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Immission based real-time control of the integrated urban wastewater system

Immissiegebaseerde real-time controle van het geïntegreerd stedelijk afvalwatersysteem

door
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Woord vooraf

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Contents

List of symbols and abbreviations

A	Area of flow cross-section (L^2)
a.s.l.	above sea level
ANN	Artificial neural networks
ASM	Activated sludge model
ATS	Aeration tank settling
BATNEEC	Best available technology not entailing excessive costs
BOD	Biochemical oxygen demand
BPR	Biological phosphorus removal
b	specific decay rate (T^{-1})
B	Water surface width (L)
C_i	concentration of component i (ML^{-3})
CFD	Computational fluid dynamics
COD	Chemical oxygen demand
CSO	Combined sewer overflow
CSTR	Continuously stirred tank reactor
CWA	Clean water act
DAE	Differential and algebraic equations
DO	Dissolved oxygen
DO_{sat}	Oxygen saturation concentration (g/m^3)
DO_{SP}	Setpoint for dissolved oxygen (g/m^3)
DWF	Dry weather flow
ELV	Emission limit value
EQO	Environmental quality objectives
EQS	Environmental quality standards
FIS	Fundamental Intermittent Standards
$F_{overload}$	The maximum overload allowed to the WWTP
GA	Genetic algorithms
GIS	Geographic information systems
ICS	Integrated catchment simulator
IE	Inhabitant equivalents
IUWS	Integrated urban wastewater system
K_1	First order degradation constant for BOD ($d-1$)
K_La	Reaeration constant ($d-1$)
K_{LAS}	First order degradation rate of LAS (T^{-1})
$K_{S,(i)}$	half-velocity constant (of component i) (ML^{-3})
LAS	Linear alkylbenzene sulfonate
LEDA	Library of efficient data types
LTI	Linear time invariant
LQG	Linear quadratic Gaussian
$M_{(i)}$	mass (of component i) (M)
$\mu_{(j)}$	specific growth rate (of biomass species j) (T)
MBPC	Model based predictive control
MIMO	Multiple input multiple output

MLSS	Mixed liquor suspended solids
MSL	Model specification language
NPDES	National pollution discharge elimination system
ν_{ij}	stoichiometric coefficient for the species j with respect to the substrate i
ODE	Ordinary differential equation
PBRTC	Pollution based real-time control
PDE	Partial differential equation
PE	Population equivalents
PRBS	Pseudo random binary sequence
Φ_{i_α}	flux of component i in the flux at terminal α (MT^{-1})
Q	Flow rate (L^3T^{-1}]
r_j	process rate for the species j ($ML^{-3}T^{-1}$)
R_i	reaction rate of component i ($ML^{-3}T^{-1}$)
ρ_i	density of component i (ML^{-3}), process rate of reaction i
RAS	Return activated sludge
RI	Robustness index
RTC	Real-time control
RWQM1	River Water Quality Model No.1
S_f	Friction slope
S_i	Concentration of soluble component i (ML^{-3})
S_o	Bed slope
SCE	Shuffled complex evolution
SS	Suspended solids
SRT	Sludge residence time
SSE	Sum of squared errors
t	Time (T)
ThOD	Theoretical oxygen demand
TKN	Total Kjeldahl nitrogen
TP	Total phosphorus
TSS	Total suspended solids
TMDL	Total maximum daily load
TOC	Total organic carbon
UES	Uniform emission standards
UPM	Urban pollution management
V	volume (L^3)
VFA	Volatile fatty acids
WAS	Waste activated sludge rate
WFD	Water framework directive
WQBRTC	Water quality based real-time control
WWTP	Wastewater treatment plant
x	Distance (L)
X_i	concentration of particulate component i or biomass (ML^{-3})
y	flow depth (L)
$Y_{(i)}$	yield coefficient for growth (on substrate i) (MM^{-1})

Subscripts

A	Autotrophic bacteria
B	Biomass
H	Heterotrophic bacteria
O	oxygen
S	biodegradable substrate

Chapter 1

Introduction

All societies, dating from the times of early civilisation, have had to deal with problems related to the provision of safe drinking water, flood protection, drainage and sanitation (Chocat *et al.*, 2001). Nevertheless, depending on the different geographical contexts and population expectations, many of those problems remain unsolved and others arise.

The construction and operation of municipal drainage systems has been historically driven by two objectives: (1) to maintain public hygiene and (2) to prevent flooding. Only later the aspect of pollution control became important and treatment facilities have been introduced to preserve the aquatic ecosystem. The advance of mathematical models as tools for design and operation of the system followed this historical development. Detailed models of sewers, treatment plants and receiving waters have been created to describe the performance according to the individual needs and objectives.

Today's challenge is to move from such individual consideration of system performance to an integrated management of the urban wastewater system. Appropriate numerical tools are required to predict the behaviour of the complete system under historical and future scenarios. Still, although the basic principles are known (Lijklema *et al.*, 1993), the development of integrated models proves to be a challenging task. The main bottleneck is the complexity of the total system that prevents a simple linkage of the existing detailed models of the individual subsystems to an entity.

This joint consideration is also required by the recently adopted Water Framework Directive (WFD) of the EU, which mainly focuses on the quality of the receiving water, which should be "good" both in terms of ecological status and chemical quality. In view of this legislation, management practices that take the immission concentrations (i.e. the concentrations in the river) into account are necessary in order to be able to comply with the requirements of the WFD.

In this work, the requirements for and possibilities of immission based real- time control (RTC) in the integrated urban wastewater system (IUWS), are explored. The urban wastewater system is composed of the sewer system and the wastewater treatment plants. These systems discharge more or less polluted water into the receiving water, either a river or a lake. The effluent from the treatment plant is continuously discharged into the receiving

water. A continuous flux of pollutants is entering the river and has a permanent influence on the river water quality downstream the treatment plant.

In dry periods the sewer system has sufficient hydraulic capacity to transport all the wastewater towards the treatment plant, where it is treated to remove a majority of the pollutants. During rain events, this situation is changed. In urban areas, large parts of the surface are covered with impervious surfaces, such as roofs, roads, parking places, ... Above a certain rainfall intensity and duration, all depressions on these impervious surfaces are filled, and the rain starts to run off the surface, entering the combined or the separate sewer system. As a consequence, the flow in the sewer system is increased, and the wastewater is diluted. This has two consequences for the efficiency of the treatment plant. First, due to the increased flow, the hydraulic residence time in the plant is reduced, leading to a decreased treatment efficiency. Second, the efficiency of the biological treatment is reduced since the incoming wastewater is diluted. Also, other effects may influence the behaviour of the treatment plant.

During medium and heavy rain events, the flow in the sewer system might exceed its hydraulic capacity, causing the water to leave via emergency overflows leading to a so-called combined sewer overflow. In this case, untreated water is entering the river, causing a sudden increase in the concentrations of pollutants. This obviously has a detrimental effect on the ecology of the river.

These interactions between the sewer system, the treatment plant and the receiving water are fairly complex and cannot be understood straightforwardly. Mathematical models can be used to increase the understanding of the behaviour of the subsystems of the urban wastewater system. Since long, models have been created to describe both the hydraulics and the quality process of the sewer system, treatment plant and rivers. These models have been used with varying levels of success. In order to design and tune an immission based RTC strategy, a simultaneously simulating model is necessary. In this way, two way interaction between the different submodels is possible. By using immission based RTC, the existing infrastructure can be used more efficiently. However, additional sensors, actuators and communication hardware and software need to be installed and operated in a fail-safe way.

Outline of the thesis

The different chapters in this thesis can be grouped in three main parts. In a first part, the state-of-the-art in integrated modelling and control will be explained, togehter with the simulator used in this work. The second part deals with the problems to be tackled when creating an integrated model and the solutions proposed in this work. The third part describes the development and application of an immission based RTC strategy.

Chapter 2 starts with a general introduction about the IUWS, followed by the legislational framework that has an influence on the management of IUWSs. The second part of this chapter gives an overview of the mathematical models used in literature for the different subsystems, together with the RTC possibilities within these subsystems. Also the state-of-the-art on integrated modelling and integrated RTC are discussed.

Chapter 3 describes the simulation software WEST that has been developed and used within this research. Special attention is paid to the implementation of the models of the sewer system and rivers.

Chapter 4 is a key chapter, and outlines the general procedure that will be used to build a model that can be used for the design and tuning of an immission based control strategy. Three key problems are outlined and a general solution proposed. In the next chapters, the different parts of this procedure are applied and evaluated.

Chapter 5 describes the model simplification and model reduction as proposed in chapter 4 to the activated sludge model No. 2d model. The simplification uses a grey box model, while the model reduction eliminates several state variables and/or processes.

Chapter 6 describes the model simplification to the river hydraulics and pollution propagation. A complex mechanistic model using the "de Saint-Venant" equations is used to generate data to calibrate the simplified model.

Chapter 7 describes the application of the general concepts of chapter 4 to the Lambro catchment in order to predict the immission concentration of biodegradable detergent, LAS, responsible for 1% of the BOD in household wastewater. Only the wastewater treatment plant (WWTP) and the river are taken into account in this case study.

Chapter 8 describes the case study of the catchment of Tielt. Both model simplification and model reduction are applied to obtain a control model that is used to tune two immission based control strategies. These strategies are evaluated both from an emission and immission point of view.

Chapter 9 describes the application of a predictive model to optimise the dissolved oxygen concentration. The predictive model is used as a software sensor which can be used to control the WWTP and the sewer systems.

Chapter 10 draws some general conclusions about the thesis. In the last part, a general discussion and perspectives are presented.

Chapter 2

Literature Review

2.1 The integrated urban wastewater system

The integrated urban wastewater system considered in this thesis consists of three main components: the sewer system, the wastewater treatment plant (WWTP) and the receiving water. This part of the global water system has of course links with other parts like groundwater, rural streams, drinking water production, agricultural runoff and seas. The focus however, lies on the effect of urban settlements on the water quality of the receiving waters in the neighbourhood of cities and villages. Therefore, only these subsystems will be discussed. A schematic overview of an urban wastewater system as dealt with in this thesis is shown in Fig. 2.1.

2.1.1 The sewer system

Provision of safe drinking water, flood protection, drainage and sanitation rank highly among the needs of all societies. Urban drainage systems with stormwater drain systems, sewers and manholes have since long been used to address these issues (Marsalek *et al.*, 1993). Pipes are used to transport both the rain water and the wastewater out of the

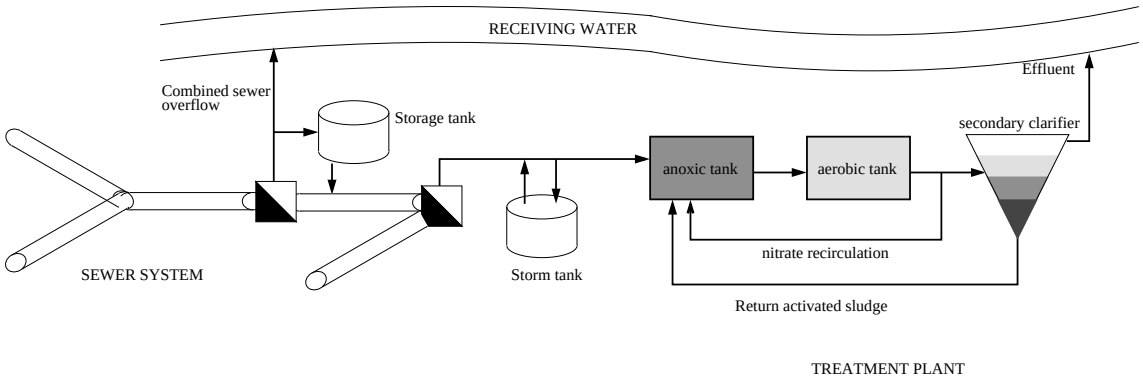


Figure 2.1: The integrated urban wastewater system studied in this thesis

urban area as quickly as possible. These sewer pipes lead the water either directly to the receiving water or to a wastewater treatment plant. The wastewater that enters the receiving water with or without treatment, will have a detrimental effect on the water quality in the river.

