM) that can be obtained without measuring BOD is 1E+21 and including BOD measurement is 1E+25. Here again it has to be checked what the consequence is for the uncertainty on the simulated DO concentrations. Further a cost analysis is needed, as for some variables, it is likely that measuring at high frequency during the whole year is more expensive than measuring during three months at a low frequency.

The usefulness of this method resides in its ability to evaluate sub-optimal sampling strategies, whereby strategies are evaluated in view of the limitations of costs and other practical

considerations. This can be of great importance for some costly and time-consuming analysis of samples, e.g. for pesticide modelling and monitoring (Holvoet et al., 2006) . By extending the OED method with a procedure for the definition of the modelling uncertainty, it thus becomes possible to define the optimal sampling strategy to obtain a given modelling accuracy.

Further extensions of the OED can be done according to the aims or possibilities of the experimental design. A first extension can be the addition of more or other parameters of sampling layout. Those can be other measurable variables such as suspended solids and water temperature or additional sampling locations. One may also try to find out if a distinction has to be made between the different variables in relation to their sampling frequency and period. As such, sampling schemes can become very efficient and advanced.

4.4. Conclusions and recommendations

It has been shown that OED methods can be used for an iterative, sequential design of a strategy for measuring water quality variables on a river, in view of the calibration of water quality models. In a first stage a relatively extensive set of measurements is needed to set up a model for the river. Using the model, the OED method enables the definition of efficient measurements strategies, to find better model parameter estimates and reduce the uncertainty in those estimates. In subsequent stages, the measurement strategy can be updated in an iterative way.

For the river Dender, it was shown that the method is able to define the most logical solution to the problems, if a maximal accuracy is aimed at, the optimal sampling strategy will be the one with the highest number of samples and the highest sampling frequency, at the maximal number of locations and whereby a maximal number of variables is measured. But this method is also able to find sub-optimal sampling strategies with acceptable accuracy. Also costs and practical matters can be considered.

The method can easily be extended with even more parameters of sampling layout to finally come to very efficient sampling layouts. Another extension can be the use different evaluation criteria for the OED because other criteria than the maximization of the det(FIM) can be more suitable for the problem under consideration. Also a method pareto optimisation for optimising for more than one evaluation criterium at the same time can be applied and is developed by De Pauw (2005) . For example, the reliability of the parameter estimates can be less important than the final uncertainty on critical values of certain parameters. So it is evident that in such cases other schemes for the OED can be applied (or a combination of different criteria). In those cases the optimisation is done on for instance the minimisation of the uncertainty of the dissolved oxygen concentrations below 5mg/l.

This research is not only applicable in river water quality models. Other fields of application are e.g. rainfall-runoff modelling for the detection of optimal gauge locations or groundwater modelling.

5. The evaluation of uncertainty propagation into river water quality predictions to guide future monitoring campaigns

5.1. Introduction

In the field of environmental modelling and assessment, uncertainty analysis (UA) is a necessary tool to provide, next to the simulation results, also a quantitative expression of the reliability of those results. Next to the expression of uncertainty bounds on the results, uncertainty studies have mainly been used to provide insight in the parameter uncertainty. However, uncertainty analysis can also be a means to prioritise uncertainties and focus research efforts on the most problematic points of a model. As such, it helps to prepare future measurement campaigns and to guide policy decisions.

In this study, the use of an UA as an evaluation tool is assumed to be applied on an already calibrated model that can simulate measured data well but with an unacceptably high uncertainty, especially in view of predicting water quality. We only consider parameter and input uncertainty that can be minimised by gathering additional data. Model structure uncertainty and mathematical uncertainty are not taken into consideration. That way the presented uncertainty bounds around the results will not contain 95% of the The aim of this research is to show how UA can be used to guide future monitoring campaigns to make model results more reliable by minimising the parameter and input data uncertainty of the model.

5.2. Methodology

To reduce the overall uncertainty on the model results for a certain variable the following steps are proposed.

1. Identify which sources contribute mainly to the overall uncertainty on the model results
2. Estimate or calculate the uncertainty related to those main contributors
3. Propagate the uncertainty through the model
4. Analyse the model results to set up a monitoring campaign
5. Perform the measurements
6. Recalibrate the model with new inputs
7. Repeat step 3 till 6 until satisfying results are obtained

For every step of this process different techniques exist that can be chosen among according to the experience of the modeller. In the practical example the methods used are described.

Step 1: Identification of the main uncertainty contributors, uncertainty characterisation

his step is mainly carried out via a global or local sensitivity analysis. Because it is assumed that an already calibrated model is available, a local sensitivity analysis should be able to identify the most important parameters and data of the model. Indeed, local analysis is done around an a priori assumed value of the parameter. For a local sensitivity analysis the following methods exist: finite difference method, (b) the direct differential method, (c) the Green's function method, (d) the polynomial approximation method and (e) automatic differentiation. Global sensitivity analysis can be done in various ways: with a Monte Carlo approach, first order or second order reliability methods and model emulators. An overview of available sensitivity techniques with advantages and disadvantages is given in the chapter "Sensitivity Analysis" of the literature study.

Step 2: Estimation or calculation of uncertainty

Parameter uncertainty can be calculated from the covariance matrix. The latter is obtained during the local sensitivity analysis or the calibration process if the optimisation methods is derivative based so that the covariance matrix is calculated during the optimisation (Beck, 1987).

If no direct calculations are possible, e.g. for the uncertainty on the inputs, the uncertainties need to be estimated. One can divide the parameters and data in uncertainty classes (accurately known, very poorly known and an intermediate class) and assign a percentage uncertainty to them. A similar approach was adopted by Reichert and Vanrolleghem (2001). Other options are expert knowledge, questionnaires or statistical calculation of uncertainties with historic data.

Step 3: *Propagate the uncertainty through the model*

For this step Monte Carlo methods can be used, in which the input data or parameters are sampled between the uncertainty bounds that are detected in the previous step. If correlation between some of the parameters and inputs exist and are known, these correlations should be considered in the analysis. Another option is to apply linear error propagation. The advantage of the latter is computational efficiency. However, if there are significant non-linearities within the uncertainty range in the model, the results will be inaccurate. Monte Carlo simulation is a simple technique but requires a large number of model runs, which is computationally very demanding. Less runs with the same results as 'ad random sampling' are needed with 'the Latin Hypercube sampling' (McKay et al., 1979). Many methods for uncertainty analysis are presented in detail in the chapter Literature review, Uncertainty Analysis.

Step 4: Analyse the model results to set up a future measurement campaign

Two different approaches can be used according to the aim for which the additional measurements are collected. If it is the aim to reduce parameter uncertainty, an automated optimal experimental design method that is explained in Vandenberghe et al (2002) can be used. It is based on maximisation of the determinant of the Fisher Information Matrix, which corresponds to the minimisation of the variance of the parameters. This method requires a lot of simulation runs but is totally automated and as such requires no additional information or knowledge from the modeller. The complete method and procedure is explained in the chapter "Optimal experimental design".

However, when only focussing on the input data uncertainty that leads to output uncertainty expert knowledge is required. It is then the aim to find a link between periods of high/low uncertainty and external circumstances (rain, discharge points, seasons, solar radiation…) This information is then used to make decisions about location, period, frequency… of future measurements.

Step 5: Perform the measurements

At this stage it is essential to ensure a good quality control on the measurements to minimise measurement errors. Important is also to carefully adding information concerning exact hour, location and depth of the sample. This information is sometimes crucial to the modeller like in situations were the water quality variable changes very fast or in rivers were the water is stagnant and there is a depth gradient for the variable.

Step 6: Recalibrate the model with new inputs

An important issue here is that the calibration method must be able to find the optimum. First, a choice is made between manual and automated methods. The former may depend on the experience of the modeller. Automated methods can differ in search method: global search methods scan the whole parameter space and are as such able to find the global optimum, but do not provide uncertainty measures. Local search methods start on a certain point in parameter space and end when they find an optimum. However, there is no assurance that this is the global optimum, so it is best to start in the neighbourhood of the optimum for those methods. With these methods covariance matrices for the optimum parameters are often calculated because they are derivative based.

Step 7: Repeat step 3 till 6 until satisfying results are obtained

The stop criterion for this 'trial and error method' is dictated by an 'a priori' desired reliability of the model results. In practice however, personnel, time and equipment matters will be the limiting factor and will indicate when this process stops.

5.3. Results and discussion

The seven steps are now demonstrated on a case study: simulations of the water quality of the river Dender, Flanders, Belgium for 1994 with a QUAL2E based model in ESWAT. The evaluation of the uncertainty on model results is performed for nitrate in the river water.

Step 1: Identification of the main uncertainty contributors

We evaluate the sensitivity of the model on the following result: the time that NO_3-N is higher than 3 mg/l at Denderbelle, near the mouth of the river in 1994. For nitrate there are almost no limits in regulation. In Belgium the sum of NO_2-N, NO_3-N needs to stay below 10 mg/l for basic water quality. The choice for this 3 mg/l is based on the fact that it is seen from simulations that periods with problem of eutrophication are linked to periods of high nitrate, here higher than 3 mg/l. A sensitivity analysis for all input data and parameters in the ESWAT model is too complex for the program we use: UNCSAM (Janssen et al., 1992), described in the chapter "Materials and methods". This program cannot handle more than 50 parameters at the time. So we split the problem in different parts: 1) sensitivity to model parameters 2) sensitivity to point pollution input and 3) sensitivity to diffuse pollution input. Each sub problem gives a ranking of the parameters by using the Standardised Regression Coefficient (SRC).

$\mathrm{SRC_i} = \dfrac{\Delta y / S_y}{\Delta x_i / S_{x_i}}$ (1) with $\Delta y / \Delta x_i$ = change in output due to a change in an input factor and S_y, S_{x_i} the standard deviation of respectively the output and the input. The input standard deviation S_{x_i} is specified and chosen by the user and presents typically the possible literature values.

This technique for sensitivity analysis is better explained in the chapter "Sensitivity analysis". For each of the subproblems the parameters or data that contribute significantly to the output (5 % level) are then taken together in one overall sensitivity analysis to compare the contribution of the different outputs. The column with the SRC as a result of that analysis is indicated in table V.19 with "combined parameter- input".

Table V.19: Results of the sensitivity analysis for the model output "hours NO3 >3mg/l" at Denderbelle, 1994. (pa16 = Amount of fertilisation on pasture in subbasin 16; fa4 = Amount of fertilisation on farming land in subbasin 4; gropa = growth date of pasture; plfa = Plant date on farming land; co5 = Amount of fertilisation on corn in subbasin 5; co15 = Amount of fertilisation on corn in subbasin 15; pa12 = Amount of fertilisation on pasture in subbasin 12; co11 = Amount of fertilisation on corn in subbasin 11; ai5 = O_2 uptake per unit of NH_3 oxidation; rk5 = denitrification rate; rk2 = oxygen reaeration rate; ai6 = O_2 uptake per unit of HNO_2 oxidation; bc2 = rate NO_2 to NO_3; rk3 = rate of loss of bod due to settling; ai4 = O_2 uptake per unit of algae respiration; Rs5 = organic phophorous settling rate)

Diffuse pollution input	SRC	Point pollution input	SRC	parameter	SRC	Combined Parameter-input	SRC
Pa16	-0.30	BOD point 6	-0.61	Ai5	-0.7	Ai5	-0.51
Fa4	0.23	NO3 point 7	0.42	Rk5	-0.34	Ai6	-0.50
gropa	-0.18	BOD point 5	-0.38	Rk2	0.32	Rk5	-0.40
plfa	0.17	BOD point 8	-0.24	Ai6	-0.21	Bc2	0.38
Co5	-0.17	NH3 point 1	0.23	Bc2	-0.2	Ai4	-0.31
Co15	-0.16	BOD point 3	-0.23	Rk3	0.17	Rk2	0.12
Pa12	0.16	BOD point 7	-0.22	Ai4	0.12	plfa	-0.08
Co11	0.15	BOD point 1	-0.14	Rs5	-0.09	BOD point 6	-0.07
		NO3 point 5	0.11			BOD point 1	-0.07
		BOD point 4	-0.09			Pa16	0.07
		NH3 point 2	0.09				
		BOD point 2	-0.08				
		NH3 point 3	0.06				

SA for the parameters

For the parameters, the sampling for the sensitivity analysis was based on own experience with the model and literature ranges. The results here are the results taken from the SA on the parameters of the QUAL2E water quality model for the Dender river as given in section 2 of this chapter.

SA for the point pollution input

Point pollution towards the Dender river is due to loads coming from households via the WWTP, from industry and from households discharging immediately into the river without treatment. These kinds of input data are provided by the Flemish Environmental Institute (Vlaamse Milieu Maatschappij, VMM). For the ranges of uncertainty of the point pollution inputs we sampled uniform between halve and double the values, as we decided that those inputs belong to the uncertainty class 'poorly known' (Reichert and Vanrolleghem, 2001). Indeed, the loads coming from point pollution were only available as yearly averages instead of varying values per day or even hourly (e.g. loads differ between day and night, week days and week-ends and official holiday periods). The inputs that were varied were discharge of the loads and the loads of NO_3-N, NH_3-N, BOD, DO and Dissolved P on 11 different points. (For the location of those points see the chapter of "Case studies").

SA for the diffuse pollution input

A previous study in SWIM (Soil and Water Integrated Model) for the same kind of nitrogen leaching model as available in ESWAT from arable land in large river basins (Krysanova and Haberlandt, 2001) showed that the relative importance of natural and antropogenic factors affecting nitrogen leaching in the Saale river basin was as follows: (1) soil, (2) climate (3)

fertilisation rate and (4) crop rotation. Reducing the uncertainty on inputs for soil and climate depends on better equipment to measure the different variables and proper use of sophisticated mathematical techniques to interpolate for places that are not measured. A lot of studies on that subject already exist (Lacasse et al., 2007; Sevruk 1986). Reducing the input uncertainty related to fertilisation rate was not studied often before. In Flanders, new legislation concerning fertilisation application was made in the late nineties. Campaigns to list the fertiliser use were then started and it is known that still a large amount of information is wrong or missing. A lot of effort is still needed to complete the information. The evaluation and quantification of the impacts of land management practices on nitrogen wash-off to surface water is therefore very important.

The focus for diffuse pollution input related uncertainty is here on fertilisation rate and time of fertiliser application on the most important crops. For the application of fertiliser for the different land uses three application dates were assumed; 1st of March, 1st of April and 1st of May. Also operations such as planting and harvesting dates can be defined. Day and months were used to specify the planting and harvesting dates. Of course, those dates depend on climate, crop and farmer. So assumptions had to be made concerning those dates.

Data on fertiliser and manure use are provided by The Flemish Institute for Land Use (VLM). They provided data on the nutrient use and production for each municipality in Flanders. In ESWAT, one has to specify for each subbasin the total amount of fertiliser and the detailed composition of the fertiliser. Some conversions of the supplied data had to be made so that they could be used in ESWAT. It consisted of recalculations of the application rates for each municipality to application rates per subbasin (Smets, 1999). Further the assumption was made that the same amount of fertiliser is applied on all crops. This is clearly different from practice, but at this stage, insufficient details are available to specify this more realistically. The fractions of mineral N, organic N, and NH_3-N in the fertilisers are considered to be known and fixed. Hence, we only analyse the total amount of fertiliser used (see table V.20). As there are a lot of differences in management practices between the different farmers and the time of planting and harvesting is different from year to year, the plant date and harvest date for the crops are also considered in the analysis. For a global sensitivity analysis we take the uniform distribution with standard deviation S_{x_i}. The ranges of the uniform distributions are given in table V.21. We assumed no correlation. To supply the information on those ranges a few farmers living in Maarkedal (situated in the Dender basin) were interviewed about their land management practices.

Table V.20: Composition of the manure as input in SWAT

Chemical	Percentage of total fertiliser (100*kg/kg)
HNO_3	28.5%
Mineral P	7.5%
Organic N	28.0%
Organic P	7.5%
Ammonia	28.5%

Table V.21: Ranges for global sensitivity analysis of management practice inputs for nitrogen

Input	Uncertainty
Plant date for the crops	+/- 1 month
Harvest date of the crops	+/- 1 month
Amount of fertiliser applied per subbasin and per crop (kg/ha)	+/- 25%

SA on parameters and inputs

The global sensitivity of the parameters and the inputs shows that some parameters, O_2 uptake per unit of NH_3 oxidation, O_2 uptake per unit of HNO_2 oxidation, denitrification rate, rate NO_2 to NO_3, O_2 uptake per unit of algae respiration and the reaeration rate are most influencing followed by the input data, plant date on farming land, amount of fertilisation on pasture in subbasin 12 and bod loads from point 1 and 6. This could not be seen from the separate analyses of inputs and parameters. So, different values of the parameters can give different model results while those results are not much influenced by the input data for this river. This again shows the importance of a well-calibrated model.

Step 2: Estimation or calculation of uncertainty

For both the point and diffuse pollution input the same uncertainties were taken as the sampling range used for the sensitivity analysis because we obtained no new information between the SA and the UA. For the uncertainty on the parameters a recalibration with the most influencing parameters with a derivative based method, in that way that uncertainty ranges can be calculated with the covariance matrix, is best, but is not done here. Uncertainties of 50 % were assigned to each of the parameters.

Step 3: Propagation of the uncertainty through the model

Here again the uncertainties are split: parameter uncertainty, diffuse pollution uncertainty and point pollution uncertainty.

Then for each an uncertainty analysis was performed in which all of the uncertainty sources are varied at the same time to see the effects of the uncertainty on parameters and inputs. For this analysis we calculate the uncertainty bands (i.e. the 5% and 95% percentiles) for the results of the time series.

Figure V.18 shows the propagation in time of the parameter uncertainty for Nitrate in the river at Denderbelle, 1994. Output uncertainty becomes high at certain moments due to parameter uncertainty.

Figure V.19 and V.20 show the time series of nitrate in the river water at Denderbelle, situated near the mouth, with the 5% and 95% uncertainty bounds with resp. uncertainty on point input and diffuse pollution input.

Step 4: Analyse the model results to set up a future measurement campaign

To cope with the parameter uncertainty optimal experimental design based on the Fisher Information Matrix should be done (as explained in the "optimal experimental design chapter) as this is the most objective method to find important measurement places to better estimate the parameters. This design of new experiments is not presented here as we focus on the uncertainty analysis and what information can be revealed from it.

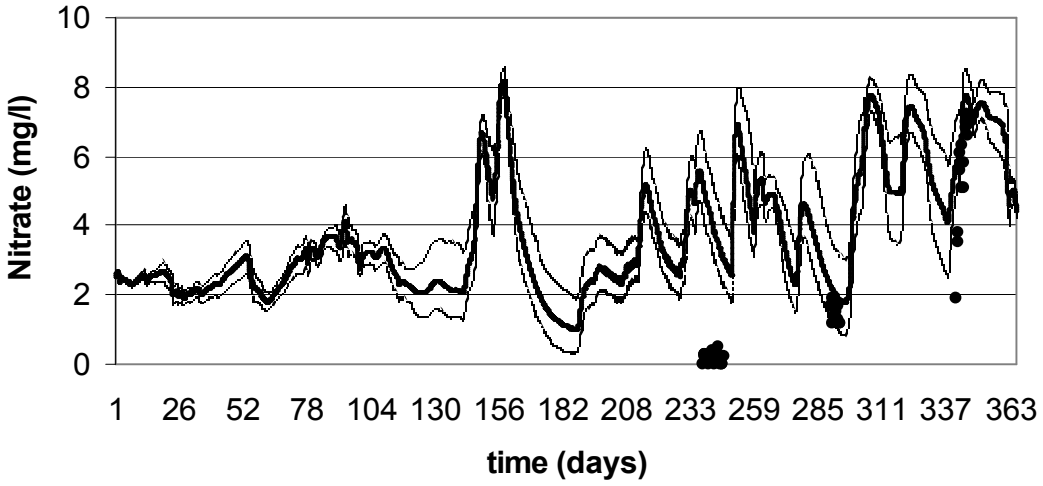


Figure V.18: Measurements (symbols) and simulation of nitrate (line) with confidence intervals (dashed line) related to parameter uncertainty at Denderbelle, 1994.

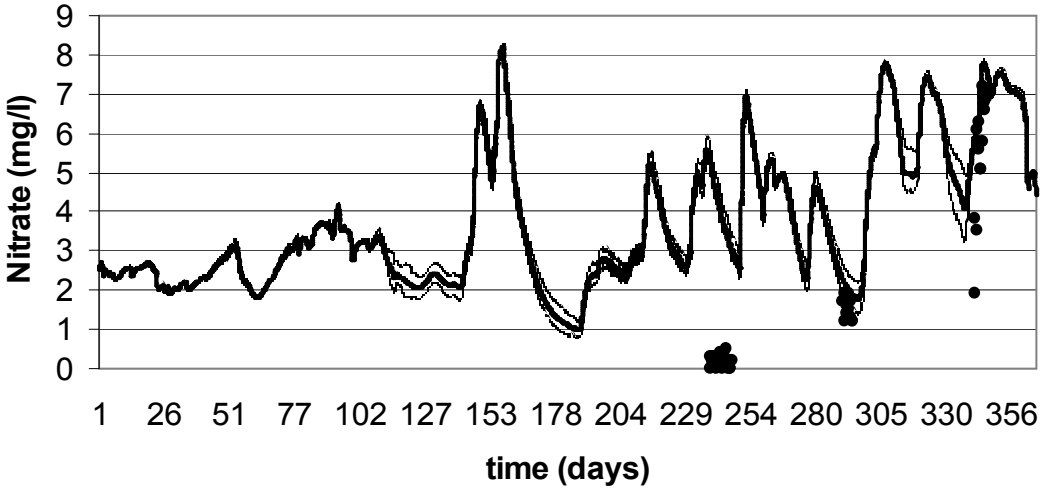


Figure V.19: Measurements (symbols) and simulation of nitrate (line) with confidence intervals (dashed line) related to point pollution input uncertainty at Denderbelle, 1994.

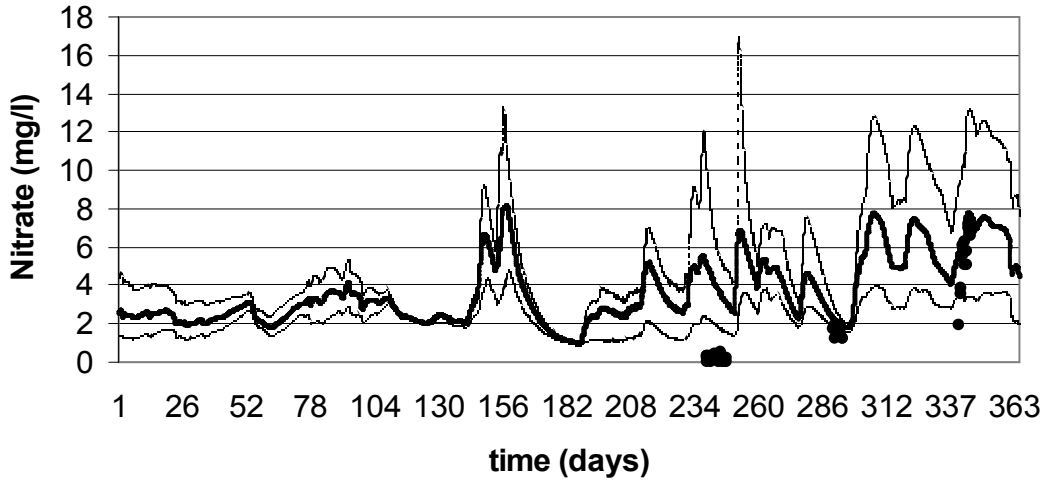


Figure V.20: Measurements (symbols) and simulation of nitrate (line) with confidence intervals (dashed line) related to diffuse pollution input uncertainty at Denderbelle, 1994.