Basically two types of sewer systems can be distinguished: separate and combined sewer systems. Separate sewer systems have two pipes for transporting the water out of the city, one for the rain water and one for the wastewater. The main advantage is that the wastewater is not diluted during rain, and can hence be treated more efficiently. Moreover, no combined sewer overflows can occur, reducing the amount of pollution leaving the sewer system. Disadvantages are the higher construction costs, the risk of misconnection, sudden and strong hydraulic impact to rivers, and higher heavy metal load to the receiving water.

Combined sewer systems have only one pipe where the stormwater and the wastewater are mixed and transported together. The advantage is that only one pipe needs to be constructed. The disadvantage is that during rain events, the flow to the treatment plant is increased while the pollutants are diluted, which reduces the efficiency of the treatment plant. If the flow in the sewer system becomes higher than the hydraulic capacity of the pipes or the WWTP, the water leaves the system via emergency exits, or combined sewer overflows (CSOs) and enters the receiving water without treatment, causing acute pollution at such a discharge point. In order to reduce the amount of combined water spilled at the CSOs, storm tanks may be built in the system, to store a certain volume of storm water before the CSOs start to spill. In this way, both the frequency and the volumes of spilling are reduced.

2.1.2 The wastewater treatment plant

The wastewater in the sewer system is transported to the treatment plant. At this point, the water may be treated in different ways before being discharged to the environment: it may receive physical treatment (like sedimentation or filtration), chemical treatment (like precipitation or flocculation) or biological treatment (degradation of the waste by bacteria) (Metcalf and Eddy, 1991). Municipal wastewater is mostly treated in biological wastewater treatment plants, where the main purification step is carried out by bacteria. Different plant layouts can be used, but most systems consist of a series of unit processes like activated sludge systems, biofilters, natural systems (like reed beds) or anaerobic systems in combination with one or more physical or chemical treatment processes.

In the past, the treatment of wastewater focused on the removal of organic carbon. Bacteria are brought in contact with the wastewater containing oxygen and the organic pollutants in the wastewater. A common measure of expressing the concentration of organic material is the chemical oxygen demand (COD). The COD is the amount of oxygen used when organic material is completely oxidised to carbon dioxide. The bacteria partially transform the COD into carbon dioxide, and partially in new bacteria. In this way, the oxygen depleting effect of the wastewater on the receiving water can be reduced drastically.

With increasing population densities and corresponding volumes of wastewater, another negative effect on the receiving water has become evident: enrichment with nutrients or eutrophication. These nutrients (mainly nitrogen and phosphorus) allow algae to grow abundantly, leading to algal blooms. These large amounts of algae consume a lot of oxygen during the night, leading to very low oxygen concentrations, which might be lethal for the aquatic fauna. For this reason, wastewater treatment plants have been forced to upgrade towards nutrient removal. For nitrogen, the nitrification - denitrification pathway (with internal recirculation of the wastewater) has been used traditionally. The oxygen used to oxidise the ammonium-nitrogen into nitrate-nitrogen is partially reused to remove organic carbon (COD) in the denitrification step where the nitrate is transformed into nitrogen gas that escapes to the atmosphere.

Phosphorus cannot be transformed into a gaseous form, so it has to be removed with the excess sludge. Two ways are used to store the phosphorus into or onto the sludge: chemical precipitation and biological phosphorus removal (BPR). In the first way, chemical precipitation, a chemical (usually iron) is added so that the insoluble ferric phosphate is formed, which attaches to the sludge flocs. In the second way, biological phosphorus removal, special bacteria are involved. When exposed to a certain sequence of anaerobic and aerobic or anoxic conditions, these bacteria are capable of storing phosphorus into polyphosphates in relatively large concentrations. In this way, phosphates can be removed with the excess sludge.

The most frequently used system in which these processes occur, is probably the activated sludge system. It basically consists of a series of activated sludge tanks in which different conditions (anaerobic, anoxic and aerobic) prevail to promote the nutrient removal processes described above. The sludge is separated from the effluent in a secondary clarifier or settling tank. This is possible since the bacteria in the activated sludge tanks tend to grow in flocs with a density greater than the density of water. They therefore settle within a reasonable time period and can be separated from the effluent. Fig. 2.1 shows a schematic overview of a simple activated sludge plant.

2.1.3 The receiving water

In general, three types of receiving waters can be distinguished: rivers, lakes and seas. In Flanders, only rivers are used frequently as a discharge point for effluents from the WWTP. Also the combined sewer overflows usually spill into brooks, rivers or streams. These urban rivers also have a lot of other functions: transport, recreation, fishing, drinking water production, irrigation and habitat for aquatic fauna. All these functions can only be maintained by the combination of two factors, the quantity and the quality of the water in the river. Only if the right quality of water is present in a sufficient quantity, all of the functions of the river can be used. It is clear that some of these functions require a better quality than others, and the minimum quality is being determined by the most stringent quality condition.

The water quality of a river system is not only determined by the inputs into the system, but also by the processes taking place. Bacteria play an important role in the conversion

processes, either in a direct way or by the production of extracellular enzymes. Bacteria can be present both on the river bottom in the sediment, or in suspension.

Water quality can be judged on the basis of several parameters, usually classified as:

Physical: temperature, turbidity, conductivity.
Chemical: dissolved oxygen, biochemical oxygen demand (BOD) or COD, hardness, pH, alkalinity, nutrients (N, P), toxic compounds, organic volatile compounds.
Biological/Ecological: biocenosis of bacteria, plants and animals, coliform bacteria and variety and complexity of the food chain.

It is clear that all these parameters influence each other and that several factors should be looked at when judging the water quality. The combination of several criteria leads to a classification of the river as having good, moderate or bad quality.

2.1.4 Interactions between sewer systems, treatment plant and rivers

There are several interactions between the three subsystems considered. There are obvious ones, like the effect of a CSO spill or the effluent of the treatment plant on the water quality of the receiving water. The impact of a single CSO event is dependent on the dilution capacity of the receiving water. As a result of this, the pollutant concentrations in the river are increased, sometimes to harmful levels for the aquatic fauna. Another, less direct effect of a CSO is the increase in oxygen demand in the river, leading to a decreased oxygen concentration, which may again be toxic for the river fauna. Also, the sewer system delivers water to the treatment plant, and a varying amount or quality of this wastewater will clearly affect the plant.

The examples above illustrate the effects related to the flow of water, with both the quality and the quantity being important. There are also effects which are not directly related to the water flow. The most known is the backwater effect. If a CSO is partially drowned in the river (i.e. the outlet of the CSO is filled with river water), the spill capacity of the CSO structure will be reduced. In the same way, the discharge capacity of an effluent pipe of the WWTP can be reduced due to the water level in the river. This is e.g. the case in Quebec, where the Saint-Lawrence river is a tidal stream, influencing the hydraulic capacity of the treatment plant (Pleau *et al.*, 2001).

Other effects relate more to the water quality than to the water quantity. The same flow rate of wastewater may have different effects on the treatment plant depending on its quality (COD concentration, C/N ratio, P content, ...). Every change of quality in an upstream compartment (sewer system or treatment plant) will have a more or less pronounced effect on the downstream compartment (treatment plant or river). The examples are numerous: changing of the cleaning frequency of a pipe, connection of a new housing area to a sewer system, disconnection of industries, disconnection of surface water from the sewer system, installation of an extra aerator in the treatment plant, etc. An overview of the effect on the water quality from the urban drainage system is given in Table 2.1. It should be noted that the environmental effects distinguished are interrelated and that the impacts might be discussed. When planning any kind of change in a subsystem, it is important to realise that it may have serious implications in other subsystems.

Table 2.1: Impacts of key contaminants on receiving waters (Lijklema *et al.*, 1993)

Contaminant	Environmental effects	Ecological Impacts[1]	Affected water use[2]
OXYGEN DEMAND			
COD from CSOs	DO reduction	3, 4	A, B, D, E
WWTPs	Biomass accumulation	1, 2, 7	A
NH_4 from CSOs	DO reduction	3, 4	A, B, D, E
WWTPs	Biomass accumulation	1, 2, 7	A
NUTRIENTS			
N_{tot} from CSOs and surface runoff	Enrichment	1, 2, 4, 7	A, B, C, D, E
P_{tot} from CSOs and surface runoff	Enrichment	1, 2, 4, 7	A, B, C, D, E
TOXICANTS			
NH_4 (+ temp. + pH)	Toxicity	2, 3, 4	D
Metals - Acute	Toxicity	2, 3, 4, 7	D
- Cumulative	Toxicity	2, 3, 4, 7	D
Organic micropollutants (cumulative)	Toxicity	2, 3, 4	D
HYGIENE			
Faecal bacteria	Public health Biomass	1, 2, 7	A, B, D
PHYSICAL			
Temperature	temp. rise + long term change	1, 2, 5, 6	D
Suspended solids	Blanketing + harm to fish	4, 6	A, B, C, D, E, F
Flow	Washout; morphology changes	2, 4, 7	D
Chloride	Excess dissolved solids	2, 5, 7	A, D, F

[1] The ecological impacts noted refer to ecosystem characteristics: 1. Energy dynamics; 2. Food web; 3. Biodiversity; 4. Critical species; 5. Genetic diversity; 6. Dispersal and migration; 7. Ecosystem development

[2] Beneficial receiving water uses affected by contamination are coded as follows: A - Water supply; B - Bathing; C - Recreation; D - Fishing; E - Industrial water supply; F - Irrigation

2.2 Legislational aspects

2.2.1 European Union policy

Many European directives have had an (direct or indirect) influence on the water quality of the European rivers. The early approaches focused on “human health protection” and “harmonisation of the environmental rules to avoid market distortion”. For the protection of human health, standards were set for the quality of water intended for drinking, bathing and fishing (Council of the European Communities, 1975, 1976b, 1978, 1979, 1980). Another important directive regulated the emissions of dangerous substances to surface waters (Council of the European Communities, 1976a).

In the beginning of the 1990s, two new directives were introduced to tackle the main sources of water quality deterioration: pollution from urban wastewater (Council of the European Communities, 1991b) and pollution from nitrates originating from agricultural

runoff (Council of the European Communities, 1991a). The urban wastewater directive set clear infrastructural targets of wastewater treatment for all European urban settlements for different classes of sensitivity of the receiving waters. The objectives of the urban wastewater directive state, as a general rule, that there should be wastewater collection and treatment for all settlements above 2000 population equivalent (PE) with biological treatment, plus nutrients removal where the affected waters show an elevated nitrates level and/or eutrophication (Zabel *et al.*, 2001).

In 2000, the Water Framework Directive (WFD) (Council of the European Communities, 2000), was adopted. The main objectives of the WFD are (Blöch, 2001):

- integrated river basin management across borders, with coordinated programmes of measures
- protection of all waters, surface waters and groundwater, in quality and quantity with a proper ecological dimension
- emissions and discharges controlled by a ”combined approach” of emission limit values and quality standards, plus the phasing out of particularly hazardous substances
- introducing water pricing policies
- strengthening public participation

For surface waters the objective is that of a “good” ecological and chemical quality status. A surface water is defined as of good ecological quality if there is only slight departure from the biological community that would be expected in conditions of minimal anthropogenic impact. These expected conditions might differ from member state to member state (Kallis and Butler, 2001). Quality elements for assessment are divided into biological elements (e.g. composition and abundance of flora and fauna), hydromorphological elements (e.g. quantity and dynamics of flow, river depth and width variation) and supporting physico-chemical elements (e.g. thermal/oxygenation conditions, salinity, nutrients, etc.). Chemical quality status is classified is classified only in two categories: “good” and “failing to achieve good”. A “good” water body fulfils all the standards set by EU legislation for the concentration of chemicals in water.

Another important goal of the WFD is that of “no-deterioration” for all waters upon implementation of the measures. In addition to the good and non-deteriorating status, more stringent requirements are set for protected zones.

Each authority is responsible for preparing and implementing a River Basin Management Plan to achieve the good ecological quality. Public and stakeholder participation is foreseen in the production, review and updating of the river basin plans. Monitoring is central to the directive as it will determine the classification of the waters’ status.