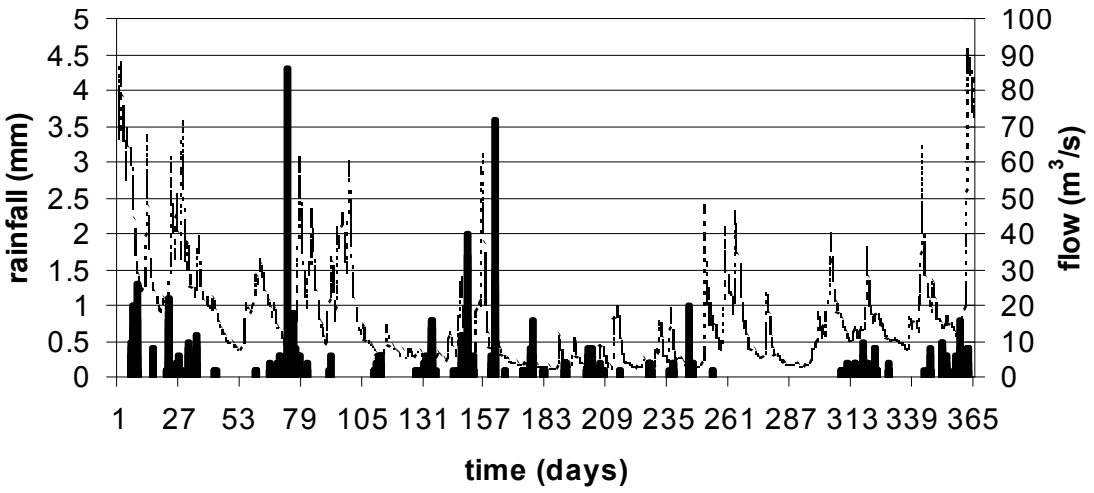


Figure V.21: Rainfall (full) and Flow (dashed) in 1994 at Denderbelle.

Linking the obtained results in step 3 to the external circumstances, rain and flow (figure V.21), we can see that diffuse pollution inputs are important during periods with high rainfall and high flows. During dry weather flows, the input uncertainty of the loads is also propagated. Hence this UA learns that we can obtain a better calibration for the diffuse pollution part of the model with data that are taken during wet periods with high flows, because the model output nitrate is more sensitive towards inputs of diffuse pollution in those periods. If one focuses on calibrating the in-stream behaviour and point pollution then measurements during dry periods are needed, as in such conditions the model is not sensitive towards input of diffuse pollution.

Further it is seen on figure V.20 that the 95 % bounds show much higher peaks than the mean concentrations time series. This means that some peak values of nitrate in the river water at Denderbelle may not be predicted properly due to an underestimation of the amount of fertiliser used. Those peaks (eg. day 156 and 260) are significantly higher than the levels of nitrate for basic water quality.

It is also of interest to know how the uncertainty is propagated from one place to the other. This analysis was done for the uncertainty propagation due to diffuse pollution inputs. The amount of time that NO_3-N was higher than 3 mg/l was calculated. This was done for the time series of the mean, the 5 % - bound and the 95% - bound (figure V.22). The uncertainty bounds become larger when approaching the mouth due to the summation of the uncertainties on all diffuse pollution inputs that enter the river. However, it is interesting to see that with the available quality of input data no conclusions can be drawn concerning the question whether the diffuse pollution causes more hours nitrate exceedance downstream than upstream. The uncertainty bounds on the model results are too wide, more accurate data are needed to draw good conclusions from the model results. This would mean that the model results show no indication that there is a difference in pollution state between the different

locations in the Dender. However, we can assume that most of the influencing uncertainties related to diffuse pollution work in the same direction, this is especially the case for the amount of fertiliser applied on the fields, which also seemed to be the most influential input in the sensitivity analysis so comparing one place to the other, we can assume that there is a significant higher amount of NO_3 critical value exceedance downstream than upstream.

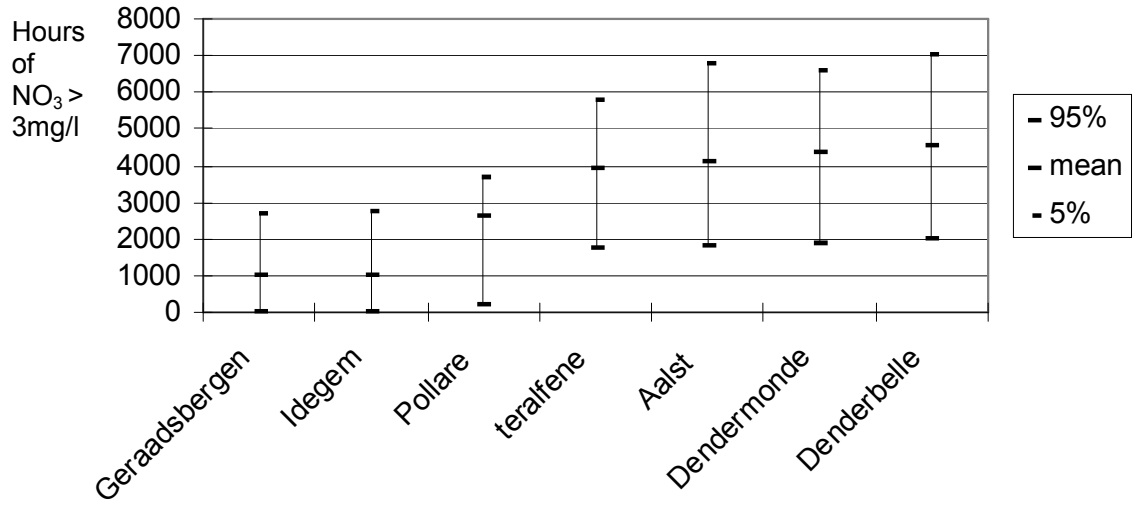


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Figure V.22: Uncertainty propagation from upstream to the mouth of the Dender in 1994 related to diffuse pollution input uncertainty.

Step 5: Perform the measurements
Step 6: Recalibrate the model with new inputs
Step 7: Repeat step 3 till 6 until satisfying results are obtained

Those three steps are only relevant for future measurement campaigns. However, no additional measurements were done until now.

5.4. Conclusions

The results of uncertainty analysis were evaluated to guide future monitoring campaigns. Diffuse and point pollution inputs are considered separately and give information of the model sensitivity to the inputs. Measurements during dry periods can be used to better calibrate the model for point source pollution because the inputs of diffuse pollution are not important then. On the other hand, periods with rainfall and high flows are needed for the calibration of the model with diffuse pollution because the model output nitrate is then very sensitive towards the inputs related to farmer's practices.

When comparing the influence of the uncertainty of the diffuse pollution inputs, the uncertainty bounds appeared to be too wide to draw reliable conclusions from the model

results. So, it showed the importance of accurate measurements and input data if the model results serve for decision support.

It is obvious from the comparison between the global sensitivity analysis for the subgroups and for all most influencing parameters together that the parameters are most important. This shows that it is best to start with a good calibration of your model and then focus on more accurate input data.

Too often a model is calibrated with only one comprehensive measurement campaign. This is mostly not the most efficient way. When e.g. only measurements during dry periods are made, the model cannot be well calibrated for the diffuse pollution part. So it is better to perform two separate smaller measurement campaigns with the first one being 'exploring', while the second campaign is guided by previous analysis of the model results. The combination of the two monitoring campaigns can assure that at least some measurements are performed at 'the right moment', making the calibration process easier and more reliable.

It is necessary to combine all previous uncertainty analysis to evaluate the total uncertainty on the model results and to compare them with the measurements. In this way, model structure uncertainty can also be quantified (Willems and Berlamont, 2002).

In this research the second monitoring campaign is missing and could have shown the possibilities of the proposed succession of steps.

6. Sensitivity analysis to define the most sensitive parameter subset for auto-calibration of a river water quality model

6.1. Introduction

A mathematical model of a system under consideration has to be calibrated in such a way that the model reproduces the measurements and that predictions made with the model are representing reality, which is checked in a validation. In hydrology, the models used vary between simple black box models and complicated, distributed physical models. There is a trend to make more use of the complicated models because next to the generation of predictions of water flows and quality they help in understanding the system. Nowadays, the computational burden of such complicated model is not an issue anymore, but the main problem is the calibration of the large amount of parameters. During calibration, parameter values are adjusted between boundaries until the model outcomes fit the measurements best.

For models with many parameters a trial and error calibration is very tedious, if not impossible. Automatic calibration procedures also pose problems, mainly due to the high correlation that often exists between the many parameters. In this chapter a sensitivity analysis procedure is proposed to reduce the number of parameters for calibration.

6.2. Methodology

The sensitivity analysis presented here focuses on the parameters of the in-stream QUAL2E based water quality model only, which includes 33 parameters. The method is a global one based on regression analysis whereby the sampling is done with Latin Hypercube sampling (McKay et al., 1979) (see literature study on sensitivity analysis). The table XX in section 2 of this chapter gives all the water quality parameters with nominal default values and boundaries. Those values come from literature, the SWAT manual and from own experience with the model.

The focus in this sensitivity analysis is on critical outputs for dissolved oxygen (DO), nitrate (NO_3) and chlorofyl a (Chl a). The critical outputs are taken as the time that the oxygen concentration in the water drops below 5 mg/l, the time that the Chl a content of the water goes above 11µg/l and NO_3 above 3mg/l. Those variables are chosen as they are most problematic for the river Dender. Dissolved oxygen becomes very low during periods of low flow, nitrates are linked to eutrophication periods and in the whole summer period algae growth is high. Other outputs could be considered like the sensitivity of the nitrate concentration averaged over the whole period or the sensitivity of the objective function for the ammonium or dissolved oxygen. This objective function is the square of the sum of the squared differences between model results and measurements. The parameters that are most important for this objective function, will be the parameters that are able to minimise this function best. The choice depends on the problem at hand and the answers that one wants to get out of the SA.

The critical value for dissolved oxygen, 5mg/l, is chosen because it is set as the basic water quality standard in Belgium. The Chl a and NO_3 limits are not defined in legislation, but values of 11µg/l and 3mg/l are attained in the investigated river during summer months with at the same time low DO concentrations which is an indication of eutrophication, so those limits can be considered as indicative for water quality problems.

Various statistical methods can be employed to quantify the sensitivity and uncertainty contribution of the sources to the model outputs. In this section the same method as explained in section 2 of this chapter is applied which is based on linear regression analysis and correlation analysis between the inputs and the simulated model outputs and whereby the parameters with significant correlation are determined to be important.

6.3. Results and discussion

6.3.1. Sensitivity analysis

The sensitivity analysis was carried out, based on simulations for the whole year of 1994 and on the water quality variables at the mouth of the river at Denderbelle.

The largest VIF value amounted to 1.68 for all the cases. Values for R^2_{adj} were 0.92, 0.95 and 0.87 for the regression between the parameters and the amount of time with too low oxygen, high algae and high nitrate concentration in the river water.

In tables V.22 and V.23 the result of the sensitivity analysis is shown. The parameters shown are those that are significant in the regression analysis on a 5 % level. It is obvious that different sets of important parameters are obtained when other evaluation criteria are used. If one wants to calibrate the Dender model for all the variables, DO, Chl a and NO_3, all parameters in tables V.22 and V.23 need to be considered in the calibration procedure, which makes in total 20 parameters. For an automatic calibration this can already be a too large number of parameters. Because of dependencies between the parameters the automatic calibration will not find a unique solution and the number of parameters need to become smaller. So it is recommended to first start with formulating the aim of the model and then to perform a SA in function of the aims. It is however always a good procedure to fix the aim of the model before choosing a model and calibrating it.

Table V.22: The normalized regression coefficient and the rank of importance in the sensitivity analysis for time of DO < 5 mg/l and time of Chl a > 11 µg/l

DO < 5 mg/l			Chl a > 11 µg/l		
Parameter	SRC	Rank	Parameter	SRC	Rank
ai5	0.521	1	rhoq	-0.626	1
Bc1	0.354	2	umax	0.577	2
ai4	0.279	3	kp	-0.255	3
rk1	0.268	4	rk6	-0.250	4
ai3	-0.240	5	Λ1	0.099	5
rhoq	0.159	6	ai5	0.069	6
ai6	0.159	7	rk4	0.065	7
umax	-0.159	8	bc2	0.051	8
rk3	-0.149	9	ai1	0.049	9
rk2	0.138	10			

Table V.23: The normalized regression coefficient and the rank of importance in the sensitivity analysis for time of NO_3-N>3 mg/l (hourly time step)

	NO_3-N >3 mg/l	
Parameter	SRC	Rank
ai5	-0.7	1
rk5	-0.34	2
rk2	0.32	3
ai6	-0.21	4
bc2	-0.2	5
rk3	0.17	6
ai4	0.12	7
rs5	-0.09	8

6.3.2. Calibration

It is chosen here to calibrate the model with the set of important parameters for time of DO<5 mg/l. This calibration is done with the PEST software. The methodology of this calibration is described in the chapter “Materials and Methods”. A calibration for the flow was done in the study by van griensven and Bauwens (2005). The flow in 1994 is given in figure V.23 and the results of the calibration are shown in figures V.24 and V.25. and V.26. The following parameter values (explanation in table V.1) were obtained during the calibration (table V.24).

Table V.24: The parameter values after calibration of the model

Parameter (table V.1)	Value after calibration	Unit
ai5	3.71	mg O_2/mg NH_3-N
bc1	0.1	day^{-1}
ai4	2.0	mg O_2/mg algae
rk1	0.064	l/day
ai3	2.3	mg O_2/mg algae
rhoq	0.2	l/day
ai6	1.0	mg O_2/mg HNO_2-N
umax	2.2	l/day
rk3	3.0	m/day
rk2	1.09	m/day

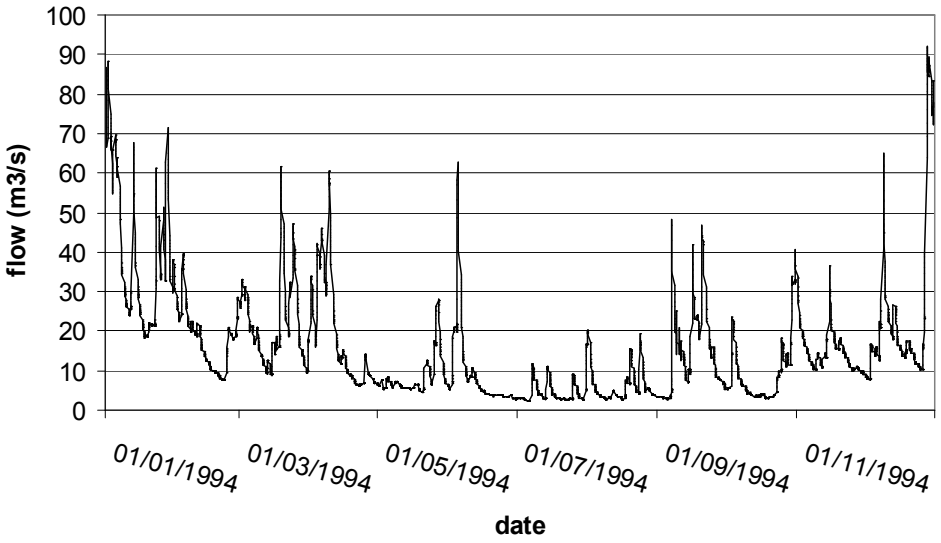


Figure V.23: Model results for flow, Denderbelle, 1994

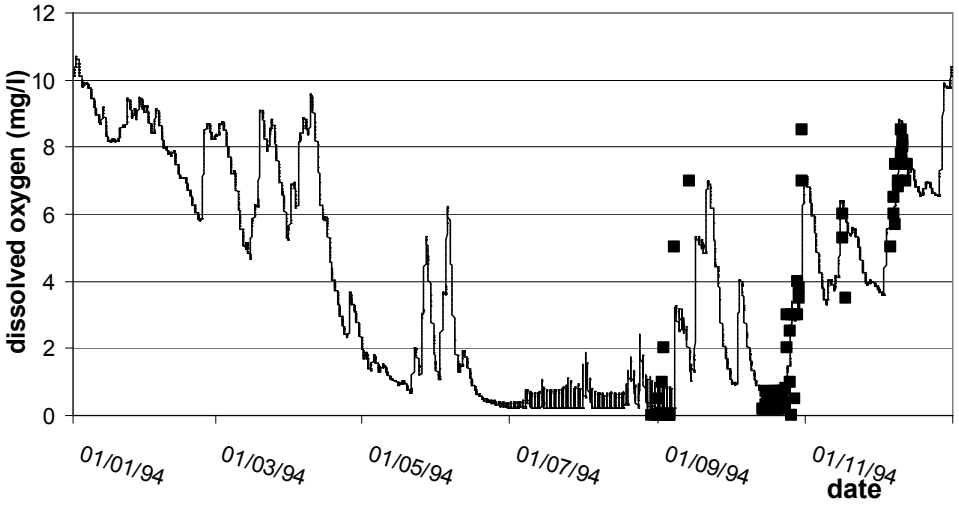


Figure V.24: Model results (line) and measurements (symbols) for DO, Denderbelle, 1994

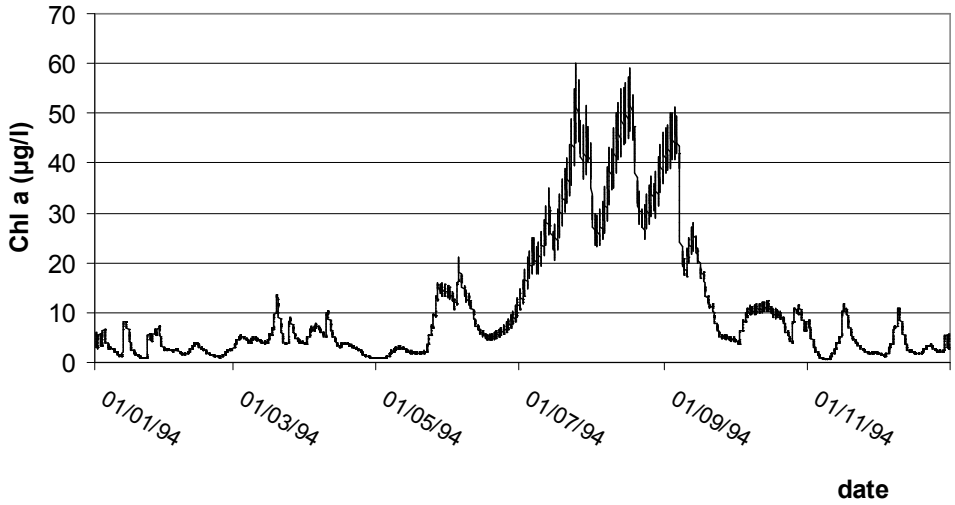


Figure V.25: Model results for Chl a, Denderbelle, 1994

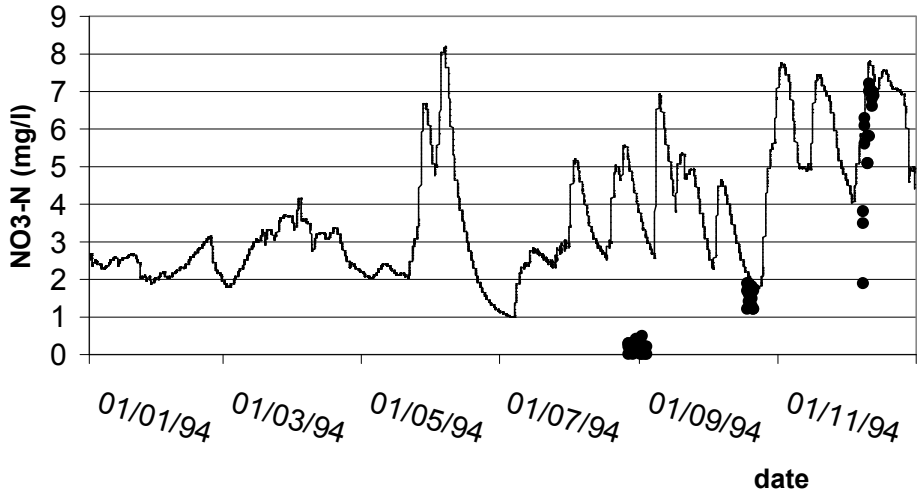


Figure V.26: Model results (line) and measurements (symbols) for NO_3-N, Denderbelle, 1994

6.3.3. Validation

The validation of this model was done for the year 2000. The measurements for 1994 were obtained in dedicated measurement campaigns but for 2000 the only measurements available were those from the Flemish Environmental Agency (VMM). On several places along the Dender the VMM measures the physico-chemical parameters around 2 times per month. Also, because measurements at Denderbelle were not available for the year 2000, the validation is done with measurements at Pollare, upstream of Denderbelle. The results for DO were very good and no additional calibration was needed. However the fit between model results and measurements for nitrates were very bad and additional calibration was then done with the parameters ai5 and rk5 (O_2 uptake per unit of NH_3 oxidation and denitrification rate resp.). Note that the results for 1994 for NO_3 after automatic calibration were overestimated but then deemed acceptable.

The results for 2000, before and after recalibration with the VMM data, are shown in figures , V.27, V.28 V.29, V30.

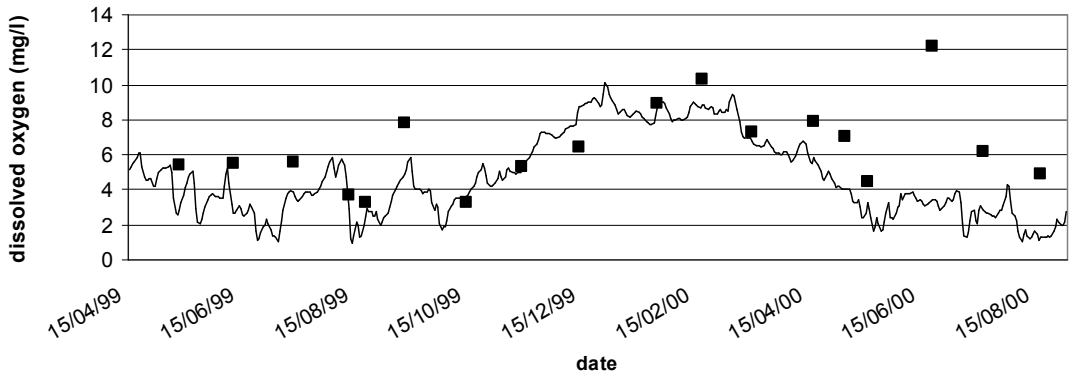


Figure V.27: Model results (line) and measurements (symbols) for DO before recalibration, Pollare, 2000

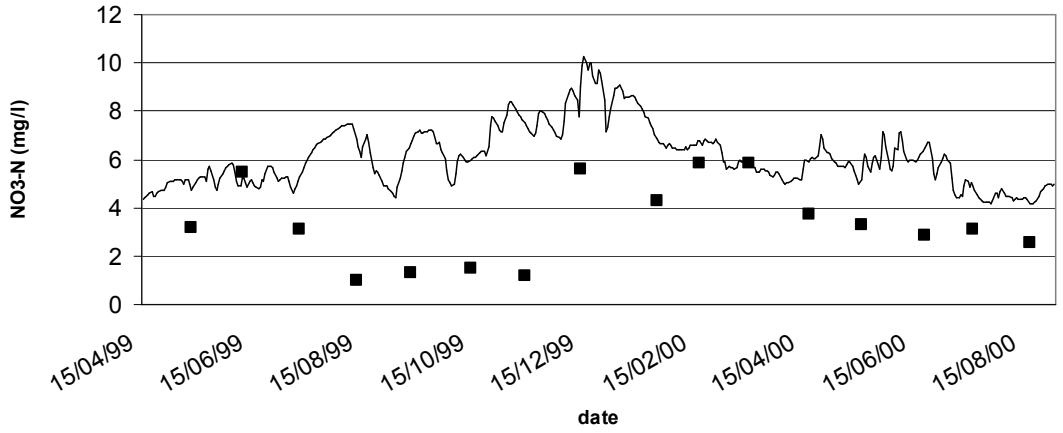


Figure V.28: Model results (line) and measurements (symbols) for NO_3-N before recalibration, Pollare, 2000

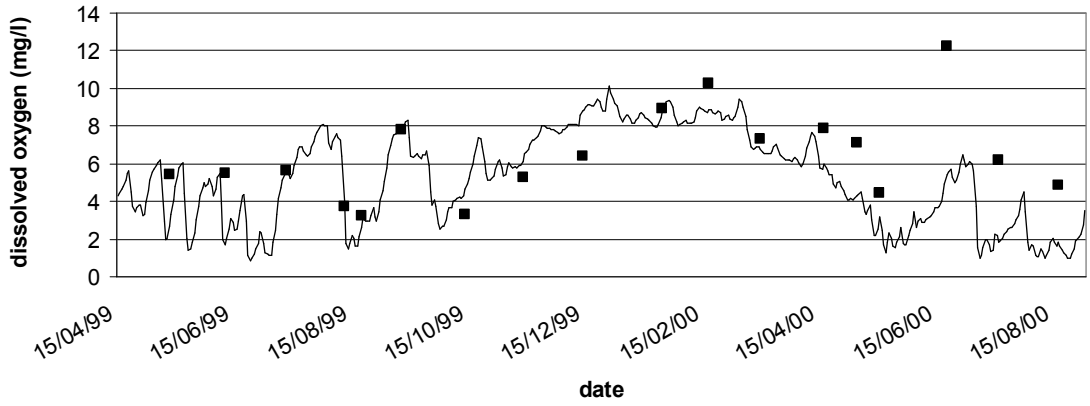


Figure V.29: Model results (line) and measurements (symbols) for DO after recalibration, Pollare, 2000

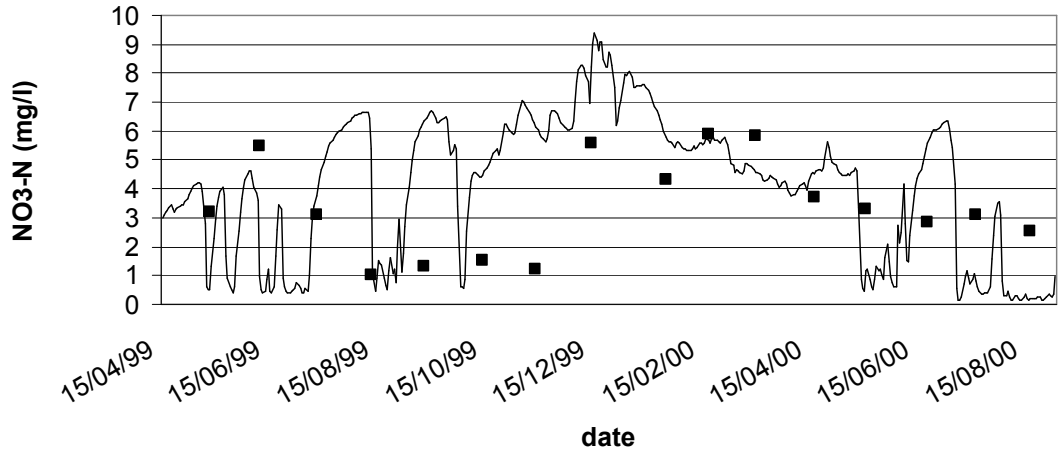


Figure IV.30: Model results (line) and measurements (symbols) for NO_3-N after recalibration, Pollare, 2000

6.4. Conclusions

A sensitivity analysis for the QUAL2E based river water quality model of the Dender river, implemented in ESWAT was performed to reduce the number of parameters to calibrate. The SA revealed that only around 10 parameters need to be changed during calibration to obtain good fits between simulated and measured values, this for a particular aim, in this case being to have good simulation results for the periods with lower DO concentrations.

Different parameters are ranked as most sensitive when different criteria are used. This means that the modeller has to decide before calibration what the aim of his model will be. If one

wants to have a good degree of reliability of the model for the low oxygen values, it is best to look at sensitivity of parameters towards low oxygen outcomes. It is seen in the validation that indeed the DO results are fitting well the measurements when the calibration was performed with the most sensitive parameters for the amount of time that DO goes below a critical value. However, an additional calibration was needed to get good results for the nitrate simulations of the validation period.

7. Importance of the selection of model parameter subsets

7.1. Introduction

Many river water quality models are available ranging from simple, conceptual models to more complex, physically based models (Rauch et al., 1998) that are preferred more and more because of their ability to make extrapolations. However, due to the complexity of such models many parameters need to be determined (= calibrated) before the model describes the system well.

Fortunately most modellers have become aware of the fact that the calibration process does not normally result in a unique parameter set because parameters are often highly correlated with each other. The question that automatically rises is "how would the model predictions change if another subset of parameters were used in the calibration of the model?" If there exists differences between the model results after calibration with different subsets of parameters, it is interesting where the differences are situated and what the influence is on some variables that are subject to legislation or are critical to biological life.

The aim of this research is to detect the variation of critical water quality variables after calibration of a complex water quality model where different subsets of parameters are changed while the other parameters are fixed, typically to literature values. It shows how far parameters can compensate for each other. Here, the modified QUAL2E model (van Griensven and Bauwens, 2002) with an application on the river Dender in Belgium is used.

7.2. Methodology

The order of steps to obtain a calibrated model is: sensitivity analysis, calibration with the most sensitive parameters and afterwards uncertainty analysis and validation. The objective of sensitivity analysis of model output can be defined as 'to evaluate how a given model depends on its input factors' (Saltelli et al., 2000). It is often assumed that the number of important parameters in a model is small compared to the total number of parameters. A sensitivity analysis can reveal those most influential parameters. In practice the step of SA is often neglected. The modeller uses his experience about the model and/or processes and starts a manual calibration in which he changes +/ - 10 parameters. The other parameters are kept on a fixed literature value.

A comparison of different calibrated models that were all assumed to be the best calibrated model would show the possible variation between results. It is the aim of this contribution to focus on critical dissolved oxygen concentrations in the river and the influence on decisions that would be taken based on the different outcomes.

First a calibration of the model with the most important parameters will be conducted and these most important parameters will be the reference subset. The most important parameters are found in section 2 of this chapter. The output of the calibrated model gives a time series, which can be compared with other time series obtained after calibration with different subsets of parameters. The selection of the different subsets is based on a questionnaire sent around to 30 water modellers in 2002. The results of that questionnaire are given in appendix A. The most commonly used subsets are given in table V.25.

Table V.25: Different sets of variable parameters most often used for the calibration of the modified QUAL2E in ESWAT (based on questionnaire (appendix A))

Name of the set	Variable set of parameters (according to table V1)
Reference	μmax, ai3, ai4, rhoq, ai0, λ1, ai5, rk2, rk1, rk4
Subset 1	rk4 , bc3, rk3, μmax, bc1, rs4, rk1, rhoq, ai6, λ1
Subset 2	μmax, rk1, rs2, rs3, rk4, bc2, kl, kp, kn, λ0, pn, kdd
Subset 3	rk2, rk4, rk1, bc1, bc2, bc3, rs2, rs3, rs4, rs5, rk3
Subset 4	rk2, rk4, rk6
Subset 5	μmax, rk4, λ1, rk1, kdd, rk2, λ2, bc1, kp, pn

7.2.1. Selection of reference parameter subset.

In order to compare the outcomes of models calibrated with different parameter sets it was decided to define a reference parameter subset. The reference set was selected to contain those parameters that are influencing the critical values most because that set gives the most reliable predictions for the critical variable under consideration. The critical value considered here is DO and the parameter subset that is chosen here is the one found in section 2: μmax, ai3, ai4, rhoq, ai0, λ1, ai5, rk2, rk1, rk4. For this set all the most important parameters can be tuned to give the best estimates for the low DO values, the values we are interested in and there is no risk to fix an influential parameter on a wrong value.

7.2.2. Calibration

The model was calibrated with different sets of parameters given in table V.1. The calibration of the model was done with the optimization program PEST (Pest Manual, 1994) (see chapter "Materials and Methods"). The objective function was the weighted sum of squared differences between measured and modelled dissolved oxygen (DO) concentrations.

$$\Phi = \sum_{k=1}^{4} \sum_{i=1}^{n} \omega_k (obs_{k,i} - calc_{k,i})^2$$

With ω_k = weight given to the observations of each variable, *obs* = observation, *calc* = calculated value and n = the number of observations for each variable, k = numbering for each variable, i = numbering for each observation .

All fixed parameters were set on the nominal value given in table V.1. The most influential parameters were varied, starting from their nominal value until the lowest objective function value was reached.

7.2.3. Analysis of the model output of the models calibrated with different subsets

In figures V.31, V.32 and V.33 the results are given of the model results after calibrating different subsets. In each of the figures one subset calibration is compared with the reference. When analysing what kind of parameters are chosen to be important, the major differences between the reference and the subsets can be summarised as in table V.26.

Table V.26: Subsets of parameters for calibration and their particular focus

Parameters for calibration	Focus on
Reference	Production, uptake and reaeration of O_2, algae growth and respiration, cBOD processes
Subset 1	cBOD processes, benthic oxygen demand, nitrification, denitrification
Subset 2	Algae processes, benthic processes
Subset 3	Reaeration, O_2 processes, benthic processes, nitrification, denitrification, phosphates

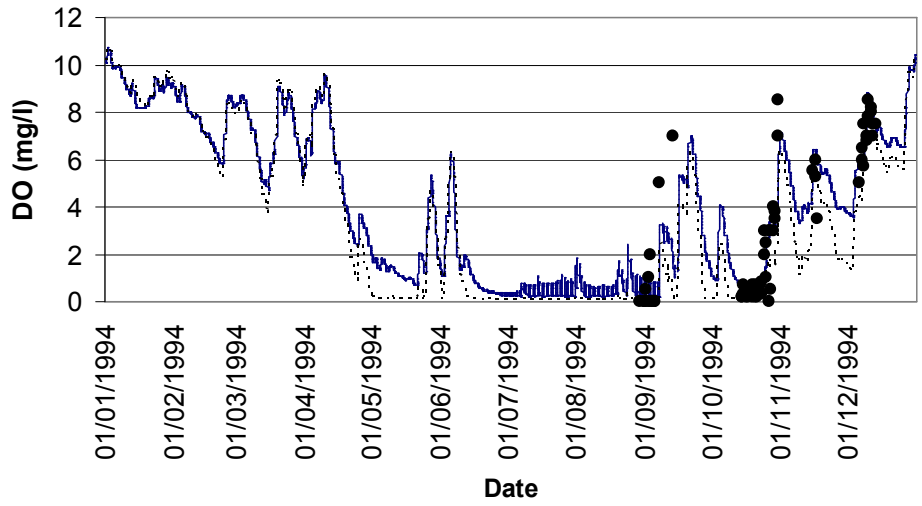


Figure V.31: Model results and measurements (symbols) of DO at Denderbelle, 1994, model calibrated with two different subsets of parameters (full line is the reference, dotted line calibrated with subset 1)

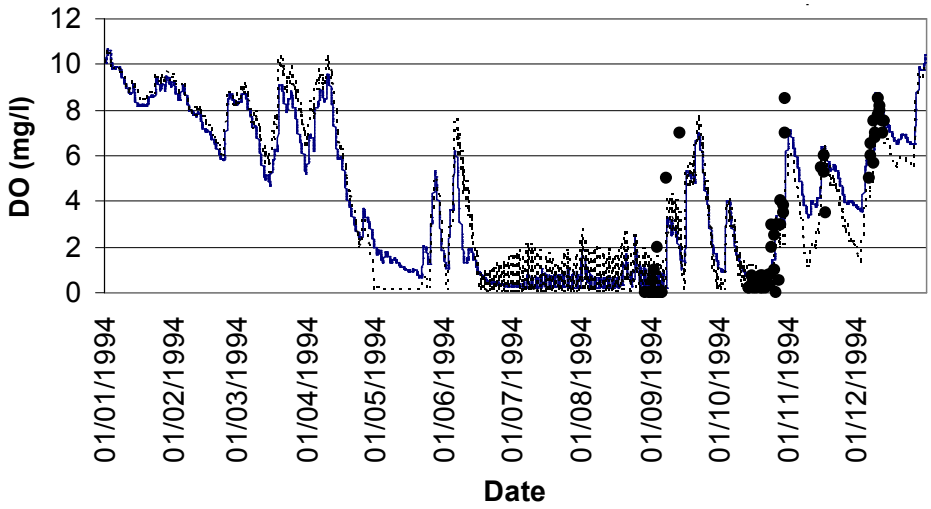


Figure V.32: Model results and measurements (symbols) of DO at Denderbelle, 1994, model calibrated with two different subsets of parameters (full line is the reference, dotted line calibrated with subset 2)

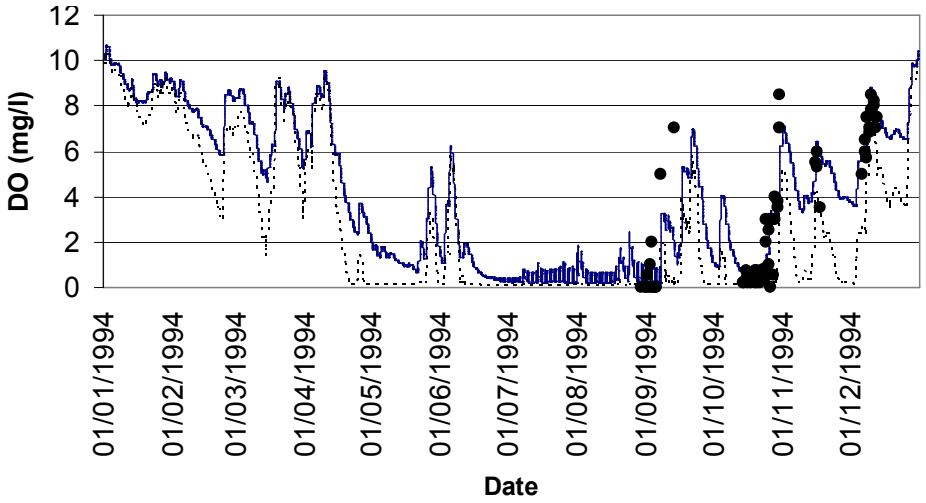


Figure V.33: Model results and measurements (symbols) of DO at Denderbelle, 1994, model calibrated with two different subsets of parameters (full line is the reference, dotted line calibrated with subset 3)

In table V.27 the values of the parameters obtained after the calibration with different subsets are presented. From this table we see that the parameters algae respiration rate (rhoq), carbonaceous biological oxygen demand deoxygenation rate coefficient (rk1), oxygen reaeration rate (rk2) and rate of loss of carbonaceous biological oxygen demand due to settling in the reach (rk3) are the parameters that are very different after the different calibrations. Apparently these parameters can compensate easily for other fixed ones to obtain good results for the dissolved oxygen concentrations in the Dender. During the calibration with subset 2 it was found that the benthic (sediment) source rate for dissolved phosphorus (rs2) and the benthic source rate for NH_4-N in the reach (rs3), could not be taken in the calibration process due to the correlation with other parameters (those two parameters are linear combinations of the other parameters which results in a singular covariance matrix which is not invertible)

Table V.27: Values of the parameters (according to table V.1) after the calibration with different subsets

	Reference	Subset 1	Subset 2	Subset 3
ai5	3.71			
bc1	0.1	0.11		0.1
ai4	2.0			
rk1	0.064	0.81	0.15	0.87
ai3	2.3			
rhoq	0.2	0.054		
ai6	1.0	1.03		
umax	2.2	2.1	1.86	
rk3	3.0	2.9		2.15
rk2	1.09			0.3
rk4		3.1	4.3	
rs4		6.26		6
λ1		0.016		
bc3		0.4		0.4
rs2		Fixed on nominal value		0.01
bc2			1.04	1
rs3		Fixed on nominal value		1
kp			0.042	
kl			5.2	
kn			0.073	
λ0			5.0	
kdd			0.01	
rs5				0,03
pn			0.3	

It can be concluded that sometimes fixing the parameter values to literature values or to values delivered with the software gives as a result that no algae growth is simulated in this river, although in reality there is a lot of algae growth during summer period. The results after

calibration with subset 1 and subset 2 give no diurnal oxygen dynamics typical for algae growth, wich means there are no processes of photosynthesis and respiration simulated. Further, the three subsets give more periods below critical oxygen levels (see table V.28). Also, when the model is calibrated with the parameters focusing on the nitrification and denitrification processes and on the benthic processes included, the oxygen concentrations go lower in spring and autumn.

Table V.28: Results for the time that DO<5mg/l at Denderbelle for the different calibrations

Calibration parameter set	Hours DO < 5 mg/l
Reference	5000
Subset 1	5520
Subset 2	5160
Subset 3	6193

7.3. Conclusions

It was demonstrated here that calibrating with different subsets of parameters gives different model predictions and can lead to different conclusions. This result is for sure particular for this case study, but it shows the importance of performing a sensitivity analysis before calibration to select the most important parameters for the particular problem at hand. That way one avoids skipping important parameters that need to be adjusted for that particular case, and which cannot be compensated by calibrating with other parameters. In the case study the consequence of a wrong calibration could be that too many measures would be taken to increase the DO levels during spring and autumn while in reality this would not be necessary.

8. Cost-effectiveness of in-stream aeration to improve river water quality

8.1. Introduction

The core issue of the European Water Framework Directive (WFD) is the achievement of good water quality in surface and ground waters on a river basin scale. To reach this goal the combined approach of emission limits and water quality standards proposed by the Directive will make new strategies available to the water managers. Interventions will not necessarily be limited to the sources of pollution but measures in the receiving water bodies will also be a possible way to achieve the water quality objectives. These measures need to be evaluated in terms of cost-effectiveness. Models can be used to perform these evaluations but uncertainty on the results is unavoidable. Hence, reliable modelling requires that the uncertainties are considered too.

One of the possible measures is in-stream aeration to compensate oxygen shortages during certain periods and to ensure fully aerobic conditions in the river at any time. Technical reaeration can be questioned as a measure to improve the receiving water quality as the philosophy behind the WFD is to go back to pristine situations in a cost-effective way and technical reaeration is a man-made intervention which consumes a lot of energy. Further, it can be questioned whether the self-purifying capacity of the river itself can be used for waste water treatment. Still, in heavily modified rivers or rivers suffering from a large diffuse pollution load, intervention might be necessary. This is obviously the case if acute fish death is occurring as a result of sudden oxygen drops.

The aim of this research is to assess the cost-effectiveness of aeration techniques in improving the water quality in surface water bodies. The Belgian Dender River is used as a real-case application. Literature review results about reaeration rates, oxygen transfer rates and energy consumption are used to run scenarios with the QUAL2E river water quality model implemented in ESWAT for the river Dender (van Griensven and Bauwens, 2001). The scenarios are then compared in terms of costs and effects on the dissolved oxygen content at the mouth of the river and uncertainty analysis is included to be able to see if there is a significant difference of the results without or with aeration.

8.2. Methodology

The river water quality model of the river Dender will be used to calculate some important values like amount of time needed for aeration and the amount of DO suppliance. First, from the model results, the duration of periods during which the dissolved oxygen is below 3 mg/l is calculated. Three mg/l is here taken as the critical value for biological life in cyprinid waters (UPM, 1998). Second, with the aid of the model, the amount of extra dissolved oxygen needed to obtain oxygen concentrations higher than 3 mg/l is calculated. Oxygen is supplied as a point load and a trial and error method provides the amount of oxygen needed. With those data a comparison was made in energy requirements for three different methods of aeration: The Clean Flo inversion/oxygenation method, a fine bubble aerator and a mechanical stirrer. This calculation provides the magnitude of costs for instream aeration that prevents the oxygen level to drop below 3 mg/l. Natural reaeration is no option for the river Dender because it is a flat river and the stream velocity is too low. At the sluices some aeration occurs but not enough.

In a second part of this research other measures which result in a reduction in pollution to the river or that avoid algae blooms during summer are discussed and compared with the in-stream aeration option. The measures looked at are: a connection of all households to the sewer system according to the General Water Plans for the Dender (AWP1), shading and reduction in diffuse pollution.

Uncertainty bounds on the results are included. These are the 5 and 95 % confidence intervals calculated with a Latin Hypercube Monte Carlo simulation. This latter technique is well explained in section 5 of chapter V. The uncertainty is caused by parameter uncertainty and

input uncertainty. Uncertainty ranges applied are according to the results in section 5 of chapter V.

8.3. Results and discussion

8.3.1. Comparison between different in-stream aeration methods

The dissolved oxygen time series for the river Dender at Denderbelle in 1994 is given in figure V.34. No in-stream aeration is applied here. The number of hours that the dissolved oxygen drops below 3 mg/l is 3810. Rather than installing an aeration system that can be switched on and off, in summer a relatively long period exists during which continuous supply of oxygen is required. The maintenance costs and follow up of the dissolved oxygen concentration would undo the benefit of the few times that the aeration can be switched off. In this year it is necessary to aerate the river from 21st of April till 13th of October i.e. 4200 hours of aeration are needed.

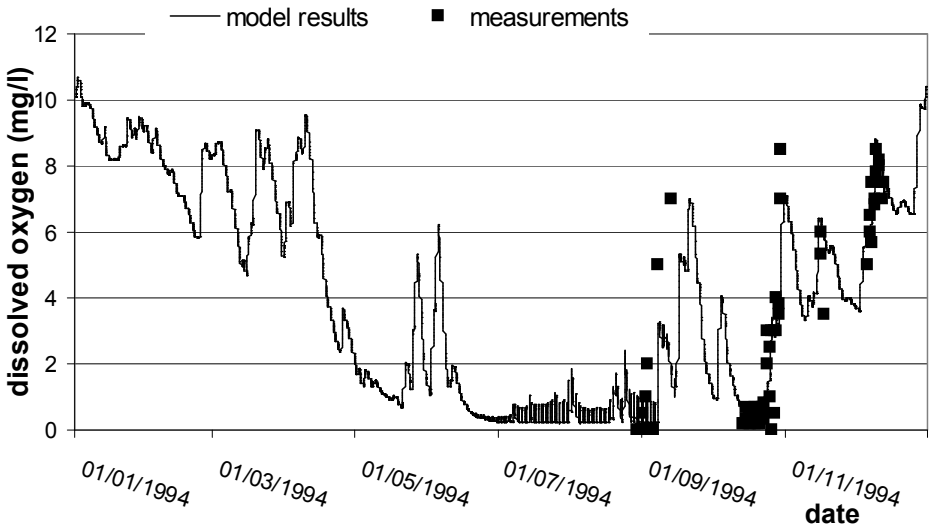


Figure V.34: Time series (line) and measurements (symbols) of dissolved oxygen at Denderbelle, 1994.