Each river basin plan should include a number of mandatory measures which are required to comply with the requirements of the directive. These include the implementation of all other relevant Community legislation for the protection of water (see Table 2.2). If application of the existing legislation does not suffice to achieve the “good” status objectives, further measures may be necessary. These should include pollution control measures based on a combination of emission limit values (ELV) and recipient quality standards

Table 2.2: Measures required under the following Directives

The Bathing Water Directive (76/160/EEC)
The Birds Directive (79/409/EEC) (1)
The Drinking Water Directive (80/778/EEC) as amended by Directive (98/83/EC)
The Major Accidents (Seveso) Directive (96/82/EC) (2)
The Environmental Impact Assessment Directive (85/337/EEC) (3)
The Sewage Sludge Directive (86/278/EEC) (4)
The Urban Waste-water Treatment Directive (91/271/EEC)
The Plant Protection Products Directive (91/414/EEC)
The Nitrates Directive (91/676/EEC)
The Habitats Directive (92/43/EEC) (5)
The Integrated Pollution Prevention Control Directive (96/61/EC)

where the more stringent will apply ("the combined approach") (Kallis and Butler, 2001). Indeed, as Tyson *et al.* (1993) already noticed, in order to achieve effective solutions to urban drainage impacts, the institutional framework must allow for all the elements of the wastewater system to be considered together.

2.2.2 Urban pollution management

In the UK, an Urban Pollution Management (UPM) procedure was first published in 1994 and updated in 1998 (FWR, 1994, 1998). The UPM procedure assists in the analysis of design variations of urban wastewater systems by providing a modelling and assessing procedure. The procedure is based on three major concepts (Morris and Clifford, 1998):

- The urban wastewater system (sewers, WWTP and receiving water) should be treated as a single entity in which a change to one part has implications for the other parts which must be taken into account in the planning process.
- Compliance with environmental standards is the main objective. The modelling process is aimed at testing the compliance of a scheme with the standards identified of the system.
- The form of integrated modelling should be appropriate to the technical needs of the study (i.e. the use of simple vs. sophisticated and complex models).

For river quality planning purposes the manual specifies two options for the design basis (Morris, 2000):

- river quality standards based on a percentile approach
- a refinement of the Fundamental Intermittent Standards (FIS)

The percentile approach states that the pollutant concentration in the river should comply with the given standard for at least 99% of the time (for the 99-percentile). The FIS are concentration/duration values for a given pollutant that should not be violated more frequently than a specified value. Three sets of FIS are used depending on the type of ecological quality aimed for (Zabel *et al.*, 2001):

Table 2.3: Fundamental intermittent standards (FIS) for un-ionised ammonia for ecosystem suitable for sustainable cyprinid fisheries-concentration/duration thresholds not to be breached more frequently than shown

Return period	Un-ionised ammonia concentration (mg NH_3-N l^{-1})		
	1h	6h	24h
1 month	0.150	0.075	0.030
3 months	0.225	0.125	0.050
1 year	0.250	0.150	0.065

Table 2.4: Fundamental intermittent standards (FIS) for oxygen for ecosystem suitable for sustainable cyprinid fisheries-concentration/duration thresholds not to be breached more frequently than shown

Return period	Dissolved oxygen concentration (mg l^{-1})		
	1h	6h	24h
1 month	4.0	5.0	5.5
3 months	3.5	4.5	5.0
1 year	3.0	4.0	4.5

- ecosystems suitable for sustainable salmonid fishery
- ecosystems suitable for sustainable cyprinid fishery
- marginal cyprinid fishery ecosystem

An example of the FIS for sustainable cyprinid fishery ecosystems is given in Table 2.3 for un-ionised ammonia and Table 2.4 for oxygen. The standards require that each concentration/duration threshold does not have a return period less than that specified. The return period is the average time between two events. For example, the 1h dissolved oxygen (DO) threshold concentration for one month is 4 mg l^{-1} (see Table 2.4). This means that the DO concentration can fall to 4 mg l^{-1} for 1 h as long as the average interval between such events is not less than one month. An application of this concept to an urban catchment is shown in Fig. 2.2 (Harremoës and Rauch, 1996). It is clear from this figure that the river does not comply with the FIS set for Carp fishery, as a DO concentration of 1 oxygen mg/l has a return period of about 1 year, while this should be 10 years to comply with the water quality criterion. Van Assel (2000b) mentions that these FIS are difficult to calculate from the current model outputs, and state that data handling remains a serious obstacle for correct application.

2.2.3 The US policy

The US policies are laid down in the so called Clean Water Acts (CWA). Waste dischargers are required to apply for a permit under the National Pollution Discharge Elimination System (NPDES).The main focus of this legislation on the control of point source dischargers. This has improved the water quality in a majority of rivers. However, a large

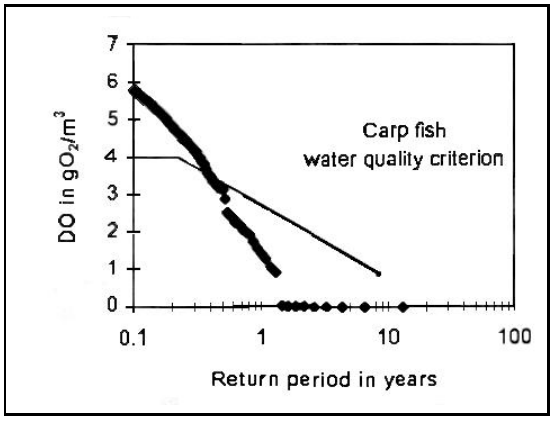


Figure 2.2: The application of the FIS concept to an urban river (Harremoës and Rauch, 1996)

number of rivers cannot meet water quality standards with point source control alone (Chen *et al.*, 1999).

The US Clean Water Act establishes a process to facilitate recovery of surface waters not meeting their established water quality standards. It is the responsibility of the state and/or federal agencies to develop an appropriate Total Maximum Daily Load (TMDL) for each water body and for each identified pollutant. The TMDL identifies the amount of pollutant loading that a water body can receive and still provide its designated uses (like drinking water production, recreation, ...) (Havens and Schelske, 2001).

The TMDL process basically involves (Freedman, 2001):

- identifying impaired waters
- defining water quality goals
- quantifying sources of impairment
- linking sources to water quality
- calculating the TMDL
- establishing a TMDL implementation plan

Hence, the TMDL only has to be calculated if the point source control doesn't succeed in meeting the water quality standards. The concept is generally agreed upon, but the tools and data to calculate these TMDLs seem inadequate at the time being (Freedman, 2001; Werblow, 2000). These authors question the quality of the calculated TMDLs, and hence the quality of the measures taken to achieve the TMDLs.

2.2.4 Comparison of approaches

Two main approaches to protect the quality of receiving waters can be followed as was already noted by Tyson *et al.* (1993), who classified the approaches as either following the Uniform Emission Standards (UES) or as following Environmental Quality Objective/Environmental Quality Standards (EQO/EQS). A similar distinction was made by Ragas *et al.* (1997) who classifies the Emission Limit Values as being either technology based (like the UES) or water quality based (like the EQO/EQS).

Under the EQO/EQS approach the principle is to establish use requirements of the water body. The designated uses become the EQO for that receiving water. The EQS for that water is then derived as a set of numerical standards (derived from modelling tools) which, if met, will protect the EQO. This approach should be followed when dealing with pollutants that impose an oxygen demand or increased nutrient levels (Tyson *et al.*, 1993).

The UES focuses on the effluent quality irrespective of the local discharge conditions of the receiving water. These standards are technology based and can be classified as Best Available Technology (BAT), Best Practicable Means (BPMs), or Best Available Technology Not Entailing Excessive Cost (BATNEEC). This approach is relevant for application to hazardous substances like heavy metals (Tyson *et al.*, 1993).

The European Urban Wastewater Directive can be considered as a mixture of the UES with the EQO/EQS approach. All wastewater should be treated and the effluents should comply with specified standards. However, in sensitive areas (like those subject to eutrophication) additional standards should be met. With the WFD, the emphasis is more on the EQO (good ecological status) but the UES are required to be met as well. For a given river, the most stringent of the two measures applies.

This has also been the case in the US, where the TMDL concept was approved. However, for a long time, only the point sources have been controlled without looking at the resulting water quality. Only recently, the TMDL (the water quality approach) has gained attention from the government. So it is clear that a regulation alone does not suffice to achieve the water quality standards set. Monitoring plays an important role as only measurement can tell if the standards are being met or not.

The European directives have been implemented by the member states into national legislation in order to comply with the directives at the deadlines set. Zabel *et al.* (2001) point to the fact that most countries have implemented laws to enforce the implementation of the urban wastewater directive, but have so far failed to regulate the design and effect of CSOs. In highly urbanised regions like Flanders (Belgium) the impact of the urban wastewater system is very important for a number of small rivers which drain the cities. The current Flemish legislation allows CSOs to spill 7 times a year. In the current situations it is possible that large CSOs spill into small rivers with little dilution capacity, turning the river water into diluted sewage with a very low quality. As a consequence of these regular spills, the ecological status of these rivers deteriorates to unacceptably low levels (Wils, 2000). It is clear that the good ecological status of the WFD will require also specific legislation for the polluting effect of the CSOs.

2.3 Modelling of the integrated urban wastewater system

Mathematical modelling of complex systems like sewers, WWTPs or rivers, is useful for several reasons. A mathematical model can serve as a compilation of knowledge available about the system, it might be used as a training tool for plant operators, it might be used in planning and management of the system or it can be useful for testing several upgrading options. Mathematical modelling in the integrated urban wastewater system (IUWS) has a long history, especially the modelling of the separate subsystems. Recently, integrated

modelling studies are being carried out, to evaluate the effect of certain measures on the other parts of the system. Every integrated model consists of several submodels. Therefore, the modelling of the subsystems is discussed before the integrated modelling approaches can be explained.

2.3.1 Modelling rainfall-runoff processes

The main source of water in the urban drainage system is not the wastewater, but the stormwater or rainwater. During a rain event, the rain falls on the surface and a part enters the sewer system via overland flow. Modelling the integrated urban wastewater system hence requires rainfall data as model input. Rain gauge stations provide precipitation data in the required resolution and accuracy (Schilling, 1991). Radar images are used to predict rainfall on a smaller spatial scale, which is useful for controlling the system (Aspegren *et al.*, 2001; Collier, 1996). Different types of input data can be used to simulate the integrated urban wastewater system: design storms, short selected rainfall series, modified single storm events and long rainfall series (Vaes *et al.*, 1999b). The type of rainfall needed depends on the problem to be solved. Often historical rainfall series are used if longer time series need to be simulated (Einfalt *et al.*, 1998).

The two most important phenomena that have to be taken into account when calculating the runoff are the losses during runoff generation and the transformation of the effective rainfall into time series of flow rates on the surface (surface flow hydrograph). The losses during runoff generation are caused by wetting of the surface material (wetting losses) and by the filling of depressions on the surface (depression losses). Models that calculate the runoff take into account several basic phenomena like infiltration, interception, evaporation and storage in depressions. The runoff is also influenced by the permeability of the surface. Different types of models can be used to describe the overland flow process ranging from very detailed (kinematic wave description) to more simple (reservoir models, time-area relations or unit hydrographs) (Butler and Davies, 2000; Chow *et al.*, 1988).

2.3.2 Hydraulic modelling of the sewer system

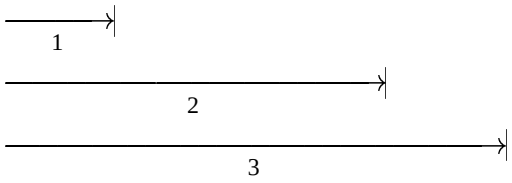
Deterministic modelling of sewer hydraulics

The deterministic modelling of the water motion in sewer systems is based on the “de Saint-Venant” equations. These equations were developed to describe gradually-varied unsteady flow in open channels in one dimension. These equations can also be used to describe the flow in partially filled pipes and have been successfully applied to describe unsteady flows in sewer networks.