To calculate the energy costs for the in-stream aeration with diffusive aerators we first calculate the actual oxygen transfer (OTR_{act}) rate needed by using the maximal transfer rate

$$OTR_{act} = OTR_{\max} * \left[\left(\frac{DO_{sat} - DO_{act}}{DO_{sat}} \right) \right]$$

(OTR_{max}) for the aeration equipment. The following formula is used:

Taking an average of 2 mg/l as actual DO and the saturation level of 9,5 mg/l DO at 15° C the maximal OTR needs to be multiplied by 0,789. We take this average over the summer period. The Actual OTR and the needed power are given in table V.29. Also the investment and maintenance costs are presented.

Inversion/oxygenation system "Clean Flo"
This system oxygenates the water and removes toxic gases**.** The process inverts and oxygenates 11000 m^3/d of water per diffuser at 2 m depth using a laminar flow principle. Laminar flow prevents mixing of anoxic, high toxic gas-content bottom water with the main water body before the water reaches the surface. At the surface, the uprising water spreads out towards the shore in a 0.04 cm deep layer. This oxygenates the water and rids the water of toxic gases. Laminar flow causes a Venturi effect to add water from the water body to the water column as it rises, causing increased water flow in deeper water.

When calculating costs for the Clean Flo system, if necessary, also land acquisition along the shore for cabinet placements has to be considered in addition to protective fencing or concrete buildings to protect against vandalism. (Clean Flo international, 2004)

Fine bubble aerators
Fine bubble aerators are the most energy efficient means of aeration but have the largest capital and maintenance costs. Fine bubble aeration is generally defined as a diffuser system that produces air bubbles in water or wastewater with bubble diameters of approximately 0.5 mm to 4 mm diameter. All diffuser systems create a spectrum of bubble sizes but high efficiency fine bubble systems have a large fraction of bubbles in the 0.5 mm to 2 mm diameter range.

The high maintenance costs are related to the problem of clogging. Diffuser clogging often occurs from the inside. It is caused by dust and dirt particles carried in by the air supply or by impurities in the water. Calcium carbonate often forms a deposit, which clogs the pore outlet. Another source of plugging is bacterial slime, which forms a layer on the external surface of the diffuser.

Mechanical surface aerator
Mechanical aerators work by creating small droplets of water using a mixer. These droplets are propelled through the atmosphere above the water's surface. Oxygen in the air is transferred into the small water droplets, which then fall back into the water.

Table V.29: Calculation of costs for aeration of the Dender in summer

	Fine bubble aerator	Mechanical surface aerator	Clean Flo system (Clean Flo international, 2004)
Maximal OTR	2,72 kg/kWh	2 kg/kWh	not available
Actual OTR	2,15 kg/kWh	1,5 kg/kWh	not available
Needed power	1953 kWh	2800 kWh	4230 kWh for oxygenation + laminar movement
Energy costs/year	574180 € for 4200 hours	823200 € for 4200 hours	1184400 €
Maintenance costs/yeqr	332700 €	not available	5 000 €
Investment costs/yeqr	50000 €	20 000 €	20 000 €
Total cost/year	936880 €	1023200 € (without maintenance)	1434400 €

8.3.2. Comparison of in-stream aeration with other measures

In the model an amount of 4000 kg O_2/day is transferred for a period of 4000 hours. This amount is obtained by trial and error in the model until reasonable results were obtained for the whole summer period. Figure V.35 (left) shows the effect on the dissolved oxygen concentration at a point close to the mouth.

AWP 1999

The total cost for the whole investment program in the Dender catchment for the period 1991-2005 amounts to 233 mio €. This investment program includes the renovation and construction of wastewater treatment plants, construction of a new sewer system and connection of households to the new and existing sewer system. The reduction in point pollution load was calculated and reported in the AWP 1999 project description (VMM, 1999). In figure V.35 (right) the effect on the dissolved oxygen by the reduction of the BOD load and of the total load according to the AWP plans, is presented. If the reduction in N and P load is also taken into account, the oxygen level is much better. Hence, it is obvious that biological nitrification and phosphorous removal are important for the river Dender to bring the oxygen levels up to acceptable levels.

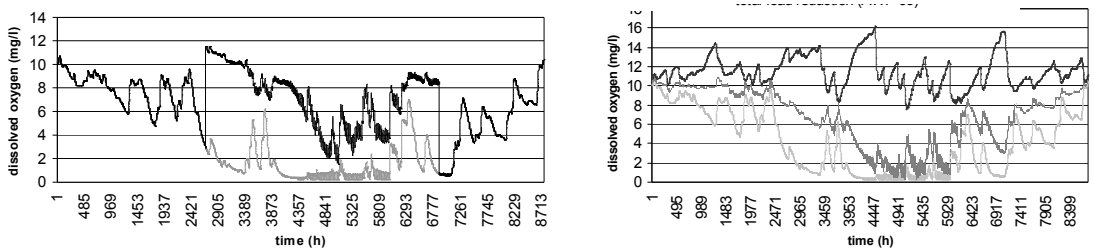


Figure VI.35: Comparison of obtained dissoved oxygen concentrations at Denderbelle without (grey) and with aeration (black) (left) and without aeration (grey), with implementation of the AWP plan (right) (with BOD load reduction (dashed) and with total load reduction (black))

Shading

Another option for reducing algae growth is the reduction of sunlight that is reaching the river water surface by planting trees along the river providing shading in this way. According to (Ghermandi, 2004) shading would produce a 15 % higher minimum dissolved oxygen content and a 30 % higher average minimum DO. To have the same effect at Denderbelle, an additional amount of 1000 kg O_2 per day introduced 8 km upstream is needed. This would increase the costs for aeration to +/- 300000 €. Hence, shading is an attractive and less expensive alternative. However it is not sufficient to avoid fish kills. When combining both measures, shading and aeration, the additional amount of aeration needed is calculated with the model results 3000 kg (4000 kg O_2 /day – 1000 kg O_2 /day). It will be less because shading also lowers the average water temperature and as processes go slower at lower temperature, less DO is needed. Further, all additional advantages of shading such as lower water temperature, less algae, recreational value and habitat for birds should be considered too.

Diffuse pollution

The reduction in diffuse pollution also leads to a reduction in phosphate and nitrogen load to the river and as a consequence less algae blooms and less respiration during night time.

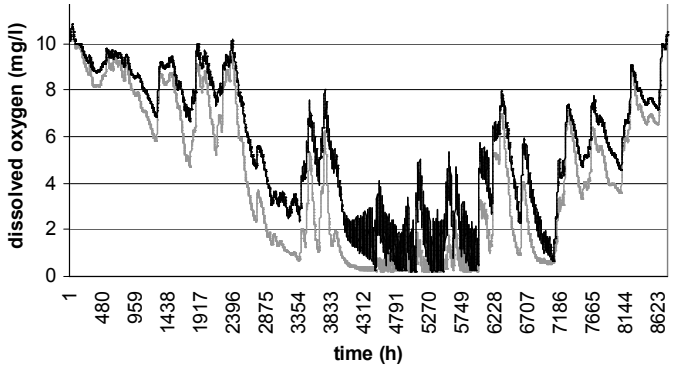


Figure V.36: Influence of 90% reduction in amount (black) of fertiliser use for the river Dender 1994. (without aeration (grey))

It is a measure that assures good oxygen levels only if the algae bloom is caused by the diffuse pollution input. If, however, the nutrients, nitrate and phosphate are not limiting algae

growth due to the discharge of nutrients via point sources, the measure will not influence much and the same situation of low oxygen during summer holds as is the case for the Dender river. As can be seen in figure V.36, the oxygen levels are better until June 10th. With higher temperature and lower flows during summer, the oxygen levels become critical again and in this case in-stream aeration is the only option for avoiding fish kills. Moreover, reducing diffuse pollution means dealing with agricultural fertiliser and manure use. Hence, the economic and political consequences are important and warrant a study on itself. It is obvious for the river Dender that reduction in diffuse pollution has to be accompanied by reduction in point pollution loads as proposed by the AWP 99.

8.3.3. Uncertainty on the results

The uncertainties on the results are shown for the scenario 'without aeration' and 'with aeration' only for the period where the aeration device is on (figure V.37). The uncertainty on the parameters of the water quality model, uncertainty on the inputs of the point pollution inputs and uncertainty in fertiliser amount and plant and harvesting dates. The uncertainty on the hydrodynamic model for the river Dender was not considered here as it is assumed that the model was well calibrated thanks to the many measurements of flow available for this river.

The uncertainty represented by the 5 % and 95 % percentiles on both scenario's shows that the river Dender benefits significantly from aeration during the summer period. The uncertainty analysis also allows concluding that it is possible for the dissolved oxygen content of the river to go below 3 mg/l even when the aeration system is installed, albeit only for very short periods.

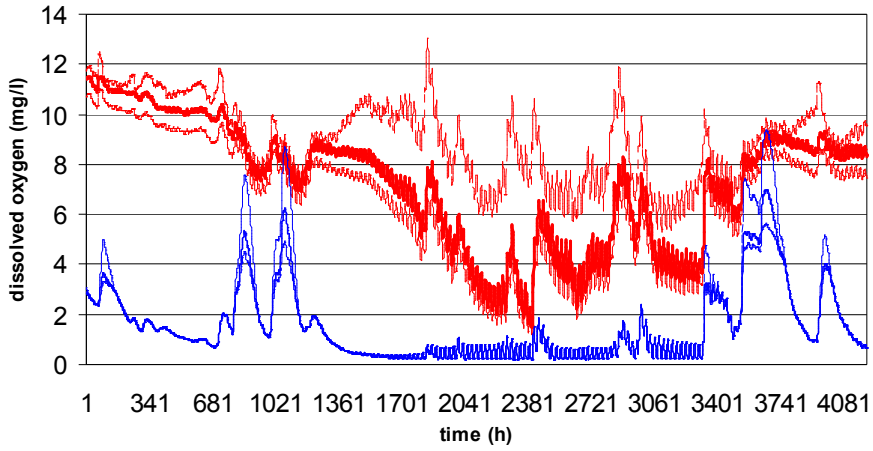


Figure V.37: DO time series during aeration period of scenario 'without aeration' (blue) and 'with aeration' (red) with uncertainty expressed as 5 % and 95% percentiles (dashed)

8.4. Conclusions

This modelling study evaluated the extent of reaeration needed to maintain a minimum of 3 mg O_2/l in the Dender River, to get an idea of aeration costs and to see whether other measures exist that can avoid the need for aeration.

In-stream aeration is found to be a very effective measure for the compliance with dissolved oxygen standards in rivers. It can be switched on when needed, e.g. during crucial periods of low oxygen e.g. in summer. This avoids excessive energy costs.

Comparison of different methods (fine bubble diffuser, meachanical aeration, the oxygenation/inversion system of Clean Flo), shows that aeration costs to obtain oxygen levels above 3 mg/l in the river Dender is about the same for all the systems.

Other measures to raise the oxygen levels in the Dender were compared in terms of their effectiveness. The fundamental option, reducing the point pollution load, following the AWP 1999 plan, is the best option and ensures that oxygen levels are above critical levels the whole year. However, it is a very expensive option and it also takes a long period before it will be fully implemented: 16 years. In the meantime in-stream aeration techniques can help overcoming critical periods.

Shading is a very attractive additional measure that can be combined with other measures in the stream. It reduces algae blooms, assures higher minimum DO levels and has also other advantages such as lower water temperature, less algae, high recreational value and a habitat for birds. Reduction in diffuse pollution input does not appear to be a valid option for the Dender as long as nitrogen and phosphates are still discharging through point pollution. Algae blooms keep occurring during summer even though diffuse pollution was reduced by 90 %.

Uncertainty analysis on the results for the scenario ‘with aeration’ shows that it is possible for the dissolved oxygen content of the river to go below 3 mg/l even when the designed aeration system is installed, albeit for very short periods. Further the UA shows that the two options, with or without aeration are significantly different.

9. Assessment of the effect of shading on river water quality for the Nete river

9.1. Introduction

In this section just like in section 8 an evaluation is made of an in-stream measure, shading, that can be applied to improve the river water quality. Ecological engineers and water managers look with increasing interest at shading by riparian vegetation for its potential positive effect on the water quality in surface watercourses.

While the role of near-stream vegetation in filtering the contaminants from diffuse pollution, in controlling erosion processes and in reducing the impact of floods has been extensively analysed, the impact of shading by riparian vegetation on the water quality is less clearly

understood. Research suggests that shading might influence the water quality in small to medium watercourses mainly by reducing the temperature of the water and the solar radiation that reaches the water surface (Beschta et al., 1987; Collier et al., 2001). Cooler water can hold a higher concentration of dissolved oxygen (DO) and therefore increase a stream's capacity to assimilate organic wastes from sewers, treatment plants or diffuse sources. Furthermore, water temperature both affects the growth and development rates of most aquatic organisms and influences the kinetics of chemical reactions. At lower temperatures, oxygen consumption rates decrease, leading to a smaller risk for oxygen depletion. Light availability, on the other hand, controls algal growth, together with nutrient availability and hydraulic mixing conditions. Light interception can inhibit excessive algal growth in streams that are particularly exposed to the risk of eutrophication.

The degree to which riparian vegetation affects water temperature and incident solar radiation depends on a series of factors, including geographic and climatic aspects, characteristics of the channel, type of vegetation and turbidity of the water. Channel width is probably the most obvious factor influencing the effect of riparian shading. The wider the channel, the smaller is the fraction of solar radiation that is intercepted by the riparian vegetation. Riparian shade is unlikely to have a significant influence on stream temperatures where the natural low-flow stream width exceeds 30 m (Washington Forest Practice Board, 1992). The characteristics of the vegetation that most influence the effect of shading include canopy height, width of the vegetated buffer zone and foliage density. Fast-growing trees, with a deep and strong root system like *Alnus glutinosa*, *Salix spp*. and *Populus nigra* seem thus to be the most indicated tree species for shading (Ministry of the Flemish Community of Belgium, 2000).

This section provides a model-based assessment of the efficiency of shading by riparian vegetation as a measure to increase the water quality in a watercourse, by evaluating its effect on five water quality parameters in a medium-sized river stretch located in the Nete river basin in Belgium. Because of data scarcity there is a large uncertainty on the model outcomes. Therefore, an uncertainty analysis is applied to identify if the measure gives a significant effect on the water quality variables. For scenario analysis it is however not always needed to comprise all possible uncertainty into the uncertainty analysis. Only those inputs and parameters for which the related uncertainties can differ under different circumstances are taken into account because decisions about the improvement caused by the implemented measures are based on the difference between the results of the scenarios. Uncertainties that are the same for the different scenarios will become zero for the difference, only the others form an uncertainty bound around the difference and form the basis of decision. It is suggested that the results found in this study have a more general validity so that they can be extended to watercourses with characteristics similar to the studied one.

9.2. Case study: the Nete river basin, model implemented in WEST

The Nete river basin is located entirely within the Flemish Region of Belgium and covers a surface of 1673 km² (see figure V.38). The main watercourses within the river basin are the

Grote Nete and the Kleine Nete. For this study a stretch of the Grote Nete of 19.5 km of length was selected. The boundaries of the stretch are the confluence with the Grote Laak (upstream) and with the Wimp (downstream). More information about the Grote Nete can be found in de chapter "Case studies" and the modelling approach is described in section 1.2 of this chapter.

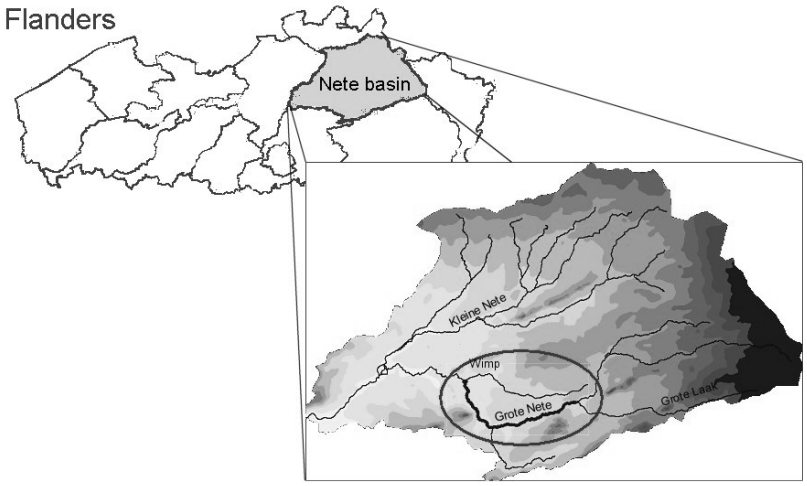


Figure V.38: The Nete river basin and the stretch of the Grote Nete selected for this study.

A model for the Nete river was implemented in the WEST® software (MOSTforWATER NV) (Vanhooren et al., 2003).

9.3. Sensitivity analysis

A global sensitivity analysis was performed in order to identify the most influential parameters of the water quality model. This helped in manually adjusting the parameter values to obtain the calibrated model. The method used is a regression and correlation technique (Saltelli et al., 2000) with Latin Hypercube Monte Carlo sampling (McKay et al., 1979). More explanation of this method can be found in the chapters about sensitivity analysis. Regression is done between the parameters under consideration and a critical output of the model. Since oxygen shortage is one of the main water quality issues in the Nete, the amount of hours that the oxygen concentration drops below 5 mg O_2/l and the average DO concentration are chosen as the critical outputs for the problem at hand.

The mean values of the parameters, distributions, variance, minimum and maximum used in the Monte Carlo sampling are given in table V.30. The variance is chosen to be either 50% or 20% around the mean value. Some of the uncertainty sources are not part of the water quality model but were included in the uncertainty analysis due to their importance for algae and oxygen dynamics. These are the atmospheric radiation factor (beta_ar), the groundwater quantity, measured as fraction of the inflow (GW_q) and its temperature in °C (GW_t). For these parameters variations coming from literature have been applied (Reichert et al., 2001b). The uncertainty in the model inputs has been accounted for multiplying the nine inputs by nine independent factors varying between 0.5 and 1.5.

Table V.30: Values of the parameters for the river Nete model with frequency distribution characteristics for the Monte Carlo sampling

Parameter	Mean	Var.	Min	Max	Dist.	Parameter	Mean	Var.	Min	Max	Dist.
alfa1	96.859	20%	77.487	116.231	t	K_HPO4_H_aer	0.02	50%	0.01	0.03	u
alfa2	48.226	20%	38.581	57.871	t	K_N_H_aer	0.2	50%	0.1	0.3	u
Beta1	11.613	20%	9.290	13.936	t	K_NH4_N1	0.5	50%	0.25	0.75	u
Beta2	16.157	20%	12.926	19.388	t	K_HPO4_ALG*	0.02	50%	0.01	0.03	u
Kla_base	1	50%	0.5	1.5	t	K_O_N1	0.5	50%	0.25	0.75	u
Pow_v	0.97	50%	0.485	1.455	t	K_NO2_N2	0.5	50%	0.25	0.75	u
Pow_h	-1.6	50%	-0.8	-2.4	t	K_NO3_H_anox	0.5	50%	0.25	0.75	u
K_gro_H_anox	1.6	50%	0.8	2.4	u	K_NO2_H_anox	0.2	50%	0.1	0.3	u
K_gro_ALG*	2	50%	1	3	u	K_N_ALG*	0.1	50%	0.05	0.15	u
K_gro_N1	0.8	50%	0.4	1.2	u	K_HPO4_H_anox	0.02	50%	0.01	0.03	u
K_gro_N2	1.1	50%	0.55	1.65	u	K_I*	30	50%	15	45	u
K_hyd	3	50%	1.5	4.5	u	K_O_ALG*	0.2	50%	0.1	0.3	u
K_resp_ALG*	0.1	50%	0.05	0.15	u	K_death_ALG*	0.1	50%	0.05	0.15	u
K_resp_H_aer	0.2	50%	0.1	0.3	u	K_ads	0.5	50%	0.25	0.75	u
K_resp_H_anox	0.1	50%	0.05	0.15	u	beta_ar*			0.8	0.9	u
K_resp_N1	0.05	50%	0.025	0.075	u	GW_q*			0.08	0.12	u
K_resp_N2	0.05	50%	0.025	0.075	u	GW_t*			10	12	u
K_O_H_aer	0.2	50%	0.1	0.3	u						

*parameter used for difference analysis (see paragraph on uncertainty analysis)
Var.=variation, Dist.=distribution, t=triangular distribution, u=uniform distribution.

Table V.31 illustrates some statistics of the performed regression. The coefficient of determination (R^2) of the regression can be used to assess the goodness of the linear approximation of the regression between parameters and outputs. R^2 is defined as:

$$R^2 = S_{\hat{y}}^2 \Big/ S_y^2$$

with $S_{\hat{y}}^2, S_y^2$ respectively the variation on the model outcomes and the variation on the approximated value after linearisation.

Since an extension of the set of regressors with additional variables invariably leads to an increase of R^2, independently from the significance of the added variable, the adjusted coefficient of determination R^2_{adj} is introduced as an alternative measure of the goodness of the approximation:

$$R_{adj}^2 = 1 - \left(1 - R^2\right)\left[\left(N-1\right)/\left(N-\left(1+p\right)\right)\right]$$

with N the number of simulations and p the number of parameters considered. The closer the value of this coefficient is to 1, the better the regression.

Furthermore, numerical problems may occur when applying a linear regression analysis if the parameters are highly correlated. The Variance Inflation Factor (VIF) is a suitable measure for the correlation. It is defined as:

$$VIF_i = \left[C_x^{-1}\right]_{ii}$$

with $\left[C_x^{-1}\right]_{ii}$ the i-th diagonal element of the inverse of the correlation matrix. It is assumed that a linear regression can be applied as long as the VIF is less than 5 for all I (Janssen et al., 1992).

Table V.31: Regression statistics for DO concentration below critical threshold (5 mg O_2/l) and average DO concentration.

	Original parameter values	Ranked parameter values
DO concentration < 5 mgO_2/l		
R^2	0.65	0.76
R^2_{adj}	0.61	0.73
Largest *VIF*	1.20	1.15
Average DO concentration		
R^2	0.92	0.92
R^2_{adj}	0.92	0.91
Largest *VIF*	1.16	1.14

In this study, standardized regression coefficients (SRC) are used as sensitivity measures:

$$SRC_i = \frac{\Delta y / S_y}{\Delta x_i / S_{x_i}}$$

with $\Delta y / \Delta x_i$ the change in output due to a change in the i-th input and S_y, S_x the standard deviations of output and input respectively. The standard deviation of the input S_{x_i} is specified by the user. If the regression is not good enough, that is if the R^2_{adj} is less than 0.7 (Saltelli et al., 2000), it is advisable to perform a substitution of the values of parameters and results by their ranks. The measure thus obtained is called ranked standardised regression coefficient (RSRC).

In the regression, 45 parameters were used and 500 Monte Carlo runs were performed. As illustrated in table V.31, the regression is not satisfying enough to get quantitative results (R^2_{adj} less than 0.7), the uncertainty contribution expressed by the SRC representing only a small fraction of the real uncertainty, but a qualitative ranking of the parameters that most influence the output results can be obtained on the basis of the rank transformed standard regression coefficient (RSRC).

The most important parameters determining the frequency of events with DO concentration below 5 mg/l, in descending order of importance are: Kla_base, pow_h, alfa1, K_growth_algae, beta1, k_gro_N1, pow_v, K_gro_H_aer, K_NO3_anox. Next to these parameters, also the nine inputs influence very much the results. It can however be expected that this load is known with good precision as it is based on direct measurements in the river. For the sensitivity analysis performed on the average value of DO, the following important parameters were obtained: K_growth_algae, alfa1, Kla_base, K_HPO4_het, K_NH'_N1, K_NO2_N2, K_NO3_H, K_N_alg. Here again the input upstream is also very important. The analysis with the average DO output gives a better regression between parameters and output

than with the exceedance frequency of low DO values. This confirms that during extreme low DO values, the model outcome reacts nonlinearly on parameter changes.

9.4. Calibration procedure

The calibration procedure was manual and included two distinct steps: hydraulic calibration and calibration of the biochemical transformations. The simulation period consisted of 100 days of steady state input followed by a dynamic input for the period from April 1st to October 31st, 2002. The steady state inputs were obtained by averaging influent flows and pollutant concentrations during the month of April. Figure V.39 illustrates the results of the hydraulic calibration 12.2 km downstream of the initial section.

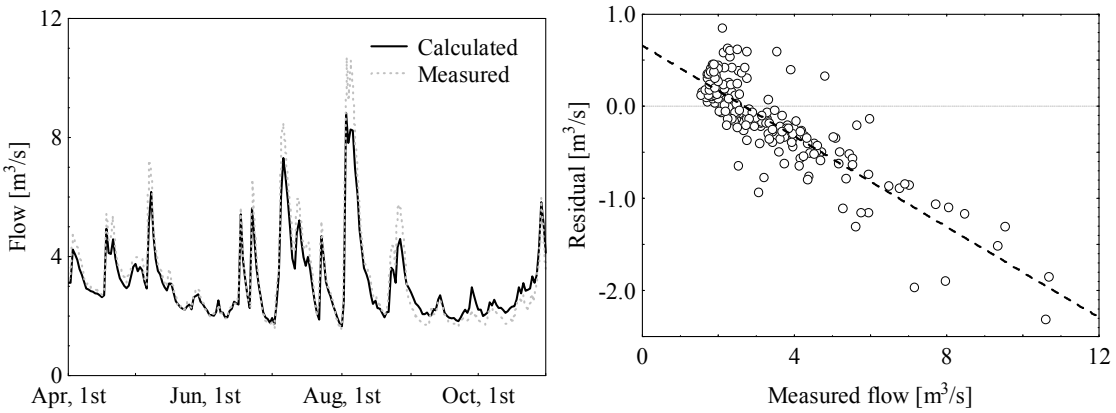


Figure V.39: Results of hydraulic calibration as comparison of measured and simulated time series (left) and as plot of residuals (measurement minus simulation) (right).

The hydraulic routing of the Nete is well reproduced by the model with exception of an underestimation of the peak flow. This may be due to the fact that the contribution of several minor tributaries of the Nete during periods of high rainfall is neglected in the model. The only calibration parameter was the number of tanks-in-series (10 tanks in the calibrated model) in which the river stretch is subdivided.

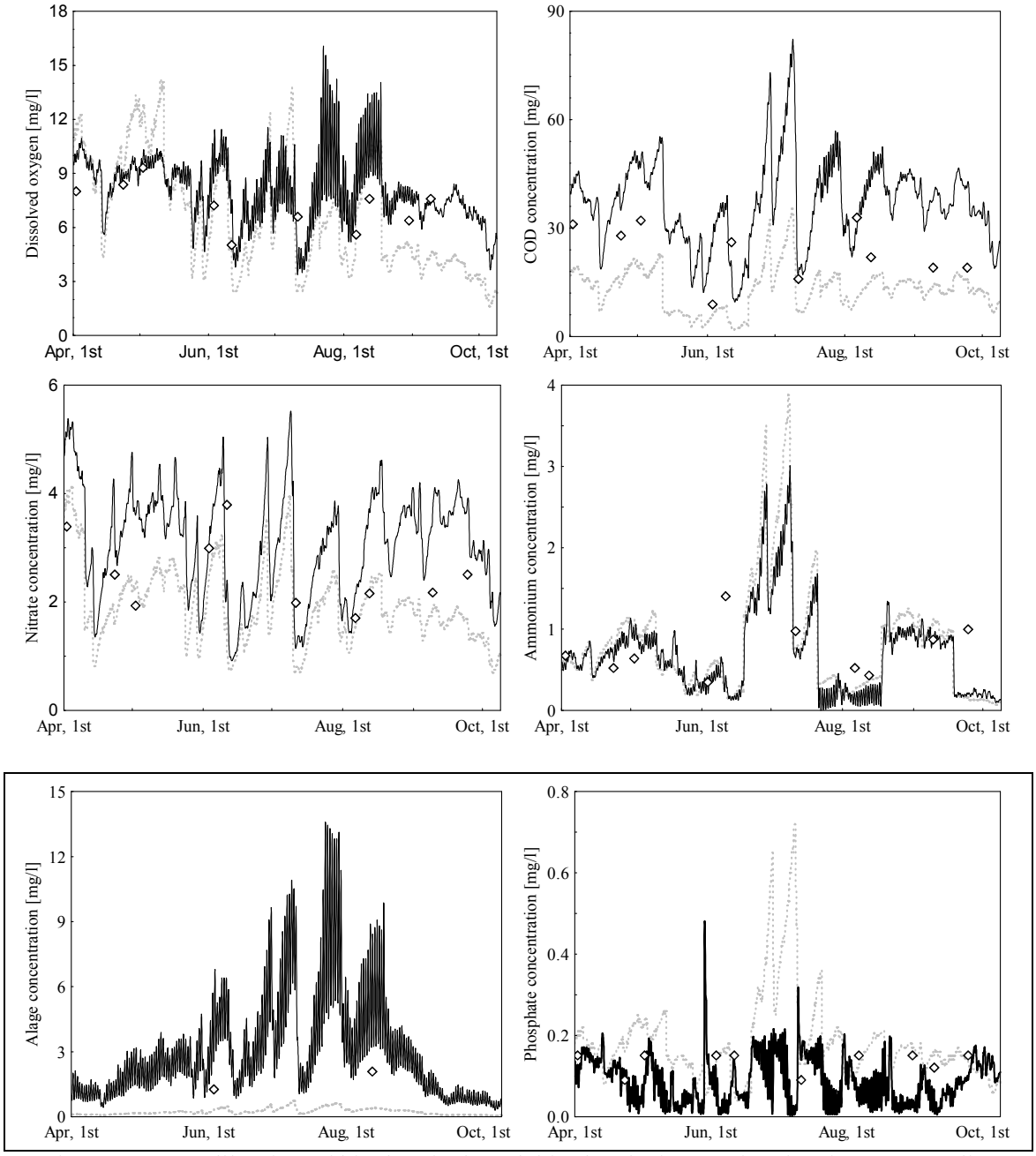


Figure V.40: Calibration of biochemical model in the closing section for six water quality parameters……..Concentration upstream ─ Concentration downstream ◊ Measured at Hulsthout

Six water quality variables were selected for the calibration of the biochemical model at different sections: DO, chemical oxygen demand (COD), nitrates, ammonium nitrogen, phosphates and algal biomass. Few significant parameters were tuned for the calibration: Monod's constants for the death of algae, the growth of algae, the algal uptake of HPO_4, the uptake of nitrogen by algae, heterotrophic (X_H) and autotrophic (X_N1 and X_N2) bacteria in the upstream section and the re-aeration coefficient (kla). In this procedure, X_H, X_N1 and X_N2 were treated as model parameters and not as state variables since, in the absence of

direct measurements, they had to be estimated on the basis of literature indications. The best results were obtained for upstream concentrations of 4 mgX_H/l, 0.3 mgX_N1/l and 0.1 mgX_N2/l.

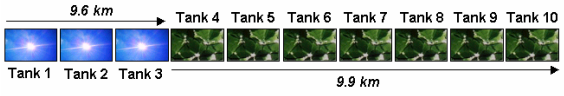
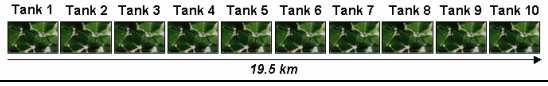
Figure V.40 shows the results of the calibration in the downstream section. The points represent the measurements made by VMM in the same section. In judging the results, it should be noted that the phosphates concentration was often below the detection limit: therefore all points in figure V.40 which indicate a concentration of 0.15 mg P/l must be intended as indicating a concentration less or equal to 0.15 mg P/l. The algae concentration might be overestimated, however this is not clear with only these two measurements.

Because of data scarcity, the evaluation of the calibration procedure had to be limited to a visual assessment of the fit between the model output and the few available measurements. For the same reason it was not possible to validate the model on a separate set of data. Due to the lack of model validation, the study must be indicated as semi-hypothetical and its results cannot be interpreted as supporting a riparian management strategy along the Nete, but as evaluating with more general validity the effects of shading in watercourses with similar characteristics.

9.5. Scenario analysis and discussion

Four scenarios were evaluated that represent different realistic shading conditions along the modelled stretch. In all scenarios, the effects of shading both on incident solar radiation and on water temperature were taken into account. The scenarios refer to the shading conditions induced by fully developed trees. The shading conditions in the four scenarios are described in table V.32.

Table V.32: Characteristics of the four considered scenarios

Scenario	Length of shaded stretch [km]	
1: alternate shading	11.9	
2: upstream shading	9.6	
3: downstream shading	9.9	
4: complete shading	19.5	

In the first scenario, shaded and unshaded conditions are assumed to alternate along the river stretch. This is reflected in the model by an alternation of tanks in shaded conditions with unshaded tanks as illustrated in table V.32. This scenario is intended to represent conditions of shading that are optimal for aquatic life (Ministry of the Flemish Community, 2000). Since

the ten tanks used in the model represent stretches of river characterized by different lengths, the total length of the shaded sections is greater than half of the total length of the stretch and amounts to 11.9 km (61% of the total length). The second scenario represents conditions of upstream shading. In this scenario, the first three tanks-in-series are modelled with shaded conditions, while the remaining seven tanks reflect unshaded conditions. Because of the different length of the tanks, the three upstream tanks account for approximately half the length of the stretch (9.6 km, 49% of the total length). The third scenario is chosen to represent the exact opposite conditions of shading of the second scenario. Only the seven tanks downstream of the stretch are in shaded conditions. This corresponds to shading along 9.9 km, 51% of the total length. The fourth and last scenario represents conditions of complete shading along the whole modelled stretch (all ten tanks-in-series are modelled in shaded conditions).

The effect of shading on the water quality of the river Nete in the four scenarios is evaluated comparing the output of the scenarios with the output of the calibrated model, which represents the current, reference shading conditions along the stretch. The effect on the algal biomass was evaluated both in terms of the change in the algal concentration in the closing section and of the algal growth within the stretch. The results of the analysis, averaged over the whole simulation period, are reported in table V.33.

Table V.33: Effect of shading on the algal concentration in the downstream section and on algal growth in the stretch

Scenario	Concentration of algae downstream	Algal growth in the stretch
1. Alternate shading	-4.4 %	-11%
2. Upstream shading	-3.3 %	-8 %
3. Downstream shading	-4.4 %	-11 %
4. Complete shading	-7.7 %	-19 %

According to table V.33, the variation in the concentration of algae within the simulated stretch is in the range between 3.3 and 7.7%, according to the scenario that is considered. This relatively low effect is explained by the small length of the simulated stretch (19.5 km): the short time of travel between upstream and downstream section does not allow for large effects on the algal concentration to take place. The highest effect on the algal concentration is given, as expected, by the scenario with complete shading. The sum of the effects of upstream and downstream shading corresponds approximately to the effect of complete shading, with upstream shading and downstream shading producing quite similar results. The effect of alternate shading is analogous to the effect of downstream shading, although in the corresponding scenarios different lengths of the stretch are in shaded conditions (61% for alternate against 51% for downstream shading).

Table V.33 shows that the effects of shading are more significant for the selected stretch when the difference in the total growth, rather than the difference in concentration, is considered. The growth of algae during the whole dynamic period is reduced by almost 20% with complete shading of the river stretch. The analysis of the variations in the modelled algal growth indicates that algae are slightly more affected by downstream shading than upstream

shading. Alternate shading does not prove to be more efficient than downstream shading in reducing the total algal production.

The effects of shading on the concentrations of DO, COD, phosphates, and ammonium nitrogen are insignificant when looking at minimal, maximal and average concentrations. During some periods of the year, however, a significant change in the profiles of the water quality variables towards better or worse conditions is clearly identifiable. This is illustrated for the variable DO in figure V.40, where the difference between DO concentrations in unshaded and completely shaded conditions is given over the whole year.

In table V.34 the effects are given as number of hours that the considered variables exceed or fall below a certain critical value. This value was assumed to be 5 mg O_2/l for DO, 14 mg/l for algae, 0.3 mg/l for phosphate and 5 mg/l for ammonia, according to legislation in Belgium concerning basic water quality. According to this analysis, shading induces slightly worse conditions for DO, its concentration being more hours under the critical level of 5 mg O_2/l with the shading option. The time of exceedance of critical concentration of algae is almost reduced to half in the case of complete shading. Exceedance of critical phosphate concentration is not affected by shading. Ammonia did not exceed the critical value in any case.

Table V.34: Number of hours of exceedance of water quality variables under different scenarios of shading.

Scenario	DO<5 mgO_2/l	PO_4>0.3 mg/l	algae>14 mg/l	NH_3>5 mg/l
0. No shading	279	19	95	0
1. Alternate shading	283	18	68	0
2. Upstream shading	282	18	75	0
3. Dowstream shading	283	18	70	0
4. Complete shading	286	18	49	0

9.6. Uncertainty analysis

To verify how much the results are influenced by the uncertainty in the parameters, a concentration-duration curve for DO with 5^{th}, 50^{th} and 95^{th} percentiles is shown in Figure 5 for the unshaded scenario and the completely shaded one. The curves express the percentage of time that DO is below a given concentration. Only these two scenarios are shown as they represent the extreme cases: the other scenarios fall in between those two. The uncertainty is calculated with Monte Carlo simulations where the parameter ranges are taken from table V.30.

The uncertainty bounds around the results of the DO and the concentrations of algae are wide. From this analysis it is therefore not possible to get to conclusions about the outcome of a scenario. However, not all the parameter and input uncertainties need to be taken into account for scenario analysis under uncertainty. Uncertainty on parameters that influence the outcomes in both scenarios in the same way, so called ‘fully dependent parameters’ (Reichert and Borsuk, 2003), will only shift the results in one direction and with the same magnitude. Therefore, an analysis on the difference of a variable in two scenarios was performed in order

to see whether the 5th and 95th percentile uncertainty bounds around the difference include or not the zero. Only the independent parameters and inputs are used in such analysis. They are indicated with asterisks in table V.30. The results of the described uncertainty analysis on the difference between scenario 0 and scenario 4 for DO concentration and average growth of algae at the end of the stretch are shown in figure V.41.

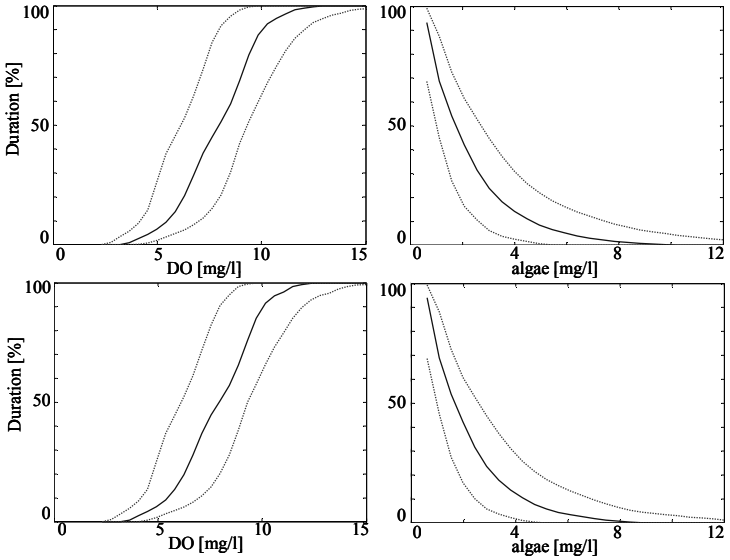


Figure V.41: The concentration-duration curves of DO and algae for the unshaded case (up) and completely shaded case (down).

From figure V.42 and figure V.43, it can be inferred that shading does not significantly reduce or increase the lowest oxygen levels in the last stretch of the river. The uncertainty concerning the difference between the scenarios contains both positive and negative values. However, a clear trend is here visible. In colder periods, when no algal growth occurs, the non-shaded scenario has higher oxygen concentrations, which become lower oxygen concentrations than the shaded scenario during warm periods with algal growth. In other words, the algae actually increase the oxygen concentration because of the production of oxygen.

The results of the uncertainty analysis for the algae indicate that there is a significant distinction between the scenarios. Shading reduces algal growth, and thus can effectively improve the conditions in rivers with excessively algal growth during summer periods.

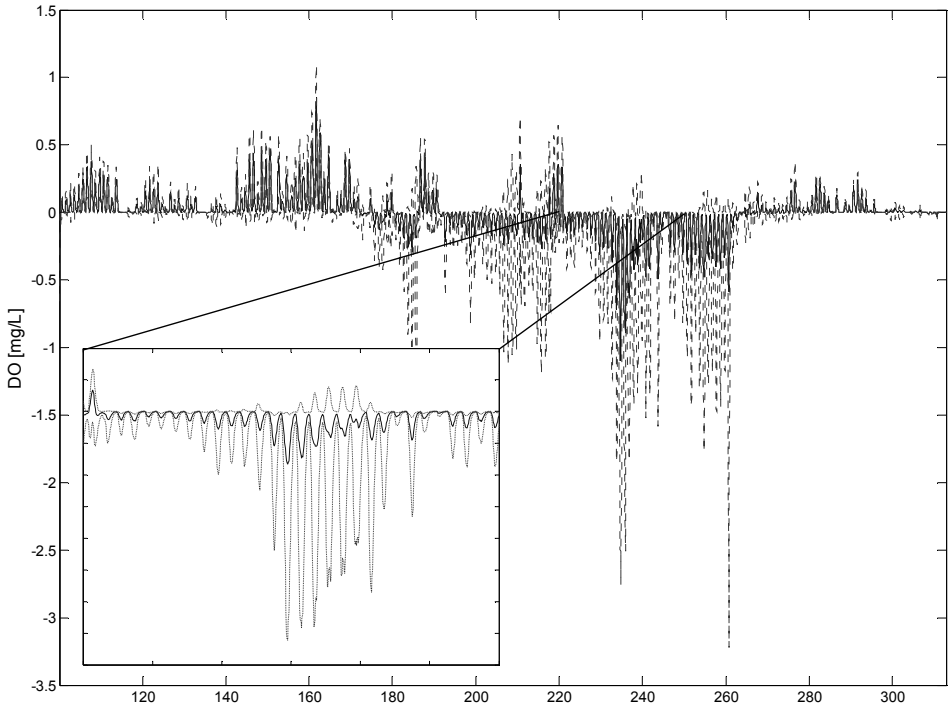


Figure V.42: Effect of shading on DO concentration during the year. Difference between scenario 0 and scenario 4 for DO; the full line represents the 50th percentile, while the dotted lines are the 5th and 95th percentiles.

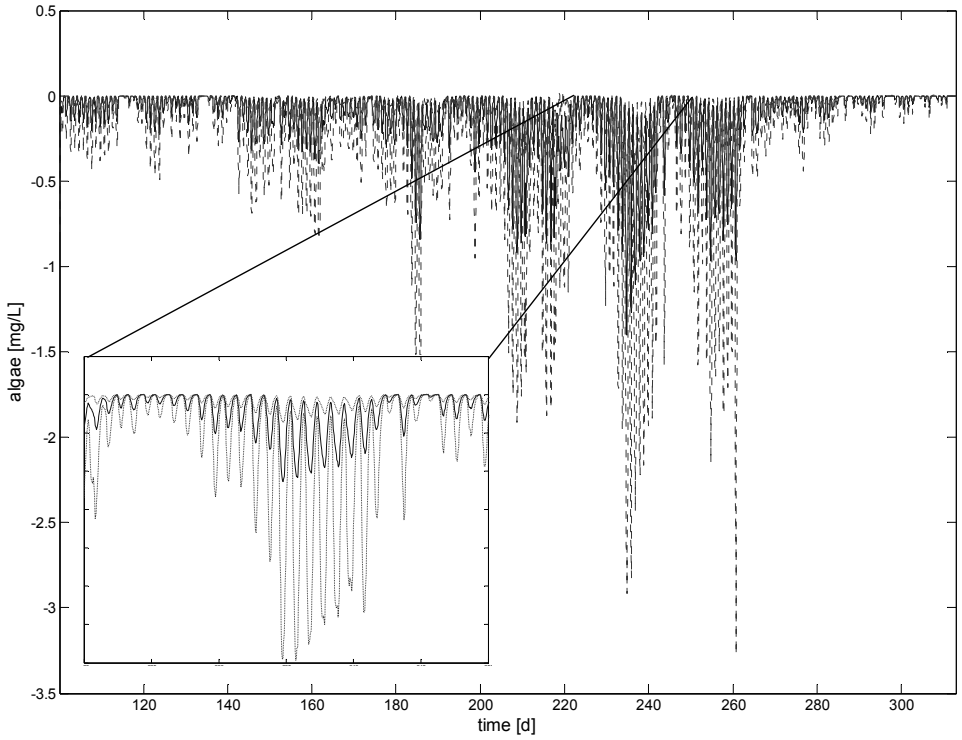


Figure V.43. Effect of shading on concentration of algae during the year. Difference between scenario 0 and scenario 4 for average concentration of algae; the full line represent the 50th percentile, while the dotted lines are the 5th and 95th percentiles.

9.7. Conclusions

The present study makes use of a dynamic modelling approach to predict water quality reactions within a river and to estimate the changes in water quality induced by shading of riparian vegetation. Such approach allowed to avoid the prohibitive costs required for extensive field measurement campaigns.

According to the analysis performed, shading can effectively influence the water quality in a surface water body, in particular in streams that suffer from excessive algal growth during the summer periods. The reduction of algal growth due to a full shading scenario was estimated to be about 20% at the outlet of a 19.5 km long stretch of the river Nete in Belgium.

No significant positive effects of shading on the minimum, maximum and average concentrations of DO, COD, phosphates, ammonium nitrogen and nitrates in the water were identified.

The influence of shading on the exceedance of critical thresholds for several compounds was examined. A positive effect is seen on algal concentration. At the downstream section of the modelled stretch, the time of exceedance of a critical concentration of algal biomass was reduced to about half by complete shading of the stretch. A slightly negative effect of shading on the exceedance of the threshold value for DO was identified.