The “de Saint-Venant” equations have two parts: a continuity equation (conservation of mass) and the dynamic equation (conservation of momentum). They can be written as:

$$B\frac{\partial y}{\partial t} + \frac{\partial Q}{\partial x} = 0 \tag{2.1}$$

$$S_f = S_o - \frac{\partial y}{\partial x} - \frac{1}{gA}\frac{\partial}{\partial x}\left(\frac{Q^2}{A}\right) - \frac{1}{gA}\frac{\partial Q}{\partial t} \tag{2.2}$$



where:

y	flow depth or water level (m)
Q	flow rate (m^3/s)
A	area of flow cross-section (m^2)
B	water surface width (m)
t	time (s)
x	distance (m)
S_o	bed slope (-)
S_f	friction slope (-)

The “de Saint-Venant” equations are valid under the following conditions (Butler and Davies, 2000):

- the pressure distribution is hydrostatic
- the sewer bed slope is small
- the velocity distribution is uniform
- the channel is prismatic
- the friction losses are the same as in steady flow conditions
- the lateral flow is negligible

Most of the time, these conditions are fulfilled in urban sewer systems, so that the equations can be used to predict the unsteady flow in sewer pipes. Some of the terms of eq. 2.2 might be less significant in some cases, giving opportunities to simplify the equations. If one takes only the bed slope and the friction slope into account (no. 1), the equations simplify to the *kinematic wave* equations. The wave does not attenuate, but translates at a certain wave speed. If one only ignores the variation of the flow rate with time (no. 2), the equations simplify to the *diffusive wave* equations. These equations are able to describe phenomena like backwater effects and wave attenuation. If no term is ignored, the *dynamic wave* equations are able to describe, next to backwater effects and wave attenuation, also flow acceleration. Depending on the situation in the system under study, one of the equations may prove adequate.

During high flows, when the pipes are completely filled with water, the flow in the pipes becomes pressurised (surcharge flow). Surcharge flow is an important phenomenon (e.g.

toward flooding or damage to sewer pipes) and has to be modelled adequately. The Preissman slot is introduced (as a numerical work around) to describe the effect of pressurised flow, while the equations 2.1 and 2.2 may still be used (Yen, 1986).

The "de Saint-Venant" equations are partial differential equations since Q and y are functions of both distance (x) and time (t). These type of equations require numerical methods to solve them. Typical examples are finite difference and finite element methods. These approaches to numerical solution can suffer from various forms of inaccuracy like "numerical oscillation" or "numerical instability". To overcome these problems small time steps have to be used (Butler and Davies, 2000). When large networks are to be modelled, these numerical techniques demand a huge amount of calculations, resulting in long computation times. This might limit the use of these models for repetitive simulation of long time series, even with the increasing processor speed of personal computers.

Several commercial software packages have implemented these equations and dedicated numerical methods to solve them. Moreover, hydraulic equations for manholes, overflows, weirs and other structures present in the sewer system are provided. Usually, a GIS interface is provided to enter information (connections, dimensions, slopes, locations, ...) about the pipes and other structures. The database containing all this information is the actual model of the sewer system and might be used to simulate the behaviour of the real system. In this way the model may be used to gain insight in the system, to test renovation options or to test control strategies. Examples of software packages are SWMM (USEPA), Hydroworks (Wallingford software), HYSTEM-EXTRAN (ITWH) and Mouse (DHI). More details about these models as well as an overview of other existing models can be found in Schütze (1998) and more recently in Zoppou (2001).

Conceptual modelling of sewer hydraulics

The deterministic modelling of sewer hydraulics has, as mentioned above, several drawbacks, e.g. long calculation times and the need for detailed information about the system. Moreover, it might not always be necessary to calculate the flow in every single pipe in the system. Often the simulation of input-output behaviour at certain important points might be sufficient. In this case, simplified conceptual models are useful.

Most conceptual models are based on the Nash cascade, which models flow in subcatchments by conceptually routing it through a series of linear reservoirs (Viessman *et al.*, 1989). In this cascade, the input of the downstream tank, is formed by the output of the previous tank. Fig. 2.3 visualises the reservoir cascade or tanks in series concept.

Some software packages, like Kosim (Paulsen, 1986) in Germany, are based on this principle. Each of the reservoirs can be described by a storage equation (2.3) and a continuity equation (2.4):

$$\frac{dS(t)}{dt} = I(t) - Q(t) \tag{2.3}$$

$$Q(t) = \frac{1}{K} S(t) \tag{2.4}$$

where:

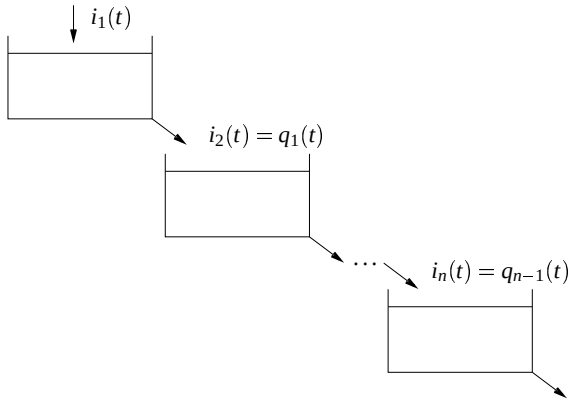


Figure 2.3: The concept of a reservoir cascade

$I(t)$ Inflow at time t (m^3/s)
$Q(t)$ Outflow at time t (m^3/s)
$S(t)$ Storage at time t (m^3)
K Storage constant (s)

Due to its simplicity, the reservoir cascade approach allows rapid simulation; on the other hand, effects such as backwater and pressurised flows cannot be simulated, which is a severe limitation, in particular for looped or flat networks. The Muskingum-Cunge method (Cunge, 1969) relates the storage to both the inflow and the outflow.

The reservoir in series concept was further developed by Vaes and Berlamont (1998, 1999). In their Remuli model, the relationship between the storage in the system and the through-flow is more complex than the relationship given in eq. 2.4. Remuli uses a multi-linear (or piece-wise linear) approach to model the relationship between the storage and the through-flow. This relationship is calibrated based on data generated with a deterministic model. Due to the fact that linear models are chosen, the differential equations can still be solved analytically, resulting in short calculation times. The authors conclude that the reservoir modelling system is an ideal tool for sensitivity and scenario analyses, the optimisation of storage, the calibration of a runoff model, etc. A detailed explanation can be found in Vaes (1999). Sartor (1999) and Motiee *et al.* (1997) each describe a system to simulate a sewer system based on hydrological methods including the capability to realistically model backwater effects. Both approaches use data generated by a dynamic deterministic model to calibrate the hydrological model.

2.3.3 Water quality modelling of the sewer system

The water quality in the sewer is the result of the mixing of the dry weather flow with the stormwater entering the sewer. The dry weather flow, i.e. the flow of wastewater produced by households and industries independent of rainfall, contains all types of pollutants: physical (like suspended and gross solids), chemical (BOD, COD, nitrogen and phosphorus) and microbiological (coliform and viruses) (Butler and Davies, 2000). The quality of the wastewater varies with both time and location. For a given catchment, a daily and weekly pattern in dry weather flow and concentration might be recognised (Heip

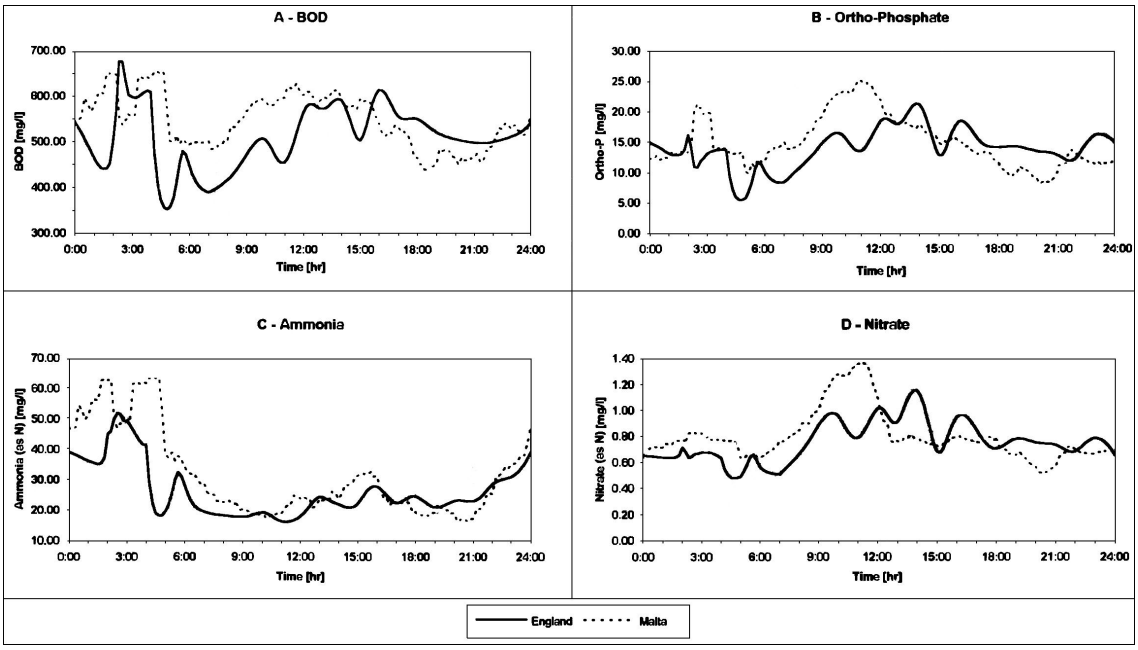


Figure 2.4: Changes in sewer dry weather flow for different pollutants (Butler *et al.*, 1995)

et al., 1997). It should be noted that external factors like public holidays or cold or warm weather disturb this average pattern since the concentrations in the wastewater strongly depend on the relative proportions of the different sources like toilets, wash basins, showers or kitchen sinks (Butler *et al.*, 1995), see also Fig. 2.4.

Pollutants in the sewer system can be divided into solubles and particulates. The soluble pollutants are transported with the water flow and might be converted by transformation processes. The particulate pollutants do not necessarily proceed at the same velocity as the water, since they are subject to sedimentation, erosion, resuspension and compaction.

Three sources of pollutants may be distinguished in a combined sewer system during storms:

- pollutants washed off from the catchment surfaces, and transported by the overland flow into the sewer system
- pollutants accumulated in the sewer pipes during dry weather and eroded during flow increases
- pollutants originating from the dry weather wastewater (from households and industries)

As Rauch *et al.* (2002a) indicate, there are four main steps that are important in the modelling of the wet weather water quality and pollutant transport in sewer systems:

- pollutant accumulation
- pollutant wash-off
- pollutant transport and transfer
- pollutant conversion processes

The most important software packages describing the water quality in sewer in combination with the "de Saint-Venant" equations are Mouse-Trap (DHI) and Hydroworks DM (Wallingford Software).

Pollutant accumulation

Pollutant accumulation is not completely understood and usually modelled using conceptual models. Pollutants accumulate during dry weather periods both on the catchment surfaces and in the sewer pipes. On the catchment surface, usually a linear accumulation or exponentially asymptotic accumulation function is used (Bertrand-Krajewski *et al.*, 1993b; Charbeneau and Barett, 1998; Schlutter, 1999). However, the field data are highly uncertain which is related to the difficulties of measuring the processes in the field (Ashley *et al.*, 1999). The factors influencing the build-up of pollutants on the surface are (Butler and Davies, 2000):

- land use
- population
- traffic flow
- effectiveness of street cleaning
- season of the year
- meteorological conditions
- antecedent dry period
- street surface type and condition

The sediment build-up in the sewer system results from the sedimentation of suspended solids during periods with low flow. This means that a sediment bed is being built-up gradually inside the sewer during dry weather. The effects of sewer sediments are threefold: blockage, loss of hydraulic capacity and pollutant storage. The first two effects might result in surcharged flows or surface flooding. The storage of pollutants, on the other hand, might lead to shock-loads to the treatment plant, washout of pollutants to the receiving water during CSO operation or increase the production of hydrogen sulfide (Butler and Davies, 2000).