CHAPTER VI
CONCLUSIONS AND PERSPECTIVES

Parts of this chapter were published as:

- Vandenberghe, V., van Griensven, A. and Bauwens, W. (2001). Sensitivity analysis and calibration of the parameters of ESWAT: Application to the river Dender. Water Science and Technology, 43(7), 295-301.
- Vandenberghe, V. , van Griensven A. and Bauwens W. (2002). Detection of the most optimal measuring points for water quality variables: application to the river water quality model of the river Dender in ESWAT, Water Science and Technology, 46(3), 1-7.
- Vandenberghe, V., Bauwens, W. and Vanrolleghem, P.A. (2004). The Evaluation of Uncertainty Propagation into River Water Quality Predictions to Guide Future Monitoring Campaigns. Environmental Monitoring and Software, 22, 275-232.
- Vandenberghe V., van Griensven A., Bauwens W. and Vanrolleghem P.A. (2006). Effect of different river water quality model concepts used for river basin management decisions Water Science & Technology, 53(10), 277-284.
- Vandenberghe V., van Griensven A., Bauwens W. and Vanrolleghem P.A. (2006). Effect of different river water quality model concepts used for river basin management decisions Water Science & Technology,53 (10), 277-284.
- Vandenberghe V. and Vanrolleghem P.A. (2005) Cost-effectiveness of in-stream aeration to improve river water quality. In: *Proceedings 10th International Conference on Urban Drainage*. Copenhagen, Denmark, August 21-26, 2005.

CHAPTER VI: CONCLUSIONS AND PERSPECTIVES

10. Conclusions

10.1. Water quality modelling

Due to the (sub-daily) variability and seasonality of weather, water quality processes and pollution sources, long time series of several water quality data should be analysed to get a picture of the stress on the ecological community. Integrated river basin water quality models can assist in the development of the pollution abatement plans to achieve the desired water quality standards and objectives. The models act as a surrogate to expensive water quality monitoring, since they can provide water quality variables whenever there are no or few data available. Catchment models can be used in watershed management to quantify the pollutant loads to a receiving water body. Once the model has been validated for a watershed's existing conditions, it can be used to predict impacts of alternative management plans to reduce pollutant loadings. To develop programmes of measures, modelling tools that account for all the important pollution sources are needed. In particular, the modelling tools must be able to quantify human impacts on river water ecology at river basin scale. Development of such tools is therefore an important issue in the European research programmes.

However, the results of modelling studies require careful evaluation and a profound uncertainty analysis is necessary. It is not only satisfactory to perform an uncertainty analysis and present the uncertainty bounds on the model results but extra attention should go also to efforts to minimise the uncertainty on model outcomes.

10.2. Calculation and reduction of output uncertainty

The modelling process can be seen as a connection of activities and products (figure VI.1).

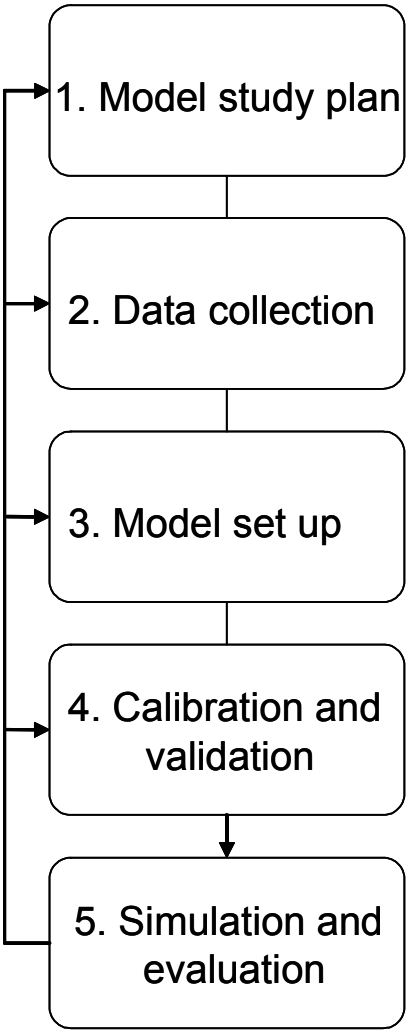


Figure VI.1: The modelling process (adapted from refsgaard et al (2004))

Every step has its own specific procedures in which different techniques and expertise are needed. During all these steps errors can be made which will accumulate into ever larger uncertainty bounds around the model results. The errors comprise of (Schnoor, 1996):

- uncertainty of the values of the parameters that appear in the identified structure of the dynamic model for the system behaviour; model parameter error (ε1)
- uncertainty of the model structure, i.e. uncertainty about the relationships among the variables characterising the dynamic behaviour of systems and uncertainty associated with predictions of the future behaviour of the system; model structure error (ε2)
- numerical errors, truncation errors, rounding errors and typographical mistakes in the numerical implementation (ε3)
- boundary condition uncertainties (ε4)

- sampling errors (i.e. the data do not represent the required spatial and temporal averages) (ε5)
- measurement errors (ε6)
- human reliability (ε7)

The model inputs can have errors ε4, ε5 and ε6, while calibration data only can have errors ε5 and ε6. An error-free model should have results that equate error-free observations and therefore we can summarise the relationship between the actual model results and the actual observations by

$$M - \varepsilon 1 - \varepsilon 2 - \varepsilon 3 - \varepsilon 4 = O - \varepsilon 5 - \varepsilon 6 - \varepsilon 7$$

It is the goal of the modeller to achieve an error-free model by reducing the errors (ε1-ε4). However, the model structure errors ε2, numerical errors ε3, and the boundary condition errors ε4 are difficult to control by the modeller. So, the aim becomes to compensate as far as possible for ε2-ε4 by identification of the optimum effective parameter values. As such the best parameter estimates compensate for the other errors.

This dissertation therefore aimed at minimising the output uncertainty on the model results of river water quality models. The focus was on the parameter uncertainty and model input uncertainty. Different methodologies were applied in several steps of the modelling process and for each part the main conclusion is given here.

10.2.1. Model study plan

10.2.1.1 Effect of different river water quality model concepts used for river basin management decisions

The two main concepts in river water quality modelling in use today are QUAL2E and RWQM1. The focus in the two concepts are somewhat different. Here they were compared in view of their role in modelling present and future states of the river and for management decision-making. After such an analysis it becomes more clear what model concept to use. It is shown that for this case study on the Dender river, QUAL2E-based water quality models their model results of DO are mainly influenced by the algae processes whereas the RWQM1 is also taking into account sedimentation and stresses processes performed separately by different microbial communities.

In view of deciding on different pollution abatement scenarios, a RWQM1 model should be preferred over a QUAL2E-based model for evaluation of a scenario of reduced diffuse pollution, because it was shown that the sediment processes then become more important and RWQM1 simulates these.

The sensitivity of the model results with respect to the processes is not the same for the 2 river water quality modelling concepts and the different models are not always able to properly answer the same management problem. This clearly shows that managers should be aware of

the possibilities and limitation of the model they use and choose a model that fits their problem and expectations. Also, knowing which processes will become important after execution of a scenario can make that during model set up extra attention is paid towards those processes in order to get more reliable results.

10.2.1.2 Sensitivity analysis to identify 'soft data' for the evaluation of a river water quality model

In ungauged basins, the modeller has no data as input or for parameter calibration. Therefore any information that can be found about what kind of measurements are most important or anything that can be known about the parameters, even if it is only based on a first visual inspection of the catchment, is of great value.

With a sensitivity analysis of the sensitivity analysis it could be concluded that the model shows different sensitivities to the parameters in different external circumstances. A table in which external circumstances, here called soft data, i.e. data that are easily collected, are related to the importance of the parameters could be established. It is a first indicator of which parameters/processes one should focus on in a particular catchment characterised by the soft data. Knowing the most influential set of parameters is important for calibration of a model, optimal experimental design, uncertainty estimations and scenario analysis where other processes can become important compared to the base case.

10.2.2. Data collection

10.2.2.1 Optimal experimental design in river water quality modelling

In literature many examples exist of the application of optimal experimental design (OED) for model parameter estimation. What is common in all these researches is that the experimental conditions that define the experiment are 'controllable' in the experimental set-ups studied (typically reactors): temperature, time, pH, measurement frequency, initial concentration,… In OED for a natural river system, things become more complicated as a combination of different factors like temperature, flow and concentration is not occurring on the desired moments and as such, a method has to be found which maximises the content of information of experimental data, without knowing the exact situations under which those measurements will occur.

In this dissertation it is shown that OED methods can be used for an iterative, sequential design of a strategy for measuring water quality variables in a river, in view of the calibration of water quality models. In a first stage a relatively extensive set of measurements is needed to set up a model for the river. Using this initial model, the OED method enables the definition of efficient measurements strategies, to find better model parameter estimates and reduce the uncertainty in those estimates. In subsequent stages, the measurement strategy can be updated in an iterative way. This methodology is able to find sub-optimal sampling strategies with acceptable accuracy and for which also costs and practical limitations can be considered.

10.2.2.2 The evaluation of uncertainty propagation into river water quality predictions to guide future monitoring campaigns

Uncertainty analysis should not only be applied to obtain an idea on the uncertainty of the final model results or to calculate risk. It can also give indications for reducing the uncertainty. Here, the results of uncertainty analysis were evaluated to guide future monitoring campaigns. Parameters, diffuse and point pollution inputs were considered separately, providing information on the model sensitivity towards these three. It is obvious from the comparison between the global sensitivity analysis for the subgroups and for all most influencing inputs together that the parameters are most important. This shows that it is best to start with a good calibration of the model and then focus on obtaining more accurate input data.

Too often a model is calibrated with only one comprehensive measurement campaign. This is mostly not the most efficient way. When, for instance, only measurements during dry periods are made, the model cannot be well calibrated for the diffuse pollution part that is driven by rainfall. So it is better to perform two separate smaller measurement campaigns with the first one being 'exploring', while the second campaign is guided by previous analysis of the model results. The combination of the two monitoring campaigns can assure that at least some measurements are performed at 'the right moment', making the calibration process easier and more reliable.

It could be concluded that for the Dender River, measurements during dry periods can be used to better calibrate the model for point source pollution because the inputs of diffuse pollution are not important then. On the other hand, periods with rainfall and high flows are needed for the calibration of the model with diffuse pollution because the model output nitrate is then very sensitive towards the inputs related to farmer's practices.

When considering the influence of the uncertainty of the diffuse pollution inputs, the uncertainty bounds appeared sometimes to be too high to draw reliable conclusions from the model results. So, it showed the importance of accurate measurements and input data if the model results serve for decision support.

10.2.3. Model set up

Also in this step of the modelling process different actions can be done to assure a minimal output uncertainty. There is the need of profound checks of the input files, performance of test runs and checking mass balances. In this work, no additional research related to this step in the modelling process is performed.

10.2.4. Calibration and validation

10.2.4.1 Sensitivity analysis to define the most sensitive parameter subset for ayto)calibration of a river water quality model

Due to the complexity of models, they contain too many parameters to be able to change them all during an automatic calibration. A sensitivity analysis was performed to reduce the number of parameters in an automatic calibration procedure for the river water quality model of the Dender river, implemented in ESWAT. In the literature a lot of methods are described for

performing SA. It was first of all decided to use a global SA because of the non-linearity of the investigated water quality model. Another main advantage is that this technique is conceptually simple and is part of many software packages. It is a technique that cannot be used if the key assumptions of the regression analysis are not met because then, the results will not be robust. Also in the case of correlated inputs, the problem of multicollinearity can affect the robustness. This is the case when two variables are highly correlated and thus essentially convey the same information. Before applying the regression analysis technique for sensitivity and uncertainty analysis on the water quality model of the Dender River, these aspects were checked and it could be concluded that the technique was suitable.

The SA revealed that only around 10 parameters needed to be changed during calibration to obtain good fits between simulated and measured values, this for a particular aim, in this case to have good simulation results for the periods with DO concentrations below a critical value. When other criteria are considered, different parameters become important. In the validation was found that indeed the DO results are fitting well the measurements when the calibration was performed with the selected parameters for the amount of time that DO goes below a critical value. However, an additional calibration was needed to get good results for the nitrate simulations of the validation period.

10.2.4.2 Importance of the selection of model parameter subsets

For the complex models that are now available for river water quality modelling it becomes a very difficult task to calibrate all the model parameters. Parameters are correlated, some are not identifiable and many automatic calibration methods cannot even handle all the parameters at the same time. Therefore, it is common practice of modellers to fix part of the parameters on literature values or values that are provided together with the modelling software and only calibrate the model with a subset of parameters. Many modellers choose that subset of parameters themselves without performing a sensitivity analysis, relying on their expert knowledge or experience. From a questionnaire held among water quality modellers, some of these subsets were taken to calibrate the model with and the results were compared.

It was demonstrated that calibrating with different subsets of parameters gives very different model predictions and can lead to different conclusions. In the case study, the Dender river, the consequence of a wrong calibration could be that too many measures would be taken to increase the DO levels during spring and autumn while in reality this would not be necessary.

10.2.5. Model evaluation

10.2.5.1 Cost-effectiveness of in-stream aeration to improve river water quality

One of the strengths of water quality models is their predicting power. Without the need to implement measures around the river for pollution control, e.g reduction in fertiliser use on the surrounding fields, aeration of a river, building extra waste water treatment capacity and evaluate their performance once they are implemented, the influence of such measures can already be evaluated beforehand by performing model simulations. For the evaluation of the

cost-effectiveness of in-stream aeration, modelling is applied to evaluate different management options. The uncertainty on the results is also calculated and presented to present the quality of the scenario results. In literature a number of in-stream aeration techniques, natural as well as artificial, are described and documented. Their capability of transferring oxygen into the water, their power needs, their investment and maintenance costs are provided. Modelling of in-stream aeration is however very useful to evaluate the effect and to get an idea about the extent of reaeration needed to maintain a minimum dissolved oxygen level in a river, the accompanying aeration costs and also to see whether other measures exist that can avoid the need for aeration.

In-stream aeration is found to be a very effective measure for the compliance with dissolved oxygen standards in rivers. It can be switched on when needed, e.g. during crucial periods of low oxygen, e.g. in summer. This avoids excessive energy costs.

Comparison of different methods (fine bubble diffuser, mechanical aeration, the oxygenation/inversion system of Clean Flo), shows that aeration costs to obtain oxygen levels above 3 mg/l in the river Dender are about the same for all systems evaluated.

Other measures to raise the oxygen levels in the Dender were compared in terms of their effectiveness. The fundamental option, reducing the point pollution load, following the AWP 1999 plan, is the best option and ensures that oxygen levels are above critical levels the whole year. However, it is a very expensive option and it also takes a long period before it will be fully implemented: 16 years. In the meantime in-stream aeration techniques can help overcoming critical periods.

Uncertainty analysis on the results for the scenario 'with aeration' shows that it is possible for the dissolved oxygen content of the river to drop below 3 mg/l even when the designed aeration system is installed, albeit for very short periods. The uncertainty analysis also shows that the two options, with or without aeration are significantly different.

10.2.5.2 Assessment of the effect of shading on river water quality for the Nete river

Simulations were performed to evaluate the effect of planting trees along the river bank for shading. Uncertainty bounds accompany the results.

In literature it is suggested that shading might influence the water quality in small to medium water courses by reducing the solar radiation that reaches the water surface and the temperature of the water. A dynamic modelling approach is performed here to estimate the changes in water quality induced by shading of riparian vegetation. Such approach allows avoiding the prohibitive costs required for extensive field measurement campaigns.

It can be concluded that shading can effectively influence the water quality in a surface water body, in particular in streams that suffer from excessive algal growth during the summer periods. The reduction of algal growth due to a full shading scenario was estimated to be about 20% at the outlet of a 19.5 km long stretch of the river Nete in Belgium.

No significant positive effects of shading on the minimum, maximum and average concentrations of DO, COD, phosphates, ammonium and nitrates in the water were identified

however. Therefore, also the influence of shading on the exceedance of critical thresholds for several compounds was examined. A positive effect is seen on algal concentration. At the downstream section of the modelled stretch, the time of exceedance of a critical concentration of algal biomass was reduced to about half by complete shading of the stretch. A slightly negative effect of shading on the exceedance of the threshold value for DO was identified in the last stretch of the river and from the scenario analysis together with uncertainty analysis it can be inferred that shading does not significantly reduce or increase the lowest oxygen levels. The uncertainty concerning the difference between the scenarios contains both positive and negative values. However, a clear trend is here visible. In colder periods, when no algal growth occurs, the non-shaded scenario has higher oxygen concentrations, which become lower during warm periods with algal growth. In other words, in this system the algae actually increase the oxygen concentration because of the production of oxygen.

11. General conclusion

In this dissertation it was the overall objective to promote good modelling practices and to provide in a systematic way methods that help the water manager or engineer to minimise the uncertainty on his model results. Therefore, the methods developed in this work were chosen to be simple, straightforward, with easy to use software or with software that can easily be developed by the user. The methods and tools were applied on real case studies, either the river Dender or the river Nete, both in Belgium. It was found that by applying different methodologies on the models, uncertainty could be made smaller and a number of suggestions for better measurement campaigns were formulated. Measurement campaigns that aim to calibrate the model better for the low DO amounts in the river should preferably hold the spring period. When calibrating the model for the Dender river for point pollution measurements during dry periods are needed and for calibration of the model with diffuse pollution measurements during periods with rainfall and high flows are needed.

12. Perspectives

12.1. The ideal model

The ideal tool for river basin water quality management should incorporate all relevant process descriptions and enable the simulation of the output variables needed by decision makers of any kind, preferably without the need for calibration and with only small uncertainty bounds around the model results. These are probably too many wishes at the same time. However, with the available computational power and the development of better modelling techniques, it should be possible to come closer and closer to this ideal tool. Large research programs are focussing on water quality models and good modelling practices. A modeller can nowadays be guided through the whole process of model set-up with literature and spread sheets, in which all necessary steps are described. But still there are gaps in the available knowledge. These are mainly related to the model structure, to modelling of

ungauged basins, to the modelling of some subsystems like sediment flow and heavy metal behaviour. Further there is still the uncertainty about how the biological status of the river will follow the improvements of the physico-chemical water quality. Next to these knowledge gaps, also budgetary reasons are limiting progress in the development of river basin models. Monitoring is expensive and still better data, with both higher temporal and spatial resolution are needed for model calibration. Another important aspect in this matter is the separation between modellers and data gatherers. Data gathering is still a matter of collecting the necessary information for evaluation of the current state of the water bodies, and these data are often not satisfactory for use in model set-up. The communication between modellers and data collectors can still improve a lot as was also one of the major conclusions from the Harmoni-CA project (van Griensven et al., 2006).

Related to the knowledge gaps also during the work for this dissertation some points were found to still require future research.

12.1.1. Sensitivity analysis

The usefulness of sensitivity analysis as a first step in the modelling process is still underestimated. Care should be taken that the set of most important parameter set is taken for the calibration of the model, considering the purpose of the model study. Otherwise wrong conclusions can be drawn. Many sensitivity analysis methods exist. Each has its own advantages and disadvantages, but often only one technique is used, the one the modeller is familiar with. Clear guidance with decision trees should exist about the choice of a technique.

12.1.2. Optimal experimental design

The optimal experimental design performed in this dissertation should be extended with even more parameters of sampling layout to finally come to very efficient sampling layouts. Another extension should be the use of different evaluation criteria for the OED because other criteria than the maximization of the det(FIM) can be more suitable for the problem under consideration. Also a method of pareto optimisation allowing to optimise for more than one evaluation criterion at the same time, should be developed.

It cannot be expected that the modeller should create extensions on the software he uses himself to detect what additional data he needs. The development of OED tools that can easily be linked with modelling software is necessary. Further, because the process of the OED in river water quality modelling is an iterative process, the ideal way of working would be the automatic incorporation of new information and data coming from automatic measurement stations into the OED tool and the automatic adaptation of the current measurement set-up when the OED requires other data. This was already developed in EAST by De Pauw (2005), however still not available to modellers.

12.1.3. Ungauged basins

The study in this dissertation about the use of soft data to get a first idea about parameter values and sensitivities of the model was only done for water quality parameters. It should be extended to other parts of a catchment model like the parameters of the rainfall/runoff module

or the diffuse pollution processes. In this research the analysis of the results of simulations with different subsets of parameters was done visually and manually, to prove the usefulness and relevance of further study. It would be better and more complete to use a cluster method. Such a method can make use of clustering techniques in which the parameter sets that give more or less identical results for one variable are clustered. An example is to cluster according to amount of time of DO limit exceedance. Within these sets of parameters again other results, for other variables, can be considered for further clustering. Within the group of parameter sets that give low amount of time of DO limit exceedance, this might then give different subsets of important parameters according to the occurrence of summer algae blooms or not. Finally, information tables could be produced in which the modeller that is facing a model study in an ungauged basin can find basic information on the basis of soft data for his model set-up. Starting from there, the modeller can decide on performing a measurement campaign for detection or calibration of those parameters that are most crucial.

12.1.4. Guidelines about model selection

Although a lot of literature exists about different model concepts, still more research is needed to indicate under which circumstances, which model concepts, are preferable. This is especially in view of future changes to the system due to, for instance, changing land use, climate change, pollution reduction. Some parameter values can change or processes that are not modelled can suddenly become important and it is essential that the modeller is aware of this and is able to make an opinion of the possibilities but also of the limitations of the chosen model concept.

12.2. Overall perspective

As the uncertainty on model results becomes smaller, the predictive power will be better and more and more trust will be put on the use of models in water management. Automatically, more river basin management studies will be supported with modelling. This generates a positive loop, as more studies are asked, more money becomes available for research in modelling, extra monitoring can be done and knowledge gaps about model use will be filled. This in turn generates newer, better and more reliable models. For the moment, with the support of the European Commision, that acknowledges the need of river basin modelling for compliance with the Water Framework Directive, we entered this positive loop. More and more guidance related to modelling tools is freely available and we enter a period in which the modelling community is progressing fast towards making models a standard, irreplaceable tool in river basin management. It is a too positive idea thinking that model results will be 100 % reliable. Therefore uncertainty calculations have to be given with every model result that serves for predictions and for scenario evaluation so that the decision process can take into account uncertainties and risk. More and more there is awareness about this and uncertainty analysis will become less a “thing” that should be avoided but a standard procedure accompanying every model study.

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APPENDIX A: QUESTIONNAIRRE

Selection of parameters to be estimated during the calibration of river water quality models

For the prediction of river water quality, good models are needed. The calibration of a model is an important step in the process of ending up with a model suitable to describe the behaviour of the river under consideration.

For the calibration of a model, the modeller typically searches for the parameter values that minimise the difference between the measured and the predicted values (the objective function). This is not straightforward as most of the time the model has a large amount of parameters, some parameters can be correlated and some parameters can even be unidentifiable from the restricted set of available data. One can either calibrate the model by trial and error or one can choose to perform an automated calibration. In the latter case it is impossible to vary all the parameters during the optimisation and only the most sensitive or most important parameters are taken into account in the calibration.

A lot of combinations of parameter values can be able to minimise the prediction errors. When the model output for one selected variable is considered in a situation different from the one used to calibrate the model with, the outputs made by calibrated models with different parameter values can be expected to be almost identical. However, perhaps a bias may be introduced around critical or extreme values (figure A.1).