Pollutant wash-off

Pollutants accumulated on catchment surfaces are washed off during storm events. The wash-off process is quite complicated. At initiation of rain, the surface and the sediments are wetted and subsequently the sediments are washed off into gully pots and into the sewer. The wash-off rate depends on the characteristics of the surface and the sediments as well as the discharge of water. Some models relate the wash-off to the rainfall intensity (Schlutter, 1999; Zug *et al.*, 1999b). The most simple, frequently used model assumes that the wash-off load is dependent on the amount of pollutant remaining on the surface. This results in an exponentially decreasing wash-off load (Charbeneau and Barett, 1998).

The wash-off of pollutants accumulated in the sewer pipes occurs during peak dry weather flow and during storm events. The mechanism of erosion of the compacted bed is complex

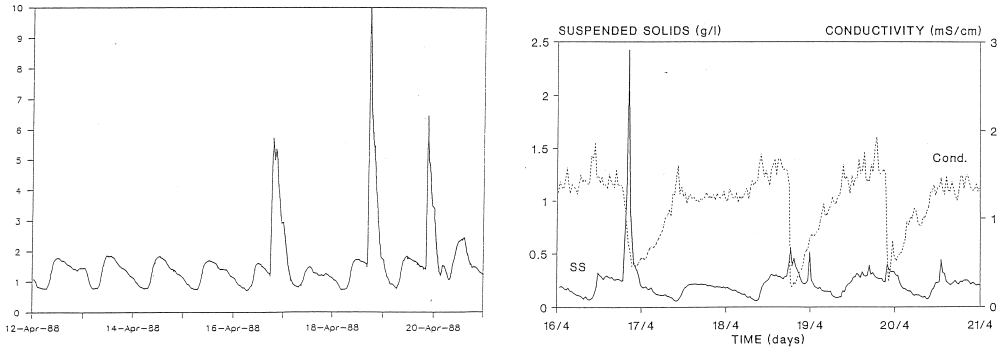


Figure 2.5: The first flush phenomena, left: flow in the sewer system; right(zoomed in): suspended solids (solid line) and conductivity (dashed line) (Verbanck *et al.*, 1994)

and not completely understood. However, it is widely agreed that the resuspension of sediment previously deposited on the invert of a sewer is a major source of the pollutants associated with the first foul flush phenomenon (De Sutter *et al.*, 1999; Larsen *et al.*, 1998; Skipworth *et al.*, 2000; Verbanck *et al.*, 1994). The first foul flush of sediments is explained as the cleaning of both the surface and sewer pipes by the water wave at the beginning of a storm. This is clearly shown in Fig. 2.5. In the left side of Fig. 2.5 the flow is shown, while on the right side, the concentration of suspended solids (solid line) and the conductivity (dotted line, as a measure of dissolved components) is shown (this plot zooms to the last part of the left plot). In the night of 16/4 to 17/4, a first storm event occurs after several days of dry weather. One can see that at the same time, the suspended solids concentrations increases dramatically, while the conductivity decreases. The rain water entering the sewer has resuspended the solids accumulated on the bottom of the pipe, while diluting the dissolved components. During the second and third storm (on 19/4 and 20/4) no major increase in suspended solids can be noted, while the conductivity is showing the same behaviour as before. One can also note that even in dry weather, the suspended solids (SS) concentration is proportional to the flow rate.

The wash-off of sediments is usually modelled with an equation depending on the accumulated mass of solids, the flow velocity or the bed shear stress. It is assumed that a minimum of shear stress is necessary to resuspend the pollutants (Ashley *et al.*, 2000; Skipworth *et al.*, 1999).

Pollutant transport

The transport of soluble components (dissolved organics, ammonia, phosphorus) can be described by both conceptual models (reservoir models) and mechanistic models (advection-dispersion). The advection-dispersion equation can be written as (Butler and Davies, 2000):

$$\frac{\partial c}{\partial t} + v\frac{\partial c}{\partial x} = \frac{\partial}{\partial x}\left(D\frac{\partial c}{\partial x}\right) \tag{2.5}$$

where:

x distance (m)

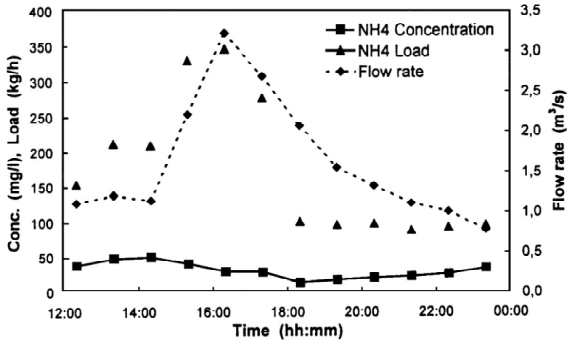


Figure 2.6: The first flush of soluble components (Krebs *et al.*, 1999a)

t time (s)
c concentration of pollutant (kg/m^3)
v mean velocity of flow (m/s)
D longitudinal dispersion coefficient (-)

One should note that, due to the hydraulic characteristics of the sewer system, a *first flush* of dissolved components is also possible. This is due to the propagation of flood waves at a velocity higher than the flow velocity of the water. In the beginning of the storm, the flow is increased at the end of the pipe by the flood wave, without the corresponding decrease in dissolved components leading to a peak load at the WWTP (Huisman *et al.*, 2000; Krebs *et al.*, 1999a). In other words, a plug of pollution is expelled from the sewer into the downstream system (WWTP or river), which is illustrated in Fig. 2.6.

The transport of particulates is more complex and can be divided in suspended load, near bed solids load and bed load (Fig. 2.7). All these transport phenomena behave differently and therefore need different equations to be described adequately (e.g. Ahyerre *et al.* (2001); De Sutter *et al.* (1999); Schlutter and Schaarup-Jensen (1998); Schmitt *et al.* (1999); Skipworth *et al.* (2000); Verbanck (2000)). The commercial software packages tend to use simple approaches, since a lot of the parameters used in the more complex models cannot be determined on a catchment wide scale.

Pollutant processes

Recently, a lot of research is trying to describe which type of biological transformation processes are important in a sewer system. A schematic overview of processes influencing BOD and oxygen in the sewer is given in Fig. 2.7. Processes can take place in the sediment, in the bulk water or in the biofilm attached to the pipe walls.

Hvitved-Jacobsen *et al.* (2002) describes the sewer as a bioreactor. According to this overview, three types of conditions can occur in the sewer system (as in the WWTP): aerobic, anoxic and anaerobic conditions.

In aerobic conditions, there is a relatively high activity of the biomass, both in the biofilm and the suspended phase. The particulate COD is transformed into soluble COD, which is subsequently degraded into carbon dioxide and new biomass. Different fractionations of COD are used by different authors (Almeida *et al.*, 1999; Huisman and Gujer, 2002;

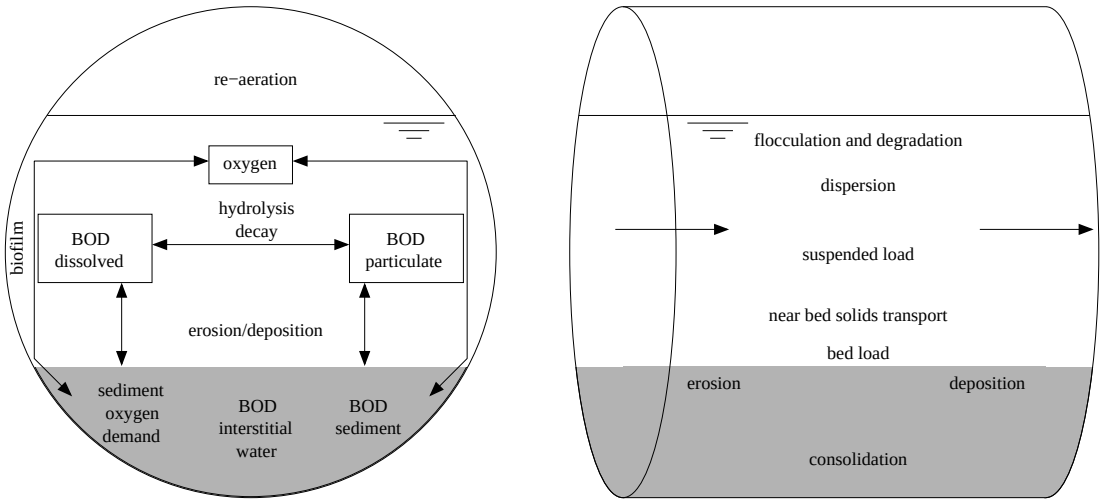


Figure 2.7: A process model related to oxygen demand (left) and transport (right) in sewer systems (Rauch *et al.*, 2002a)

Vollertsen and Hvitved-Jacobsen, 2000). Fractionation of the COD is necessary since not all organic material degrades or settles at the same rates in the sewer system. In some cases, these models allow to describe changes in COD concentrations and composition, an oxygen balance and nutrient related processes.

Normally, anoxic conditions don't occur in sewer systems, but sometimes nitrate is added to pressure sewers to prevent the formation of hydrogen sulfide. Abdul-Talib *et al.* (2002) describes the known two-step denitrification process (nitrate $\rightarrow$ nitrite $\rightarrow$ nitrogen gas) taking place in the sewer.

In anaerobic conditions anaerobic hydrolysis, fermentation (formation of volatile fatty acid (VFAs)), methanogenesis (formation of methane) and sulfate reduction (formation of hydrogen sulfide) can take place (Hvitved-Jacobsen *et al.*, 2002). The formation of hydrogen sulfide is problematic for several reasons: it is the source of odour problems, it is a toxic substance and it might be oxidised into sulfuric acid, leading to corrosion problems in the sewer pipes (Tanaka and Hvitved-Jacobsen, 2002).

Huisman (2001) recently described a complete sewer model implemented in Aquasim (Reichert, 1998). The biological model is based on the ASM3 model (Henze *et al.*, 2000), completed with a model to describe the sulphur cycle. Moreover, both bulk processes and processes taking place in the biofilm are described. The biofilm process are limited by the diffusion and conversion processes (resulting in a penetration depth of a substrate), resulting in a reduced activity if some type of substrate is no longer available in the bottom layers of the biofilm. A biofilm attachment and detachment model is also included. In combination with a hydrodynamic model (diffusive wave approximation of the "de Saint-Venant" equations) and a gas exchange model with the sewer atmosphere, this model can be considered a summary of current knowledge available in the field of sewer quality modelling.

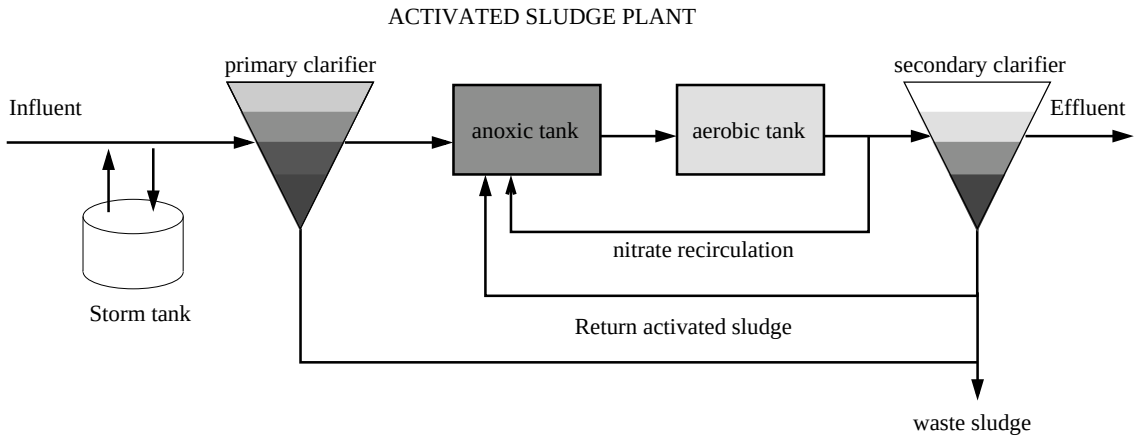


Figure 2.8: General overview of an activated sludge treatment plant

2.3.4 Modelling of biological wastewater treatment plants

Many types of treatment plants exist, but this review limits itself to activated sludge treatment plants, since this is the type of treatment plant mostly used to treat municipal wastewater (Metcalf and Eddy, 1991). A general scheme of an activated sludge plant is shown in Fig. 2.8. Typical units include: screen, sand trap, primary clarifier, activated sludge tanks, secondary clarifier.