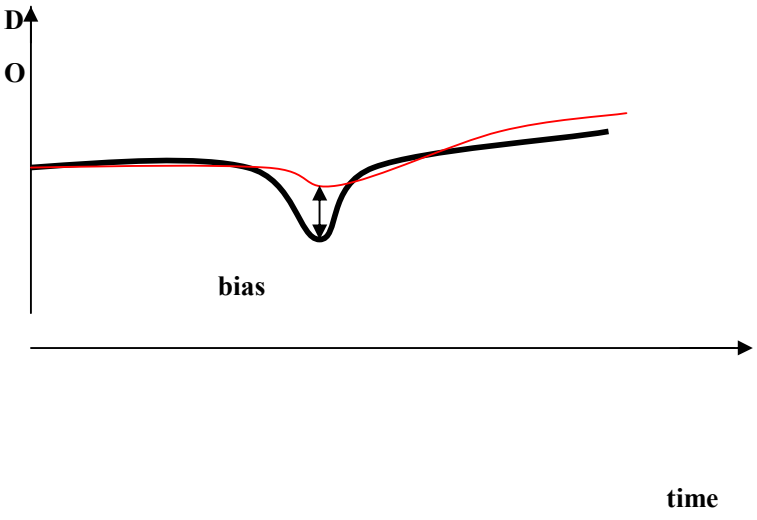

Figure A.1: the introduction of a bias when using two “different calibrated” models

It is difficult to decide what parameter set to use in the calibration in case the number of parameters is too large for the available data. Possibility is to first perform a sensitivity analysis on the model and to take the most sensitive parameters for the calibration. However,

in most cases the modeller starts to calibrate without first performing such a global sensitivity analysis.

The question remains whether the models used to predict river water quality are still useful when one doesn't know which calibration is best.

The following questionnaire is to get an idea on which parameters are considered to be a logical choice by modellers that calibrate a river water quality model, which parameters are varied during a calibration and which are set on a fixed value based on literature or previous research.
Many modellers today are now using calibrated models, both simple or very complex ones, and everyone is facing the same problems during calibration. It would be interesting to see how you are working during calibration, methods can be compared and the bias introduced by taking different parameter sets can be evaluated.

I will use the results of this questionnaire for my Phd-research "sensitivity and uncertainty analysis in river water quality modelling". First of all, the results of this questionnaire will be published and commented in a report (eventually a paper) which will be sent to everyone who filled in this questionnaire. Secondly, based on the results different selected parameter sets will be determined and used in the calibration of a modified QUAL2E model and a RWQM1 model, both implemented in ESWAT.

I think if everyone takes the time to fill in this questionnaire, we will all learn from it. In literature one finds a lot of model results and applications of a model but it is hard to find how one calibrated his/her model.

Thanks in advance.

This questionnaire takes 30 minutes to fill in the answers. Just follow the instructions on the questionnaire and when finished return it to the address below. If anything isn't clear, please feel free to contact me or my promotors, W. Bauwens (wbauwens@vub.ac.be) and P. Vanrolleghem (peter.vanrolleghem@biomath.rug.ac.be).

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The questionnaire

1. What kind of water quality model are you using now:

O Streeter-Phelps (Simple or extended)
O QUAL1
O QUAL2E
O RWQM1

2. You performed model calibration…

O many times
O a few times
O never

3. Which procedure are you using for calibration?

O trial and error, calibration for one variable
variable: …….
objective function:…….

O trial and error, calibration for different variables
variables: ……
objective function:…….

O auto-calibration, for one variable
variable: …….
objective function:…….

O auto-calibration, different variables at the same time
variables: ……
objective function:…….

4. When calibrating your model you take…

O the whole parameter set variable
O only a selected set of parameters variable

5. Are you first performing a sensitivity analysis before calibration?

O yes
O no
O sometimes

6. If Yes on question 5, what kind of sensitivity analysis?

O global sensitivity analysis
O local sensitivity analysis

7. If yes on question 5, which measures are you using to evaluate the sensitivity?

……
……
……
……
……

8. Are you first performing an identifiability analysis before calibration?

O yes
O no
O sometimes

9. **If yes on question 8, which measures are you using to evaluate the identifiability?**

……
……
……
……
……

10. Can you indicate the importance of the following parameters in the calibration process? (X = of little importance, XX = important, XXX = of many importance, indicate only those who are used during calibration!).
If some parameters are not used in your model, just cross them out, if some parameters are missing that also seem important, add them please. There is also an extra column to indicate the ranges of the parameters that you use.

QUAL2E

Variable	description	importance	range	units
Aio	ration of chlorophyll_a to algae biomass			
ai1	fraction of algae biomass that is nitrogen			
ai2	fraction of algae biomass that is phosphorus			
ai3	O2 production per unit algae growth			
ai4	O2 uptake per unit of algae respiration			
ai5	O2 uptake per unit of NH3 oxidation			
ai6	O2 uptake per unit of HNO2 oxidation			
μmax	maximum algae growth rate			
Rhoq	algae respiration rate			
Kl	Michaelis-Menton half-saturation constant for light			
kN	Michaelis-Menton half-saturation constant for Nitrogen			
kP	Michaelis-Menton half-saturation constant for Phosphor			
$\Lambda 0$	Minimum light intensity for algae bloom			
$\Lambda 1$	algal light self shading coefficient			
$\Lambda 2$	sediment shading coefficient			
pN	Algae preference factor for ammonia			
Kdd	Algae die-off rate			
RS1(:)	Local algae settling rate in the reach.			
RS2(:)	Benthic (sediment) source rate for dissolved phosphorus in the reach).			
RS3(:)	Benthic source rate for NH_4-N in the reach.			

Variable	description	importance	range	units
RS4(:)	Rate coefficient for organic N settling in the reach.			
RS5(:)	Organic phosphorus settling rate in the reach..			
RK1(:)	Carbonaceous biological oxygen demand deoxygenation rate coefficient in the reach.			
RK2(:)	Oxygen reaeration rate in accordance with Fickian diffusion in the reach.			
RK3(:)	Rate of loss of carbonaceous biological oxygen demand due to settling in the reach.			
RK4(:)	Benthic oxygen demand rate in the reach. If no value for RK4 is entered, the model sets RK4 = 2.0.			
RK5(:)	Coliform die-off rate in the reach.			
RK6(:)	Decay rate for arbitrary non-conservative constituent in the reach.			
BC1(:)	Rate constant for biological oxidation of NH_4 to NO_2 in the reach.			
BC2(:)	Rate constant for biological oxidation of NO_2 to NO_3 in the reach.			
BC3(:)	Rate constant for hydrolysis of organic N to NH_4 in the reach.			
BC4(:)	Rate constant for mineralization of organic P to dissolved P in the reach.			
Rktemp	rate constant for heat exchange			

RWQM1

Variable	description	importance	range	units
$Y_{H,aer}$	Yield for aerobic heterotrophic growth			
$Y_{H,anox,NO_3}$	Yield for anoxic heterotrophic growth with nitrate			
$Y_{H,anox,NO_2}$	Yield for anoxic heterotrophic growth with nitrite			
$f_{I,BAC}$	Fraction of respired heterotrophic and autotrophic biomass that becomes inert			
Y_{N1}	Yield for growth of 1st step nitrifiers			
Y_{N2}	Yield for growth of 2nd step nitrifiers			
$F_{I,ALG}$	Fraction of particulate organic matter that becomes inert during death of algae			
$Y_{ALG,death}$	Yield for death of algae (set to a value that avoids consumption of nutrients and oxygen)			
Y_{CON}	Yield for grazing (set to a value that avoids consumption of nutrients and oxygen)			
F_e	Fraction of incorporated biomass that is excreted as faecal pellets			
$f_{I,CON}$	Fraction of particulate organic matter that becomes inert during death of consumers			
$Y_{CON,death}$	Yield for death of consumers (set to a value that avoids consumption of nutrients and oxygen)			
Y_{YD}	Yield for hydrolysis (set to a value that avoids consumption of nutrients and oxygen)			

Variable	description	importance	range	units
$k_{death,ALG,To}$	Specific death rate for algae			
$k_{death,CON,To}$	Specific death rate for consumers			
$k_{gro,ALG,To}$	Maximum specific growth rate for algae			
$k_{gro,CON,To}$	Maximum specific growth rate for consumers per mass unit of grazed organisms			
$k_{gro,H,aer,To}$	Maximum aerobic specific growth rate of heterotrophs			
$k_{gro,H,anox,To}$	Maximum anoxic specific growth rate of heterotrophs			
$k_{gro,N1,To}$	Maximum specific growth rate of 1st stage nitrifiers			
$k_{gro,N2,To}$	Maximum specific growth rate of 2nd stage nitrifiers			
$k_{hyd,To}$	Hydrolysis rate constant			
$k_{resp,ALG,To}$	Maximum specific respiration rate of algae			
$k_{resp,CON,To}$	Maximum specific respiration rate of consumers			
$k_{resp,H,aer,To}$	Maximum aerobic specific respiration rate of heterotrophs			
$k_{resp,H,anox,To}$	Maximum anoxic specific respiration rate of heteroptrophs			
$k_{resp,N1,To}$	Maximum specific respiration rate of 2nd stage nitrifiers			
$k_{resp,N2,To}$	Maximum specific respiration rate of 1st stage nitrifiers			
$k_{eq,1}$	Rate constant for CO_2-HCO_3^- equilibrium*			
$k_{eq,2}$	Rate constant for HCO_3^--CO_3^{2-} equilibrium*			
$k_{eq,w}$	Rate constant for H_2O-OH^- equilibrium*			
$k_{eq,N}$	Rate constant for NH_4^+-NH_3 equilibrium*			
$k_{eq,P}$	Rate constant for $H_2PO_4^-$-HPO_4^{2-} equilibrium*			
$k_{eq,so}$	Rate constant for calcium carbonate equilibrium (in contrast to the equilibria above, in this case kinetic effects due to slow calcite precipitation or dissolution are typical)			
k_{ads}	Phosphate adsorption rate constant			
k_{des}	Phosphate desorption rate constant			
$K_{HPO4,ALG}$	Saturation coefficient for growth of algae on phosphate			
$K_{HPO4,H,aer}$	Saturation coefficient for aerobic growth of heterotrophs on phosphate			
$K_{HPO4,H,anox}$	Saturation coefficient for anoxic growth of heterotrophs on phosphate			
$K_{HPO4,N1}$	Saturation coefficient for growth of 1st stage nitrifiers on phosphate			
$K_{HPO4,N2}$	Saturation coefficient for growth of 2nd stage nitrifiers on phosphate			
$K_{N,ALG}$	Saturation coefficient for growth of algae on nitrogen			
$K_{NH4,ALG}$	Saturation coefficient for growth of algae on ammonia			
$K_{N,H,aer}$	Saturation coefficient for aerobic growth of heterotrophs on nitrogen			
$K_{NH4,N1}$	Saturation coefficient for growth of 1st stage nitrifiers on ammonia			
K_I	Saturation coefficient for growth of algae on light			
$K_{NO3,H,anox}$	Saturation coefficient for anoxic growth of heterotrophs on nitrate			
$K_{NO2,H,anox}$	Saturation coefficient for anoxic growth of heterotrophs on nitrite			
$K_{NO2,N2}$	Saturation coefficient for growth of 2nd stage nitrifiers on nitrite			
$K_{O2,ALG}$	Saturation/inhibition coefficient for endogenous respiration of algae			
$K_{O2,CON}$	Saturation/inhibition coefficient for endogenous respiration of consumers			
$K_{O2,H,aer}$	Saturation/inhibition coefficient for aerobic endogenous respiration of heterotrophs			

Variable	description	importance	range	units
$K_{O2,N1}$	Saturation/inhibition coefficient for aerobic endogenous respiration of 1st stage nitrifiers			
$K_{O2,N2}$	Saturation/inhibition coefficient for aerobic endogenous respiration of 2nd stage nitrifiers			
$K_{S,H,aer}$	Saturation coefficient for aerobic growth of heterotrophs on dissolved organic substrate			
$K_{S,H,anox}$	Saturation coefficient for anoxic growth of heterotrophs on dissolved organic substrate			
β_{ALG}	Temperature correction factor for algae growth rate			
β_{CON}	Temperature correction factor for consumer growth rate			
β_{H}	Temperature correction factor for heterotroph growth rate			
β_{hyd}	Temperature correction factor for hydrolysis			
β_{N1}	Temperature correction factor for 1st stage nitrifier growth rate			
β_{N2}	Temperature correction factor for 2nd stage nitrifier growth rate			

11. Did you consider correlation between your parameters during sensitivity analysis or calibration?

O yes
O no
O I will in the future

RESULTS

Qual2E: 14 answers
RWQM1: 3 answers

10 persons performed model calibration already a lot of times. Four persons did it a few times. The last ones use a trial and error method and if they first performed a sensitivity analysis they use a local sensitivity analysis.

Following procedures are used for calibration:

Trial and error, calibration for different variables
- NO_3, P, org C, org N, chl a with maximum likelihood method , root of mean squared residuals or boolean measures
- DO, BOD, NH_4, P, chl a, NO_3, curve fitting

Auto-calibration, different variables at the same time
- DO, HNO_3, NH_3, BOD, aggregation of mean squared errors by transformation in probabilistic scale, weighted sum of squared errors
- DO, BOD, SS, maximum likelihood method

Persons who make use of both methods prefer trial and error when there are not many data available and with sufficient data they use an auto-calibration.

Most persons are first performing a sensitivity analysis before calibration. That sensitivity analysis is for 8 persons a global sensitivity analysis and for the others a local sensitivity. People who do their calibration with trial and error perform only a local sensitivity analysis. Some people answered that they think that the sensitivity of the parameters is known by now so SA becomes unnecessary.

The measures used for sensitivity analysis are, the relative sensitivity coefficient, the normalised regression coefficient and even just the absolute change of the output due to changes of the input.

No one performs an identifiability analysis.

The following parameter sets are indicated as being important for the calibration (X = of little importance, XX = important, XXX= of many importance). (for the meaning of the parameters see appendix B)

QUAL2E	RWQM1
(Rk4 , bc3, rk3 (XXX)), (μmax, bc1, rs4, rk1, rhoq(XX)), (ai6, Λ1(X))	(F_e, $fi_{,bac}$, $k_{,death,alg,To}$, $k_{,death,conc,To}$(XXX))
(μmax, rk1(XXX)), (rs2, rs3, rk4, bc2(XX)), (kl, kp, kn, Λ0, pn, kdd, (X))	
(Rk2, rk4(XXX)), (rk1, bc1, bc2, bc3, bc1(XX)), (rs2, rs3, rs4, rs5, rk3 (X))	
Reaeration coefficient, decay rates, SOD	
(μmax, rk4, Λ1, rk1(XXX)), (kdd, rk2, Λ2, bc1(XX)), (kp, pn(X))	

No one considered correlation between the parameters.

5 CONCLUSIONS

This survey was send around to +/-100 persons who are working in the field of river water modelling. The response on this survey was positive but not many useful questionnaires have been returned. Most people work with already calibrated models to perform their research. They rely on the model results as being able to represent more or less the concentration levels and the seasonal variation in the river. The model is not calibrated for a particular river.
For the RWQM1-model only one person returned a completely filled in questionnaire. The use of this model is relatively new in the field and therefor not many people are using it in practical applications yet.
The people, who perform calibrations on the model they use, can be divided into two groups. The first group uses the power of computers to perform first a global sensitivity analysis and use the results of that analysis in an auto-calibration for different variables at the time. The other group still uses trial and error and performs first a local sensitivity analysis.
The calibrations are always done for different variables and only a selected set of the parameters is taken variable. From the results of this survey it is clear that if people start to calibrate their model with only the parameters that they consider “important” or of “many importance”, this set of parameters is not the same for everyone.

No one did take the effort to indicate the range of the parameters they vary in the calibration. Identifiability analysis seems a tool that is not used by river water quality modellers. No one considers correlation between his parameters.

DISCUSSION

Although there are many techniques available for the calibration of river water quality models, those techniques are not commonly used. The reasons can be that those techniques are too difficult, are not described to be understandable to everyone, are time-consuming or are not known to river water quality modellers. The model outputs of models that are not well calibrated can become very unreliable. It will be necessary to evaluate the uncertainty of critical values of river water quality variables related to the calibration process. Such an evaluation can help people to decide if it is worth to put time and effort into the calibration process.

APPENDIX B: BIOGEOCHEMICAL CONVERSION PROCESSES OF RWQM1

In this appendix a complete description of the biogeochemical process of RWQM1 equations is given. In order to apply the model, these biochemical process equations must be supplemented by transport equations, equations for substance transfer between adjacent river compartments and to the atmosphere, geometrical conversions between concentrations in the water column and surface densities of sessile organisms, etc.

The qualitative stoichiometric matrix of the model is given in Table B1; the stoichiometric parameters required to make all stoichiometric coefficients unique are listed in Table B2; the kinetic parameters are defined in Table B3; and the formulations of the process rates are given in Table B4. These definitions make the model stoichiometry unique up to the numerical values of the parameters.

In Table B1, the signs of all nonzero stoichiometric coefficients are given: "+" indicates a positive stoichiometric coefficient, "–" a negative coefficient, "?" indicates a coefficient the sign of which depends on the composition of the organic substances involved in the process and on the stoichiometric parameters, and "(+)" is the same as "?", but in this case, the composition of compounds and the stoichiometric parameters should be chosen in a way that guarantees that this coefficient is nonnegative (because there is no limiting factor to the corresponding compound in the process rate). In Table B4, limiting terms in square brackets can be omitted if the chosen stoichiometry is such that the corresponding component is not consumed.

Table B.1: Qualitative stoichiometric matrix of the complete River Water Quality Model No. 1

Component → *i*		(1)	(2)	(3)	(4)	(5)	(6)	(7)	(9)	(10)	(11)	(12)	(13)	(14)	(15)	(16)	(17)	(18)	(19)	(20)	(21)	(22)	(23)	(24)
j	Process ↓	S_S	S_I	S_{NH4}	S_{NH3}	S_{NO2}	S_{NO3}	S_{HPO4}	S_{O2}	S_{CO2}	S_{HCO3}	S_{CO3}	S_H	S_{OH}	S_{Ca}	X_H	X_{N1}	X_{N2}	X_{ALG}	X_{CON}	X_S	X_I	X_P	X_{II}
(1a)	Aerobic Growth of Heterotrophs with NH4	-		?				?	-	+			?			1								
(1b)	Aerobic Growth of Heterotrophs with NO3	-					-	?	-	+			?			1								
(2)	Aerobic Respiration of Heterotrophs			+				+	-	+			-			-1						+		
(3a)	Anoxic Growth of Heterotrophs with NO3	-				+	-	?		+			?			1								
(3b)	Anoxic Growth of Heterotrophs with NO2	-				-		?		+			?			1								
(4)	Anoxic Respiration of Heterotrophs			+			-	+		+			-			-1						+		
(5)	Growth of 1st-stage Nitrifiers			-		+		-	-	-			+				1							
(6)	Aerobic Respiration of 1st-stage Nitrifiers			+				+	-	+			-				-1					+		
(7)	Growth of 2nd-stage Nitrifiers					-	+	-	-	-			-					1							
(8)	Aerobic Respiration of 2nd-stage Nitrifiers			+				+	-	+			-					-1				+		
(9a)	Growth of Algae with NH4			-				-	+	-			-						1					
(9b)	Growth of Algae with NO3						-	-	+	-			-						1					
(10)	Aerobic Respiration of Algae			+				+	-	+			-						-1			+		
(11)	Death of Algae			(+)				(+)	(+)	?			?						-1		+	+		
(12a)	Growth of Consumers on XALG			(+)				(+)	-	?			?						-	1	+			
(12b)	Growth of Consumers on XS			(+)				(+)	-	?			?							1	-			
(12c)	Growth of Consumers on XH			(+)				(+)	-	?			?			-				1				
(12d)	Growth of Consumers on XN1			(+)				(+)	-	?			?				-			1				
(12e)	Growth of Consumers on XN2			(+)				(+)	-	?			?					-		1				
(13)	Aerobic Respiration of Consumers			+				+	-	+			-							-1		+		
(14)	Death of Consumers			(+)				(+)	(+)	?			?							-1	+	+		
(15)	Hydrolysis	+		(+)				(+)	(+)	?			?								-1			
(16)	Equilibrium CO2 ↔ HCO3									-1	1		+											
(17)	Equilibrium HCO3 ↔ CO3										-1	1	+											
(18)	Equilibrium H2O ↔ H +												1	1										
(19)	Equilibrium NH4 ↔ NH3			-1	1								+											
(20)	Equilibrium H2PO4 ↔ HPO4							1					+											
(21)	Equilibrium Ca ↔ CO3											+			1									
(22)	Adsorption of Phosphate							-1															1	
(23)	Desorption of Phosphate							1															-1	

Table B.2: Stoichiometric parameters

Symbol	Description	Unit
$Y_{H,aer}$	Yield for aerobic heterotrophic growth	gX_H/gS_S
$Y_{H,anox,NO_3}$	Yield for anoxic heterotrophic growth with nitrate	gX_H/gS_S
$Y_{H,anox,NO_2}$	Yield for anoxic heterotrophic growth with nitrite	gX_H/gS_S
$f_{I,BAC}$	Fraction of respired heterotrophic and autotrophic biomass that becomes inert	gX_I/gX_H
Y_{N1}	Yield for growth of 1st step nitrifiers	gX_{N1}/gS_{NH4}-N
Y_{N2}	Yield for growth of 2nd step nitrifiers	gX_{N2}/gS_{NO2}-N
$F_{I,ALG}$	Fraction of particulate organic matter that becomes inert during death of algae	$gX_I/g(X_S+X_I)$
$Y_{ALG,death}$	Yield for death of algae (set to a value that avoids consumption of nutrients and oxygen)	$g(X_S+X_I)/gX_{ALG}$
Y_{CON}	Yield for grazing (set to a value that avoids consumption of nutrients and oxygen)	gX_{CON}/gX_{ALG}
F_e	Fraction of incorporated biomass that is excreted as faecal pellets	gX_S/gX_{CON}
$f_{I,CON}$	Fraction of particulate organic matter that becomes inert during death of consumers	$gX_I/g(X_S+X_I)$
$Y_{CON,death}$	Yield for death of consumers (set to a value that avoids consumption of nutrients and oxygen)	$g(X_S+X_I)/gX_{CON}$
Y_{HYD}	Yield for hydrolysis (set to a value that avoids consumption of nutrients and oxygen)	gS_S/gX_S