The modelling of activated sludge WWTPs has a long history (Henze *et al.*, 1987). The IWA Task Group on mathematical modelling introduced the matrix format developed by Petersen (1965) for presentation of the biochemical conversion models in the wastewater treatment field. This matrix format is now widely used to describe biological conversion models in sewer, treatment plant and receiving water modelling. Therefore, it is useful to describe this concept before discussing the modelling of wastewater treatment plants in detail.

Modelling biochemical conversions: The Petersen matrix

Introduction Crucial in modelling the biochemical conversions in a wastewater treatment plant is to realistically model the inter-component biochemical reactions. These reactions must be representative of the most important fundamental processes occurring within the system. Furthermore, the model should quantify both the *kinetics* (rate-concentration dependence) and the *stoichiometry* (relationship that one component has to another in a reaction) of each process. Identification of the major processes and selection of the appropriate kinetic and stoichiometric expressions for each are the major conceptual tasks during development of a mathematical conversion model.

The first step in setting up this matrix is to identify the *components* of relevance in the model. The second step in developing the matrix is to identify the biological *processes* occurring in the system; i.e. the conversions or transformations which affect the components listed. Next, the kinetics vector listing the rate of every process as a function of the concentration of the different components and parameters has to be defined. Finally,

Table 2.5: Process stoichiometry and kinetics for heterotrophic growth in an aerobic environment

Component $i \rightarrow$ **Process** $j \downarrow$	1. Biomass X_B	2. Substrate S_S	3. Oxygen S_O	**Process Rate** ρ_j ($ML^{-3}T^{-1}$)
1. Growth	1	$-\frac{1}{Y}$	$-\frac{1-Y}{Y}$	$\frac{\mu S_S}{K_S+S_S}X_B$
2. Decay	-1		-1	bX_B
Stoichiometric Parameters:	M(COD).L^{-3}	M(COD).L^{-3}	M(-COD).L^{-3}	Kinetic Parameters:
Growth yield Y				Maximum specific growth rate: μ Half-velocity constant K_S Specific decay rate b

the stoichiometry matrix, relating the processes to the production or consumption of the components has to be set up.

A simple example Consider the situation in which heterotrophic bacteria are growing in an aerobic environment by utilising a soluble substrate for carbon and energy. In one - simple- conceptualisation of this situation, two fundamental processes occur: the biomass increases by cell growth and decreases by decay. Other activities, such as oxygen utilisation and substrate removal, also occur, but these are not considered to be fundamental because they are the result of biomass growth and decay and are coupled to them through the system stoichiometry. The simplest model of this situation must consider the concentrations of three components: biomass, substrate and dissolved oxygen. The matrix incorporating the fate of these three components in the two fundamental processes is shown in Table 2.5.

As mentioned in the introduction, the first step in setting up the matrix is to identify the *components* of relevance in the model. In this scenario these are biomass, substrate and dissolved oxygen, which are listed, with units, as columns in Table 2.5. In conformity with IWA nomenclature (Grau *et al.*, 1982), particulate constituents are given the symbol X and the soluble components S. Subscripts are used to specify individual components: B for biomass, S for substrate and O for oxygen.

The second step in developing the matrix is to identify the *biological processes* occurring in the system; i.e. the conversions or transformations which affect the components listed. Only two processes are included in this example: aerobic growth of biomass and its loss by decay. These processes are listed in the leftmost column of Table 2.5. The *kinetic expressions* or *rate equations* for each process are recorded in the rightmost column of the table in the appropriate row. Process rates are denoted by ρ_j where j corresponds to the process index.

If we were to use the simple Monod-Herbert model for this situation, the rate expressions would be those in Table 2.5. The Monod equation, ρ_1, states that growth of biomass is proportional to biomass concentration in a first order manner and to substrate concentration in a mixed order manner. The expression ρ_2 states that biomass decay is first order with respect to biomass concentration.

The elements within the table comprise the stoichiometric coefficients, ν_{ij}, which set out the mass relationships between the components in the individual processes. For example, growth of biomass $(+1)$ occurs at the expense of soluble substrate $(-\frac{1}{Y}$, Y is the yield parameter); oxygen is utilised in the metabolic process $(-\frac{1-Y}{Y})$. The coefficients ν_{ij} can easily be deduced by working in consistent units. In this case, all organic constituents have been expressed as equivalent amounts of chemical oxygen demand (COD); likewise, oxygen is expressed as negative oxygen demand. The sign convention used in the table is negative for consumption and positive for production.

In matrix form, we obtain a stoichiometry matrix

$$\nu = \begin{pmatrix} 1 & -\frac{1}{Y} & -\frac{1-Y}{Y} \\ -1 & 0 & -1 \end{pmatrix} \tag{2.6}$$

and a kinetics vector

$$\rho = \begin{pmatrix} \frac{\mu S_S}{K_S+S_S} X_B \\ bX_B \end{pmatrix} \tag{2.7}$$

Within a system, the concentration of a single component may be affected by a number of different processes. An important benefit of the matrix representation is that it allows rapid and easy recognition of the fate of each component, which helps in the preparation of mass balance equations. This may be seen by moving down the column representing a component.

The system reaction term, r_i, is obtained by summing the products of the stoichiometric coefficients ν_{ij} and the process rate expression ρ_j for the component i being considered in the mass balance (i.e. the sum over a column):

$$r_i = \sum_j \nu_{ij}\rho_j \tag{2.8}$$

For example, the rate of reaction, r, for oxygen, S_O, at a point in the system would be:

$$r_{S_O} = -\frac{1-Y}{Y}\frac{\mu S_S}{K_S+S_S}X_B - bX_B \tag{2.9}$$

Another benefit of the Petersen matrix is that continuity may be checked per process by horizontally moving across the matrix. This can only be done provided consistent units have been used, because then the sum of the stoichiometric coefficients must be zero. This can be demonstrated by considering the decay process. Bearing in mind that oxygen

is negative COD so that its coefficient must be multiplied by -1, all COD lost from the biomass through decay must be balanced by oxygen utilisation. Similarly, for the growth process, the substrate COD lost from solution due to growth minus the amount converted into new cells must equal the oxygen used for cell synthesis.

The Activated Sludge Models (ASMs)

At the moment, the modelling of activated sludge systems is widely practised, both in research and practical applications. With the introduction of ASM No. 1 in the 1980s, a first "standard" model was introduced to describe carbon removal and nitrification-denitrification processes. This model has been widely used as a basis for further model development Henze *et al.* (2000). In the mid-1990s, ASM No. 2 and its later extension ASM No. 2d were introduced. This model describes, next to the carbon and nitrogen removal of ASM No. 1, also processes related to biological phosphorus removal. In 1998, ASM No. 3 was developed to overcome some defects of the ASM1 model which became apparent during the intensive research performed on the basis of ASM No. 1.

As an example of an ASM-model, the ASM3 model is presented here. In this model, the conservation of Theoretical Oxygen Demand (ThOD) is used extensively in the development of process stoichiometry. For organic substances the ThOD may be approximated by the COD. For inorganic materials, the ThOD must be calculated based on redox equations relative to the redox reference of H_2O, CO_2, NH_4^+, PO_4^{3-}, SO_4^{2-}. ASM3 includes cell internal storage, like the ASM2(d). An overview of the components of the ASM3 model is given in Table 2.6, while all reactions are enumerated in Table 2.7. A detailed description of each component and reaction can be found in Henze *et al.* (2000). A relatively new concept used by ASM3 is the composition matrix. This matrix indicates the amount of conservatives that is contained in 1 g of each component. Three conservatives are used: ThOD, nitrogen and ionic charge. Applying a mass balance for these conservatives for every reaction, results in j x k mass conservation equations, which can be used to calculate the stoichiometric coefficients:

$$\sum_i \nu_{i,j} \cdot i_{k,i} = 0 \qquad \text{for } i = 1 \text{ to } 12 \tag{2.10}$$

where:

$\nu_{i,j}$ The stoichiometric coefficient for component i in reaction j
$i_{k,i}$ Element from the composition matrix of component i for conservative k (k=ThOD, N and ionic charge)

The same concept is used to predict the suspended solids concentration in the activated sludge tanks. This is useful since the SS concentration is frequently measured by treatment plant operators. One can write:

$$\nu_{j,13} = \sum_i \nu_{j,i} \cdot i_{4,i} \qquad \text{for } i = 8 \text{ to } 12 \tag{2.11}$$

where the subscript 13 denotes component 13, i.e. suspended solids, and the subscript 4

Table 2.6: List of state variables in ASM3 (Henze *et al.*, 2000)

State variables in ASM3		
1	S_{O_2}	Dissolved oxygen (M(O_2)L^{-3})
2	S_I	Inert soluble organic material (M(COD)L^{-3})
3	S_S	Readily biodegradable organic substrates (M(COD)L^{-3})
4	S_{NH_4}	unionised plus ionised ammonia nitrogen (M(N)L^{-3})
5	S_{N_2}	Dinitrogen (M(N)L^{-3})
6	S_{NO_x}	Nitrate plus nitrite nitrogen (M(N)L^{-3})
7	S_{ALK}	Alkalinity of the wastewater (mole(HCO_3)L^{-3})
8	X_I	Inert particulate organic material (M(COD)L^{-3})
9	X_S	Slowly biodegradable substrates (M(COD)L^{-3})
10	X_H	Heterotrophic organisms (M(COD)L^{-3})
11	X_{STO}	All cell internal storage products of heterotrophic biomass (M(COD)L^{-3})
12	X_A	Nitrifying organisms (M(COD)L^{-3})
13	X_{SS}	Suspended solids (M(SS)L^{-3})

denotes the fourth row in the composition matrix, i.e. the amount of suspended solids per g of component.

The kinetics in ASM3 are based on continuous switching functions, like $S/(K+S)$ for all soluble compounds that are consumed. These functions stop a process when one of the components consumed in that process is no longer available. Inhibition is modelled with a different switching function, like $K/(K+S)$. An example of a kinetic expression is given in eq. 2.12:

$$\rho_7 = b_{H,NO_X} \frac{K_{O_2}}{K_{O_2} + S_{O_2}} \frac{S_{NO_X}}{K_{NO_X} + S_{NO_X}} X_H \tag{2.12}$$

(Anoxic endogenous respiration)

One can see from the kinetics that the anoxic endogenous respiration of heterotrophs is inhibited by oxygen (S_{O_2}) and consumes, and is limited by, nitrate (S_{NO_X}). All kinetic parameters are assumed to be temperature dependent and can, for instance, be interpolated from values at 10 °C and 20 °C using the Arrhenius equation:

$$k(T) = k(20\ ^\circ\mathrm{C}) \cdot \exp(\theta_T \cdot (T - 20\ ^\circ\mathrm{C})) \tag{2.13}$$

where θ_T (in °C) may be obtained from

$$\theta_T = \frac{\ln(k(T_1)/k(T_2))}{T_1 - T_2} \tag{2.14}$$

Like every model, ASM3 has some limitations. ASM3 has been developed based on experiences in the temperature range 8-23 °C, other temperatures may lead to significant

Table 2.7: The processes defined in ASM3

Processes in ASM3	
1	Hydrolysis
Heterotrophic organisms, aerobic and denitrifying activity	
2	Aerobic storage of S_S
3	Anoxic storage of S_S
4	Aerobic growth of heterotrophs
5	Anoxic growth of heterotrophs
6	Aerobic endogenous respiration
7	Anoxic endogenous respiration
8	Aerobic respiration of storage products
9	Anoxic respiration of storage products
Autotrophic organisms, nitrifying activity	
10	Aerobic growth of X_A
11	Aerobic endogenous respiration
12	Anoxic endogenous respiration

errors. ASM3 does not include anaerobic processes. The pH is assumed to be about 7 and nitrite should not be present in elevated concentrations. Further, ASM3 is not designed to deal with activated sludge systems with very high load or small sludge residence times (SRT) (Henze *et al.*, 2000).

Hydraulics in treatment plants

The hydraulics are nearly always approximated crudely in WWTP models. If flow propagation through reactors is modelled explicitly, it is done in a simplified way, using the variable volume tank approach or using transfer functions (De Clercq *et al.*, 1999). Usually, instantaneous flow propagation is assumed, i.e. the outflow rate is assumed to be equal to the inflow rate at any time.

Mixing is usually modelled using the continuously stirred tank reactors (CSTR) in series approach (Levenspiel, 1972). This approach mimics the advection-dispersion behaviour in different unit processes. Basically, any mixing behaviour can be approximated by properly determining the number of tanks and their respective volumes (Rauch *et al.*, 2002a).

Modelling of clarifiers

The sedimentation process is one of the most important unit processes in wastewater treatment. It can be used as an unaccompanied process, as a preliminary phase before the following treatments (primary clarification) and finally as a concluding phase of the biological treatment (secondary clarification). Sedimentation utilises the gravity force to separate settleable solids from water.

Basically four types of settling are encountered in WWTP (Takács *et al.*, 1991) : discrete particle settling (the solids settle as individual entities), flocculent particle settling (typical

for primary clarifiers and for the upper layers of secondary settlers), hindered settling (suspension in which inter-particle forces hinder the settling process), and compression settling (achieved by compression of the mass of particles).

Modelling the primary clarification hardly ever takes into account its dynamic behaviour: most models are based on a steady-state approach. This tendency is legitimated by the fact that only one operational control option (the schedule of desludging) is possible on primary clarifiers. Anyway, the primary clarification acts upon the performance of the subsequent treatment processes and the sludge treatment and it is, for this reason, considered as a fundamental treatment unit. Lessard and Beck (1988) describe a model with five state variables: total suspended solids, volatile suspended solids, COD, soluble COD and ammonium. All solids are divided in a settleable and a non-settleable fraction to explain the observed behaviour of the clarifier. Gernaey *et al.* (2000) presented a model based on the approach of Takács *et al.* (1991), paying particular attention to the representation of the behaviour of particulate and soluble COD. The advantage of their work is that the model is compatible with the ASM1 models.

In modelling of the secondary clarification, more advanced models have been developed. Ekama *et al.* (1997) classifies the models according to their spatial scale, from simple 0- to complex 3-dimensional models. The 0-order models separate the incoming flow in a concentrated stream (with respect to solids) and in a (nearly) solid-free stream. In a more advanced 0-D model, Holzer and Krebs (1998) are able to predict the height of the sludge bed, by assuming a linear concentration profile in this sludge bed.

The 1-D models, which only describe processes along the vertical axis, can be used to describe particle separation and mass accumulation in the clarifier. The model of Takács *et al.* (1991) is the most known and applied one. It uses a double exponential settling function, resulting in low settling velocities at low and very high concentrations. It is based on the solid flux theory and it uses 10 layers to describe the settling tank.

The 2-D and 3-D models are able to describe flows and turbulence inside the settling tank. Computational fluid dynamics (CFD), together with turbulence models are used to describe the dynamic behaviour of the sludge bed. The complexity of the equations in this CFD-model, leads to huge calculation times for dynamic simulations (Krebs *et al.*, 2000).

The 0- and 1-D models are useful for the simulation of a complete treatment plant, allowing to model the displacement of the sludge during high inflows. The 2- and 3-D models are used to understand the interactions between flow and settling behaviour and might be used in the design of inlet, outlet and return sludge intake areas (Krebs *et al.*, 2000).

All these models require a given settling velocity function of the sludge, which has to be quantified from measurements. Models to predict changes in settling velocity and floc formation due to changes in bacterial community are not available yet. Also, problematic phenomena like sludge bulking or dispersed sludge cannot be predicted by the current models.

2.3.5 Hydraulic modelling of river systems

Deterministic modelling of river hydraulics

As for sewer systems, the flow of river systems can be described by deterministic models based on the conservation of momentum and mass, known as the "de Saint-Venant" equations (see eq. 2.1 and eq. 2.2). However, some differences with sewer systems are apparent. The channel is not prismatic as in sewer pipes, but by division of the river in different stretches, a reasonable approximation may be made. The different simplifications of the "de Saint-Venant" equations (kinematic wave and diffusion wave, see section 2.3.2) might also prove sufficient to describe the flood wave propagation reliably. These equations are implemented in numerous river modelling software packages like Aquasim (Reichert, 1998), Duflow (Aalderink *et al.*, 1995), Isis (Wallingford), Mike11 (DHI), QUAL2E (USEPA), ...

Conceptual modelling of river hydraulics

The flow propagation in rivers might also be approximated by CSTRs in series, a method known as hydrological routing. The following equations are used (Shaw, 1996):

$$\frac{dS(t)}{dt} = I(t) - Q(t) \tag{2.15}$$

and for the relationship between the storage, inflow and outflow

$$S = f_1(Q(t)) + f_2(I(t) - Q(t)) \tag{2.16}$$

where:

$I(t)$ Inflow at time t (m^3/s)
$Q(t)$ Outflow at time t (m^3/s)
$S(t)$ Storage at time t (m^3/s)
K storage constant (T)

Another conceptual approach is the unit hydrograph approach, in which the response at the end of the cascade of reservoirs can be calculated analytically (by convolution). When trying to include (non-linear) reactions of pollutants, complex calculations are necessary, making these models less suitable for water quality modelling (Shaw, 1996).

Beck and Reda (1994) have improved this modelling of river hydraulics by means of CSTRs in series. Reda (1996) mentions the following limitations of the CSTRs in series model (the following phenomena cannot be modelled with CSTRs):

- the travel of fluid-mass waves in the upstream direction
- the downstream propagation of flood waves within a tank
- water-surface slope within a tank

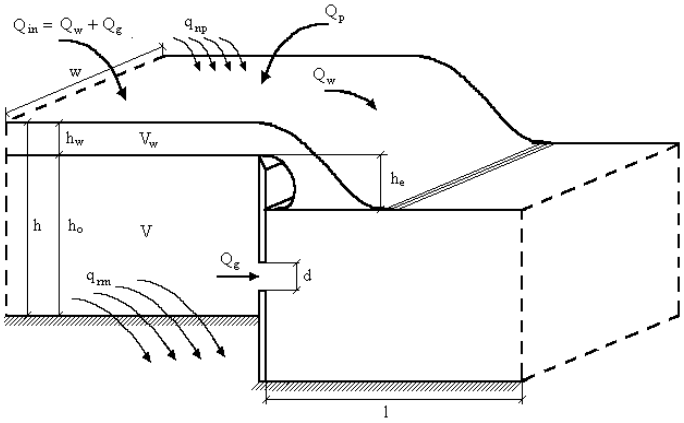


Figure 2.9: Schematic of a CSTRs element in the river model developed by Reda (1996)

This is due to the properties of a CSTR in which the water level is considered horizontal within one tank, while water can only flow from one reservoir into another in the downstream direction.

The model was applied to the river Cam, which was controlled by sluices, at which the water flowed both over the weir and through a gate near the bottom of the tank (see Fig. 2.9). Two types of flow were modelled: one through the gate and one over the weir. The flow over the weir $Q_{in,w}$ was a function of the water level in the tank, while the flow through the gate was a function of the difference in water level between this tank and the downstream tank.

The authors also introduced two extra parameters, h_a, the added depth and V_d, the dead volume. The parameter h_a was used to improve the phase lag of a flood wave of the model compared to the observed flood wave. The transport and dispersion of solubles was improved by adding a dead volume, V_d, to the tanks. This volume is not taken into account when calculating the retention time of the solubles, which is hence artificially reduced. The authors showed that with these extra parameters, both the hydraulics and the transport of solubles could be approximated well.

2.3.6 Water quality modelling

As in sewer water quality modelling, the routing of pollutants in river systems can be modelled with the advection-dispersion equation (eq. 2.5), or by using CSTRs in series. For the conversion process, different models have been developed. A general scheme of the different processes in a river, is shown in Fig. 2.10. Organic material (either in suspension or in the sediment) is decomposed, while oxygen is added by photosynthesis (by plankton or benthic flora) or reaeration through the water surface. The nitrogen cycle includes formation and degradation of organic nitrogen (e.g. incorporation in bacteria or algae), nitrification-denitrification processes and exchange with the atmosphere. The phosphorus cycle includes formation and degradation of organic phosphorus, precipitation and dissolution depending on the redox potential.

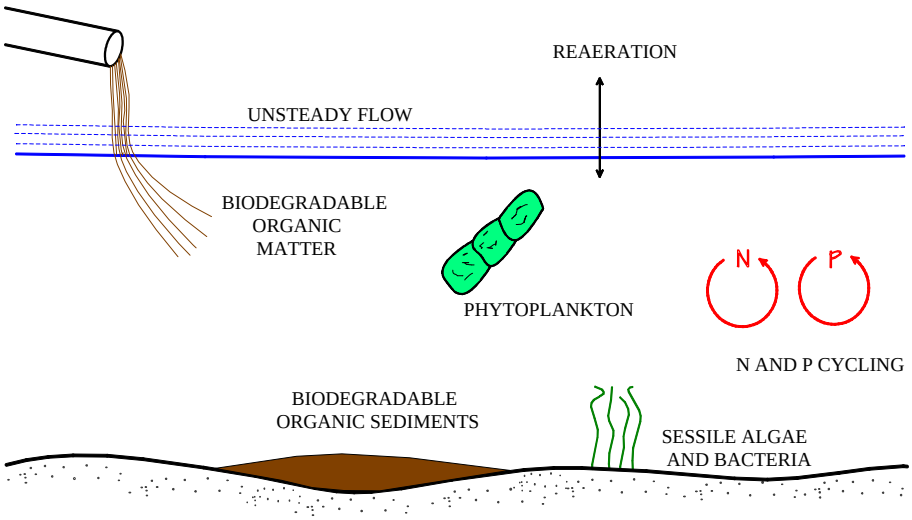


Figure 2.10: Schematic overview of river processes (Shanahan *et al.*, 1998)

Streeter-Phelps

The first water quality model was described by Streeter and Phelps (1925). The model describes the degradation of soluble organic BOD and the related oxygen consumption in the river. When solved under steady state conditions, this model results in the oxygen-sag curve. The equations can be written as:

$$\frac{dBOD}{dt} = -K_1 BOD \tag{2.17}$$

$$\frac{dDO}{dt} = -K_1 BOD + K_L a(DO_{sat} - DO) \tag{2.18}$$

where:

BOD	BOD concentration (g/m^3)
DO	Dissolved oxygen concentration (g/m^3)
DO_{sat}	Oxygen saturation concentration (g/m^3)
K_1	First order degradation constant for BOD (d^{-1})
$K_L a$	Reaeration constant (d^{-1})

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 BOD and sediment oxygen demand; dissolved oxygen; coliforms and radionuclides. Shanahan *et al.* (1998) point toward problems with the use of QUAL2E, like non-closed mass balances.

A schematic overview of the inter-relationships between the different components used in QUAL2E is shown in Fig. 2.11.

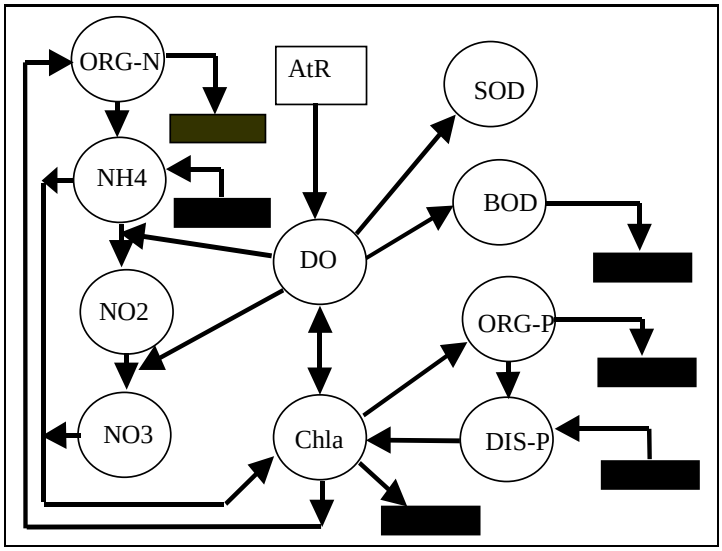


Figure 2.11: Interactions between the components in QUAL2E (Brown and Barnwell, 1987)

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, the RWQM1 was aimed to be compatible with the existing ASM models since they are both COD-based models. The RWQM1 introduced bacterial biomass as a 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. The RWQM1 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. An overview of the components is shown in Table 2.8, while the reactions are listed in Table 2.9.