Table B.3:Kinetic parameters

Symbol	Description	Units
$k_{death,ALG,To}$	Specific death rate for algae	T^{-1}
$k_{death,CON,To}$	Specific death rate for consumers	T^{-1}
$k_{gro,ALG,To}$	Maximum specific growth rate for algae	T^{-1}
$k_{gro,CON,To}$	Maximum specific growth rate for consumers per mass unit of grazed organisms	$L^3M^{-1}T^{-1}$
$k_{gro,H,aer,To}$	Maximum aerobic specific growth rate of heterotrophs	T^{-1}
$k_{gro,H,anox,To}$	Maximum anoxic specific growth rate of heterotrophs	T^{-1}
$k_{gro,N1,To}$	Maximum specific growth rate of 1st stage nitrifiers	T^{-1}
$k_{gro,N2,To}$	Maximum specific growth rate of 2nd stage nitrifiers	T^{-1}
$k_{hyd,To}$	Hydrolysis rate constant	T^{-1}
$k_{resp,ALG,To}$	Maximum specific respiration rate of algae	T^{-1}
$k_{resp,CON,To}$	Maximum specific respiration rate of consumers	T^{-1}
$k_{resp,H,aer,To}$	Maximum aerobic specific respiration rate of heterotrophs	T^{-1}
$k_{resp,H,anox,To}$	Maximum anoxic specific respiration rate of heteroptrophs	T^{-1}
$k_{resp,N1,To}$	Maximum specific respiration rate of 2nd stage nitrifiers	T^{-1}
$k_{resp,N2,To}$	Maximum specific respiration rate of 1st stage nitrifiers	T^{-1}
$k_{eq,1}$	Rate constant for CO_2-HCO_3^- equilibrium*	T^{-1}
$k_{eq,2}$	Rate constant for HCO_3^--CO_3^{2-} equilibrium*	T^{-1}
$k_{eq,w}$	Rate constant for H_2O-OH^- equilibrium*	$L^3M^{-1}T^{-1}$
$k_{eq,N}$	Rate constant for NH_4^+-NH_3 equilibrium*	T^{-1}
$k_{eq,P}$	Rate constant for $H_2PO_4^-$-HPO_4^{2-} equilibrium*	T^{-1}
$k_{eq,so}$	Rate constant for calcium carbonate equilibrium (in contrast to the equilibria above, in this case kinetic effects due to slow calcite precipitation or dissolution are typical)	$L^3M^{-1}T^{-1}$
k_{ads}	Phosphate adsorption rate constant	T^{-1}
k_{des}	Phosphate desorption rate constant	T^{-1}
$K_{HPO4,ALG}$	Saturation coefficient for growth of algae on phosphate	ML^{-3}
$K_{HPO4,H,aer}$	Saturation coefficient for aerobic growth of heterotrophs on phosphate	ML^{-3}
$K_{HPO4,H,anox}$	Saturation coefficient for anoxic growth of heterotrophs on phosphate	ML^{-3}
$K_{HPO4,N1}$	Saturation coefficient for growth of 1st stage nitrifiers on phosphate	ML^{-3}
$K_{HPO4,N2}$	Saturation coefficient for growth of 2nd stage nitrifiers on phosphate	ML^{-3}
$K_{N,ALG}$	Saturation coefficient for growth of algae on nitrogen	ML^{-3}
$K_{NH4,ALG}$	Saturation coefficient for growth of algae on ammonia	ML^{-3}
$K_{N,H,aer}$	Saturation coefficient for aerobic growth of heterotrophs on nitrogen	ML^{-3}
$K_{NH4,N1}$	Saturation coefficient for growth of 1st stage nitrifiers on ammonia	ML^{-3}
K_I	Saturation coefficient for growth of algae on light	EL^{-2}
$K_{NO3,H,anox}$	Saturation coefficient for anoxic growth of heterotrophs on nitrate	ML^{-3}

$K_{NO2,H,anox}$	Saturation coefficient for anoxic growth of heterotrophs on nitrite	ML^{-3}
$K_{NO2,N2}$	Saturation coefficient for growth of 2nd stage nitrifiers on nitrite	ML^{-3}
$K_{O2,ALG}$	Saturation/inhibition coefficient for endogenous respiration of algae	ML^{-3}
$K_{O2,CON}$	Saturation/inhibition coefficient for endogenous respiration of consumers	ML^{-3}
$K_{O2,H,aer}$	Saturation/inhibition coefficient for aerobic endogenous respiration of heterotrophs	ML^{-3}
$K_{O2,N1}$	Saturation/inhibition coefficient for aerobic endogenous respiration of 1st stage nitrifiers	ML^{-3}
$K_{O2,N2}$	Saturation/inhibition coefficient for aerobic endogenous respiration of 2nd stage nitrifiers	ML^{-3}
$K_{S,H,aer}$	Saturation coefficient for aerobic growth of heterotrophs on dissolved organic substrate	ML^{-3}
$K_{S,H,anox}$	Saturation coefficient for anoxic growth of heterotrophs on dissolved organic substrate	ML^{-3}
β_{ALG}	Temperature correction factor for algae growth rate	$°C^{-1}$
β_{CON}	Temperature correction factor for consumer growth rate	$°C^{-1}$
β_{H}	Temperature correction factor for heterotroph growth rate	$°C^{-1}$
β_{hyd}	Temperature correction factor for hydrolysis	$°C^{-1}$
β_{N1}	Temperature correction factor for 1st stage nitrifier growth rate	$°C^{-1}$
β_{N2}	Temperature correction factor for 2nd stage nitrifier growth rate	$°C^{-1}$

- * Rate constant need not have a value realistic for the chemical processes; the value simply must be large enough to guarantee that the concentrations are always very close to their equilibrium values.

The following processes are considered in the model (numbers correspond to rows in Tables B1 and B4):

- *(1) Aerobic Growth of Heterotrophs*: Growth of heterotrophic organisms using dissolved organic substrate, dissolved oxygen, and nutrients. If the organic substrate contains enough phosphorus ($\alpha_{P,XH} < Y_{H,aer}\ \alpha_{P,SS}$), no phosphate uptake from the surrounding water is necessary and the limiting term with respect to phosphate can be neglected. If there is not enough nitrogen in the substrate ($\alpha_{N,XH} > Y_{H,aer}\ \alpha_{N,SS}$), ammonia is consumed by process (1a). If ammonia concentrations become very low, there is a switch to the nitrate uptake process (1b). The ammonia limitation term in process (1a) and the whole process (1b) can be omitted if there is enough nitrogen in the substrate ($\alpha_{N,XH} < Y_{H,aer}\ \alpha_{N,SS}$). In this case, the excess nitrogen is released as ammonia by process (1a).
- *(2,6,8,10,13) Aerobic Endogenous Respiration*: Loss of biomass by aerobic endogenous respiration.

- *(3) Anoxic Growth of Heterotrophs*: Growth of heterotrophic organisms with oxygen gained by reducing nitrate to nitrite or nitrite to molecular nitrogen (denitrification; processes 3a and 3b, respectively). If $\alpha_{P,XH} < Y_{H,aer}\ \alpha_{P,SS}$, S_{HPO4} must be available for growth. In the process rate, the phosphate limitation term (square brackets in Table 3.5) is only present if this condition is fulfilled. This process is inhibited by the presence of dissolved oxygen.
- *(4) Anoxic Endogenous Respiration of Heterotrophic Organisms*: Loss of heterotrophic biomass in the absence of dissolved oxygen by endogenous respiration with nitrate (for simplicity this process is formulated as a one-step reduction of nitrate to molecular nitrogen in contrast to anoxic growth).
- *(5) Growth of 1st Stage Nitrifiers*: Growth of organisms that oxidise ammonia to nitrite.
- *(7) Growth of 2nd Stage Nitrifiers*: Growth of organisms that oxidise nitrite to nitrate. In order to avoid problems in the absence of ammonia, it is assumed that the nitrogen source for build up of biomass is also nitrite (due to the small contribution to nitrite consumption this assumption is not important).
- *(9) Growth of Algae*: Growth of algae by primary production. This process is divided into two subprocesses describing growth with ammonia (preferred) or nitrate as the nitrogen source. The Steele (1965) function is used to describe light limitation and light inhibition.
- *(11,14) Death of Algae or Consumers*: Conversion of algae or consumers to slowly degradable and inert organic matter by death, lysis, etc. With the degree of simplification in this model, which uses a constant composition of organic substances for each class, death of algae and consumers is difficult to describe. This is because dead organic material may have a composition other than algae or consumers. This problem is solved with the introduction of a yield coefficient for the death process that is used to make mass conservation of all elements possible without requiring an uptake of oxygen, nitrogen, phosphorus, or carbon during the death process. The disadvantage of this concept is that, depending on differences in the composition of algae and particulate organic matter, the process may release oxygen, ammonia, phosphate, and carbon dioxide. If there is not strong evidence for different composition of different classes of organic material, this problem can be solved by using the same composition for algae, consumers, and dead organic substances and setting these yield coefficients to unity.

- *(12) Growth of Consumers*: Growth of consumers by grazing on algae, on particulate organic matter, and on heterotrophic and autotrophic organisms (subprocesses 12a and 12e, respectively) with production of faecal pellets in the form of slowly biodegradable particulate organic matter. It is assumed that organic matter is homogeneously distributed. Note that this assumption may be violated for sessile organisms. A simple way to consider this fact is discussed in the case study of the River Glatt in Chapter 5. The yield coefficient must be small enough to guarantee the availability of enough nitrogen and phosphorus in the food for building consumer biomass. A very simple process rate proportional to the product of food and consumer concentrations was chosen. In some cases limiting terms with respect to food or consumers may be necessary.
- *(15) Hydrolysis*: Dissolution of slowly biodegradable particulate organic matter to dissolved organic matter catalysed by heterotrophic biomass. Similarly to the death processes, a yield coefficient is introduced to guarantee that no oxygen, ammonia, or phosphate be consumed during the hydrolysis process. If there is not strong evidence that the composition of particulate and dissolved organic matter is different, the same composition should be used and the yield coefficient set equal to unity.
- *(16-21) Chemical Equilibria*: Chemical equilibria between CO_2 and HCO_3^-, between HCO_3^- and CO_3^{2-}, between H_2O and H^+ and OH^-, between NH_4^+ and NH_3, between $H_2PO_4^-$ and HPO_4^{2-}, and between Ca^{2+} and CO_3^{2-} and $CaCO_3$(s).
- *(22) Adsorption of Phosphate*: Any type of binding of phosphate on particulate matter.
- *(23) Desorption of Phosphate*: Release of phosphate previously bound on particulate matter.

Note that all process formulations given above are based on *in-situ* concentrations of substrates and *in-situ* light conditions.

Table B.4: Process rates (terms in square brackets are omitted under certain circumstances, see text).

No.	Process	Rate
(1a)	Aerobic Growth of Heterotrophs with NH_4	$k_{gro,H,aer,To}e^{\beta_{gr}(T-T_o)}\frac{S_S}{K_{S,H,aer}+S_S}\frac{S_{O2}}{K_{O2,H,aer}+S_{O2}}\left[\frac{S_{NH4}+S_{NH3}}{K_{N,H,aer}+S_{NH4}+S_{NH3}}\right]\left[\frac{S_{HPO4}+S_{H2PO4}}{K_{HPO4,H,aer}+S_{HPO4}+S_{H2PO4}}\right]X_H$
(1b)	Aerobic Growth of Heterotrophs with NO_3	$\left[k_{gro,H,aer,To}e^{\beta_n(T-T_o)}\frac{S_S}{K_{S,H,aer}+S_S}\frac{S_{O2}}{K_{O2,H,aer}+S_{O2}}\frac{K_{N,H,aer}}{K_{N,H,aer}+S_{NH4}+S_{NH3}}\frac{S_{NO3}}{K_{N,H,aer}+S_{NO3}}\left[\frac{S_{HPO4}+S_{H2PO4}}{K_{HPO4,H,aer}+S_{HPO4}+S_{H2PO4}}\right]X_N\right]$
(2)	Aerobic Endogenous Respiration of Heterotrophs	$k_{resp,H,aer,To}e^{\beta_n(T-T_o)}\frac{S_{O2}}{K_{O2,H,aer}+S_{O2}}X_H$
(3a)	Anoxic Growth of Heterotrophs with NO_3	$k_{gro,H,anox,To}e^{\beta_n(T-T_o)}\frac{S_S}{K_{S,H,anox}+S_S}\frac{K_{O2,H,aer}}{K_{O2,H,aer}+S_{O2}}\frac{S_{NO3}}{K_{NO3,H,anox}+S_{NO3}}\left[\frac{S_{HPO4}+S_{H2PO4}}{K_{HPO4,H,anox}+S_{HPO4}+S_{H2PO4}}\right]X_H$
(3b)	Anoxic Growth of Heterotrophs with NO_2	$k_{gro,H,anox,To}e^{\beta_n(T-T_o)}\frac{S_S}{K_{S,H,anox}+S_S}\frac{K_{O2,H,aer}}{K_{O2,H,aer}+S_{O2}}\frac{S_{NO2}}{K_{NO2,H,anox}+S_{NO2}}\left[\frac{S_{HPO4}+S_{H2PO4}}{K_{HPO4,H,anox}+S_{HPO4}+S_{H2PO4}}\right]X_H$
(4)	Anoxic Endogenous Respiration of Heterotrophs	$k_{resp,H,anox,To}e^{\beta_n(T-T_o)}\frac{K_{O2,H,aer}}{K_{O2,H,aer}+S_{O2}}\frac{S_{NO3}}{K_{NO3,H,anox}+S_{NO3}}X_H$
(5)	Growth of 1st-stage Nitrifiers	$k_{gro,N1,To}e^{\beta_{n1}(T-T_o)}\frac{S_{O2}}{K_{O2,N1}+S_{O2}}\frac{S_{NH4}+S_{NH3}}{K_{NH4,N1}+S_{NH4}+S_{NH3}}\frac{S_{HPO4}+S_{H2PO4}}{K_{HPO4,N1}+S_{HPO4}+S_{H2PO4}}X_{N1}$
(6)	Aerobic Endogenous Respiration of 1st-stage Nitrifiers	$k_{resp,N1,To}e^{\beta_{n1}(T-T_o)}\frac{S_{O2}}{K_{O2,N1}+S_{O2}}X_{N1}$
(7)	Growth of 2nd-stage nitrifiers	$k_{gro,N2,To}e^{\beta_{n2}(T-T_o)}\frac{S_{O2}}{K_{O2,N2}+S_{O2}}\frac{S_{NO2}}{K_{NO2,N2}+S_{NO2}}\frac{S_{HPO4}+S_{H2PO4}}{K_{HPO4,N2}+S_{HPO4}+S_{H2PO4}}X_{N2}$
(8)	Aerobic Endogenous Respiration of 2nd-stage Nitrifiers	$k_{resp,N2,To}e^{\beta_{n2}(T-T_o)}\frac{S_{O2}}{K_{O2,N2}+S_{O2}}X_{N2}$

(9a)	Growth of Algae with NH_4	$k_{gro,ALG,To} e^{\beta_{ALG}(T-T_o)} \frac{S_{NH4}+S_{NH3}+S_{NO3}}{K_{N,ALG}+S_{NH4}+S_{NH3}+S_{NO3}} \frac{S_{NH4}+S_{NH3}}{K_{NH4,ALG}+S_{NH4}+S_{NH3}} \frac{S_{HPO4}+S_{H2PO4}}{K_{HPO4,ALG}+S_{HPO4}+S_{H2PO4}} \frac{I}{K_I} \exp\left(1-\frac{I}{K_I}\right) X_{ALG}$
(9b)	Growth of Algae with NO_3	$k_{gro,ALG,To} e^{\beta_{ALG}(T-T_o)} \frac{S_{NH4}+S_{NH3}+S_{NO3}}{K_{N,ALG}+S_{NH4}+S_{NH3}+S_{NO3}} \frac{K_{NH4,ALG}}{K_{NH4,ALG}+S_{NH4}+S_{NH3}} \frac{S_{HPO4}+S_{H2PO4}}{K_{HPO4,ALG}+S_{HPO4}+S_{H2PO4}} \frac{I}{K_I} \exp\left(1-\frac{I}{K_I}\right) X_{ALG}$
(10)	Aerobic Endogenous Respiration of Algae	$k_{resp,ALG,To} e^{\beta_{ALG}(T-T_o)} \frac{S_{O2}}{K_{O2,ALG}+S_{O2}} X_{ALG}$
(11)	Death of Algae	$k_{death,ALG,To} e^{\beta_{ALG}(T-T_o)} X_{ALG}$
(12 a-e)	Growth of Consumers on X_i	$k_{gro,CON,To} e^{\beta_{CON}(T-T_o)} \frac{S_{O2}}{K_{O2,CON}+S_{O2}} X_i X_{CON}$, i = ALG, S, H, N1, N2
(13)	Aerobic Endogenous Respiration of Consumers	$k_{resp,CON,To} e^{\beta_{CON}(T-T_o)} \frac{S_{O2}}{K_{O2,CON}+S_{O2}} X_{CON}$
(14)	Death of Consumers	$k_{death,CON,To} e^{\beta_{CON}(T-T_o)} X_{CON}$
(15)	Hydrolysis	$k_{hyd,To} e^{\beta_{hyd}(T-T_o)} X_S$
(16)	Equilibrium $CO_2 \leftrightarrow HCO_3^-$	$k_{eq,1}(S_{CO2} - S_H S_{HCO3} / K_{eq,1})$
(17)	Equilibrium $H^+ \leftrightarrow OH^-$	$k_{eq,2}(S_{HCO3} - S_H S_{CO3} / K_{eq,2})$
(18)	Equilibrium $HCO_3^- \leftrightarrow CO_3^{2-}$	$k_{eq,w}(1 - S_H S_{OH} / K_{eq,w})$
(19)	Equilibrium $NH_4^+ \leftrightarrow NH_3$	$k_{eq,N}(S_{NH4} - S_H S_{NH3} / K_{eq,N})$
(20)	Equilibrium $H_2PO_4^- \leftrightarrow HPO_4^{2-}$	$k_{eq,P}(S_{H2PO4} - S_H S_{HPO4} / K_{eq,P})$
(21)	Equilibrium $Ca^{2+} \leftrightarrow CO_3^{2-}$	$k_{eq,s0}(1 - S_{Ca} S_{CO3} / K_{eq,s0})$
(22)	Adsorption of Phosphate	$k_{ads} S_{HPO4}$
(23)	Desorption of Phosphate	$k_{des} X_P$

APPENDIX C: BIOCHEMICAL PROCESSES IN QUAL2E

Water column processes

The river column variables are expressed in mg/l, the river bed variables as g/m^2 and the river depth H in m.

Table C.1: Water column processes

Process	*rate*	*O_2*	*C/BOD*	*org. N*	*org.P*	*diss. P*	*abs. P*	*NH_3-N*	*HNO_2-N*	*HNO_3-N*	*algae*	*Bed C/BOD*	*Bed Org N*	*Bed Org P*	*Bed AdsP*	*Plants*
Reaeration	R *(DOsat-DO)	+1														
C/BOD degradation	rk1*γrk1*f(DO)*C/BOD	-1	-1													
Algal growth	if light > λ f(light)*f(algae)*f(sediment)*min(fN, fP)*μmax*γμ*algae	+ai3				-ai2		-F*ai1		-(1-F) ai1	+1					
Algal respiration	rhoc*γrhoc *algae	-ai4				+ai2		+F*ai1		+(1-F) ai1	-1					
Algal death	rd*algae		+ai3	+ai1	+ai2						-1					
Hydrolysis org N	bc3* γbc3*organic N			-1				+1								
Hydrolysis org P	bc4*γbc4*organic P				-1	+1										
Nitrification to nitrite	bc1*(1-exp(-0.6*DO) *γbc1*NH3-N	-ai5						-1	+1							
Nitrification to nitrate	bc2*(1-exp(-0.6*DO)*γbc2*HNO2-N	-ai6							-1	+1						
De-nitrification	if DO < 2 mg/l rk5*γrk5*HNO_3-N									-1						
P adsorption/ desorption	rk6*γrk6 (P_{abs-eq}-P_{ads})					-1	+1									

Water bed exchange

The river column variables are expressed in mg/l, the river bed variables as g/m^2 and the river depth H in m.

Table C.2: Water bed exchange

Process	*rate*	*O_2*	*BOD*	*org. N*	*org. P*	*diss. P*	*abs. P*	*NH_3*	*HNO_2*	*HNO_3*	*algae*	*Bed C/BOD*	*Bed Org N*	*Bed Org P*	*Bed AdsP*	*Plants*
Algal settling	rs1*γrs1*algae										-1/H	+ai3	+ai1	+ai2		
C/BOD settling	rk3*γrk3*C/BOD		-1/H									+1				
Organic N settling	rs4*γrs4*organic N			-1/H									+1			
Organic P settling	rs5*γrs5*organic P				-1/H									+1		
Benthic diss P production	rs2*γrs2					+1/H								-1		
Benthic ammonia production	rs3*γrs3							+1/H					-1			
Benthic oxygen uptake	rk4*γrk4*DO	-1/H										-1				
Sedimentation/bed degradation	power equation						-AdsP/SS								+H*(adsP/SS)	
Plant photosynthesis	f(light)*rp1*γrp1*plants	+1/H														+1
Plant respiration	rp2*γrp2* plants	-1/H														-1

The extended QUAL2E processes

Table C.3: Extended QUAL2E processes

Process *rate*	S_O	X_S	X_N	X_P	S_P	X_{ADP}	S_{NH}	S_{NO2}	S_{NO3}	X_A	$X_{S,S}$	$X_{N,S}$	$X_{P,S}$	$X_{ADP,S}$	$X_{A,S}$
Reaeration $R*(S_{O,sat}-S_O)$	+1														
COD decay $rk1*\gamma rk1*f(S_O)*X_S$	-1	-1													
Algae growth *if light* > λ $f(light)*f(X_A)*f(sediment)*min(f(S_N),f(S_P))*\mu max*\gamma\mu*X_A$	+ai3				-ai2		-F* ai1		-(1-F) ai1	+1					
Algae respiration rhoc*γrhoc *X_A	-ai4				+ai2		+F* ai1		+(1-F) ai1	-1					
Algal death $rd*X_A$		+ai 3	+ai1	+ai2						-1					
Hydrolysis org N $bc3*\gamma bc3*X_N$			-1				+1								
Hydrolysis org P $bc4*\gamma bc4*X_P$				-1	+1										
Nitrification to nitrite $bc1*(1-exp(-0.6*DO)*\gamma bc1*S_{NH}$	-ai5						-1	+1							
Nitrification to nitrate $bc2*(1-exp(-0.6*S_O)*\gamma bc2*S_{NO2}$	-ai6							-1	+1						
De-nitrification if S_O < 2 mg/l $rk5*\gamma rk5*S_{NO3}$									-1						
P adsorption/ desorption $rk6*\gamma rk6\ (X_{ADP-eq}-P_{ads})$					-1	+1									
Algal settling $rs1*\gamma rs1*X_A$										-1/H	+ai3	+ai1	+ai2		
Org Carbon settling $rk3*\gamma rk3*X_S$		-1/H									+1				
Organic N settling $rs4*\gamma rs4*X_N$			-1/H									+1			
Organic P settling $rs5*\gamma rs5*X_P$				-1/H									+1		
Benthic diss P production rs2*γrs2					+1/H								-1		
Benthic ammonia production $rs3*\gamma rs3$							+1/H					-1			
Benthic oxygen uptake $rk4*\gamma rk4*S_O$	-1/H										-1				
Sedimentation/bed degradation						-(X_{ADP}								+H*(X	

power equation						$/X_I)$								$_{ADP}/X_I)$	
Plant photosynthesis $f(light,X_{A,S})*f(X_{A,S})*rp1*\gamma rp1*X_{A,S}$	+1/H														+1
Plant respiration $rp2*\gamma rp2*X_{A,S}$	-1/H														-1

APPENDIX D: EMISSION LIMITS IN EUROPE

Table D.1: Emission limits in Europe

			BOD				COD		Total Nitrogen		Total Phosphorous		Ammonia		
Country	Legislation	Category	General	Monthly	Weekly	Removal	General	Removal	General	Removal	General	Removal	General	Monthly	Weekly
			[mg/l]	[mg/l]	[mg/l]	[%]	[mg/l]	[%]	[mg/l]	[%]	[mg/l]	[%]	[mg/l]	[mg/l]	[mg/l]
general	EU UWWTD 91/271/EEC	2 000 – 10 000 PE	25			70 – 90	125	75							
		10 000 – 100 000 PE	25			70 – 90	125	75	15	70 – 80	2	80			
		> 100 000 PE	25			70 – 90	125	75	10	70 – 80	1	80			
Germany	wastewater Ordinance June 2004 (Federal Law Gazette I p. 1106)	Size Category 1 Less than 60 kg/d BOD_5	40				150								
		Size Category 2 60 to 300 kg/d BOD_5	25				110								
		Size Category 3 300 to 600 kg/d BOD_5	20				90						10		
		Size Category 4 600 to 6,000 kg/d BOD_5	20				90		18		2		10		
		Size Category 5 larger than 6,000 kg/d BOD_5	15				75		10		1		10		