The RWQM1 is designed to have closed mass and elemental balances. For every organic component a fixed composition is given, described by the mass fractions α_C (carbon), α_H (hydrogen), α_O (oxygen), α_N (nitrogen), α_P (phosphorus) and α_X (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 (see section 4.4 on page 108). From this, the composition matrix as described in section 2.3.4, can be constructed for all elements considered. For all reactions the ionic charge balance is closed as well.

A decision procedure for model building in six steps has been outlined.

Define temporal representation Different water quality processes manifest themselves over different time scales. Eutrophication processes in lakes are the result of an annual nutrient loading, while CSOs effect the water quality of the receiving waters in minutes. Therefore, the time constants of the system need to be determined. A time constant is

Table 2.8: The components considered in the RWQM1 (Reichert *et al.*, 2001b)

State variables in RWQM1		
1	S_S	Dissolved organic substances (M(COD)L^{-3})
2	S_I	Inert soluble organic material (M(COD)L^{-3})
3	S_{NH_4}	Ammonium nitrogen: NH_4^+ (M(N)L^{-3})
4	S_{NH_3}	Ammonia nitrogen: NH_3 (M(N)L^{-3})
5	S_{NO_2}	Nitrite nitrogen: NO_2^- (M(N)L^{-3})
6	S_{NO_3}	Nitrate nitrogen: NO_3^- (M(N)L^{-3})
7	S_{HPO_4}	Part of inorganic dissolved phosphorus: HPO_4^{2-} (M(P)L^{-3})
8	$S_{H_2PO_4}$	Part of inorganic dissolved phosphorus: $H_2PO_4^-$ (M(P)L^{-3})
9	S_{O_2}	Dissolved oxygen O_2 (M(O)L^{-3})
10	S_{CO_2}	Sum of dissolved carbon dioxide (CO_2) and H_2CO_3 (M(C)L^{-3})
11	S_{HCO_3}	Bicarbonate: HCO_3^- (M(C)L^{-3})
12	S_{CO_3}	Dissolved carbonate: CO_3^{2-} (M(C)L^{-3})
13	S_H	Hydrogen ions: H^+ (M(H)L^{-3})
14	S_{OH}	Hydroxyl ions: OH^- (M(H)L^{-3})
15	S_{Ca}	Dissolved calcium ions: Ca^{2+} (M(Ca)L^{-3})
16	X_H	Heterotrophic organisms (M(COD)L^{-3})
17	X_{N1}	Bacteria oxidising ammonia to nitrite (M(COD)L^{-3})
18	X_{N2}	Bacteria oxidising nitrite to nitrate (M(COD)L^{-3})
19	X_{ALG}	Algae (M(COD)L^{-3})
20	X_{CON}	Consumers (M(COD)L^{-3})
21	X_S	Particulate organic material (M(COD)L^{-3})
22	X_I	Inert particulate organic material (M(COD)L^{-3})
23	X_P	Inorganic phosphorus adsorbed to particles (M(P)L^{-3})
24	X_{II}	Particulate inorganic material (M(COD)L^{-3})

defined as $\tau = \frac{l}{\overline{u}}$, where τ is the system time constant and $\overline{u}$ is the average velocity over the length scale l. If the lowerbound (τ_1) and upperbound (τ_2) time constants of the system are determined, a decision on a process of interest with time constant τ_c may be taken. If $\tau_1 < \tau_c < \tau_2$, then a dynamic model is required, if $\tau_c >> \tau_2$, the process may be omitted and if $\tau_c << \tau_1$, a steady state model is sufficient (Fig. 2.12).

Determine model spatial dimensions In this step, the number of dimensions to be considered is determined. The choice of the vertical compartments (atmosphere, water body, sediments) to be included is determined by the type of problem. If the number of vertical compartments is determined, the dimensionality can be chosen. Possible dimensions in-

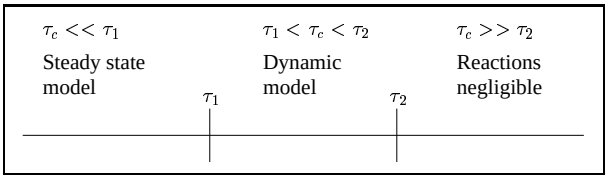


Figure 2.12: Selection of the type of model for a given process, with respect to the time constants of the system under consideration

Table 2.9: The reactions considered in the RWQM1 (Reichert *et al.*, 2001b)

	Processes in the RWQM1
1	Aerobic growth of heterotrophs
2	Aerobic endogenous respiration of heterotrophs
3	Anoxic growth of heterotrophs
4	Anoxic endogenous respiration of heterotrophs
5	Growth of 1^{st}-stage nitrifiers
6	Aerobic respiration of 1^{st}-stage nitrifiers
7	Growth of 2^{nd}-stage nitrifiers
8	Aerobic respiration of 2^{nd}-stage nitrifiers
9	Growth of algae
10	Aerobic respiration of algae
11	Death of algae
12	Growth of consumers
13	Aerobic respiration of consumers
14	Death of consumers
15	Hydrolysis
16	Equilibrium $CO_2 \leftrightarrow HCO_3^-$
17	Equilibrium $HCO_3^- \leftrightarrow CO_3^{2-}$
18	Equilibrium $H^+ \leftrightarrow OH^-$
19	Equilibrium $NH_4^+ \leftrightarrow NH_3$
20	Equilibrium $H_2PO_4^- \leftrightarrow HPO_4^{2-}$
21	Equilibrium $Ca^{2+} \leftrightarrow CO_3^{2-}$
22	Adsorption of phosphate
23	Desorption of phosphate

clude length, depth and width of the water body. While for rivers, the length dimension will be important in most cases, depth is the important dimension for most lakes. Possibilities are three-, two-, one- and zero-dimensional. If the water body is represented by one or more fully-mixed tanks, the model is called zero-dimensional. The choice of dimensionality may be influenced by the consideration of length scales, which are dependent on river width and depth, flow velocity and lateral and vertical dispersion coefficients.

Determine representation of mixing If less than three spatial dimensions are represented in the model, mixing is represented as dispersion due to velocity gradients. If three dimensions are taken into account, the turbulent diffusion is the most important mixing mechanism.

Determine representation of advection This is related to the way the movement of water is calculated (the "de Saint-Venant" or conceptual). Depending on the goal of the modelling study one or the other might be used.

Determine reaction terms In this task, the components and reactions to be included in the model are selected. The complete RWQM1 considers 24 components (Table 2.8) and

23 reactions (Table 2.9). It is clear that not all components and reactions are to be taken into account for a given river. By looking which situations are important, processes and components might be left out. A known example is nitrite which may not be present in relevant concentrations, and may hence be left out of the model. The same applies to algae, consumers, anoxic conditions, ... More hints on submodel selection are also given in Reichert *et al.* (2001b).

Determine boundary conditions A boundary condition has to be given for each dimension and each component considered in the model. The upstream flow and concentration profiles determine what enters the river stretch under study and has a significant impact on the resulting water quality predictions.

2.3.7 Modelling of the integrated urban wastewater system

In the previous sections, the mathematical modelling of the subsystems of the IUWS have been outlined. The application of these submodels has many advantages for planners, operators and managers. However, as is apparent from many studies conducted in the last few years, a major challenge in water quality management is the application of an integrated approach to the management of municipal water systems, in view of the increasing knowledge of dynamic interactions. Indeed, the expansion of system boundaries allows to determine and potentially model interactions with bordering subsystems which may uncover new management options (Krebs, 1996).

Two approaches are available to develop an integrated model: a *sequential approach* and a *simultaneous approach*. The first one implies the use of the three models that are run one after the other over the whole simulation period, using the output of one model to feed the next model. In this case, fluxes proceed in the forward direction. Conversely, in a simultaneous approach, all elements in the system are computed simultaneously. Parallel mode simulations are necessary as soon as feedback fluxes appear (e.g. information used upstream within real-time control applications or backwater effects from one subsystem to another (Pleau *et al.*, 2001)). Evidently, simultaneous mode simulations are much heavier from a computational point of view and, as a consequence, they are generally only carried out when such an effort is required, e.g. when real-time control is applied.

Related to the two approaches mentioned above, is the approach to the software implementation of the integrated model. One can either merge different software tools in such a way that sequential simulation of the integrated system is possible. When simultaneous simulation is necessary, a coordinating program is necessary to exchange information (either directly or via files) between the different software tools used. Another possibility is to use a common simulation platform where the IUWS is created by assembling a set of elements (pipes, structures, basins, river reaches, etc.).

The first option has been more often applied so far, even if the incompatibility of the state variables among the three pre-existing models is a difficult problem that cannot be avoided (Fronteau *et al.*, 1997). Indeed, the different existing models that one wants to merge in order to build an integrated model have been developed without the intention of joint use.

For instance, an important difference between the models is found in the expression of the organic material. In fact, existing sewer models (like Mousetrap or Hydroworks) or river models (ISIS, MIKE11, etc.) use BOD as a state variable to quantify organic pollution. Conversely, the state-of-the-art WWTP models, the ASM models (Henze *et al.*, 2000), use COD as a state variable. An exact relationship between BOD and COD does not exist, which makes it difficult to link these models. The RWQM1 is a COD based model (Reichert *et al.*, 2001b), but the state variables are not exactly the same as in the ASM-models. Consequently, linking is still a non-trivial task.

In the field of integrated modelling, 5 important groups can be distinguished. As many of this research was carried out during overlapping periods, an exact chronological overview is not possible. In the next paragraphs, the approach of every group towards integrated modelling is explained. In a last paragraph, other relevant projects will be highlighted.

The Imperial College Group: Beck, Lessard, Reda, Schütze

One of the first suggestions to use the models of all parts of the urban wastewater system within an integrated approach was made by (Beck, 1976). Later, Lessard and Beck (1988, 1991) developed models and control strategies for the treatment plant system, which were later on used by Reda (1996); Reda and Beck (1999) and Schütze (1998).

This work was continued in the integrated modelling studies done by Reda and Beck (1999). The hydraulic river model described in section 2.3.5, was used in a study to optimise the river water quality while dealing with combined sewer overflows and wet weather control strategies for the WWTP. The extra control options added were the opening or closing of the gates in the river which could provide extra dilution capacity during CSO events.

Schütze *et al.* (1999, 2002a) carried out the assembly and the implementation of the integrated simulation and optimisation tool SYNOPSIS (Fig. 2.13). The authors created an integrated model in which:

- The sewer system was modelled as a reservoir cascade and assumed complete mixing of pollutants. It consists of the software package EWSIM, which is an extended (research) version of the commercial Kosim package (itwh, 1995; Paulsen, 1986).
- The biological treatment was based on the model of Lessard (1989)
- The river quality model mainly encompassed dissolved oxygen and organic matter (expressed in terms of BOD) in two fractions (slowly and readily biodegradable matter). The water quality was simulated using DUFLOW (Aalderink *et al.*, 1995).

The sewer system and the treatment plant software were incorporated in one single package. Attempts were also made to link the river system in a similar way, but in 1998 the river model could only be run as a sequential process after the simulation of the sewer system and treatment plant had finished. As the authors noticed, the sequential approach limited the extent of control actions that could be evaluated, but still allowed the analysis of a large number of integrated control strategies (see section 2.4.7). When merging the submodels, the authors encountered the problem of the “reconciliation of the different

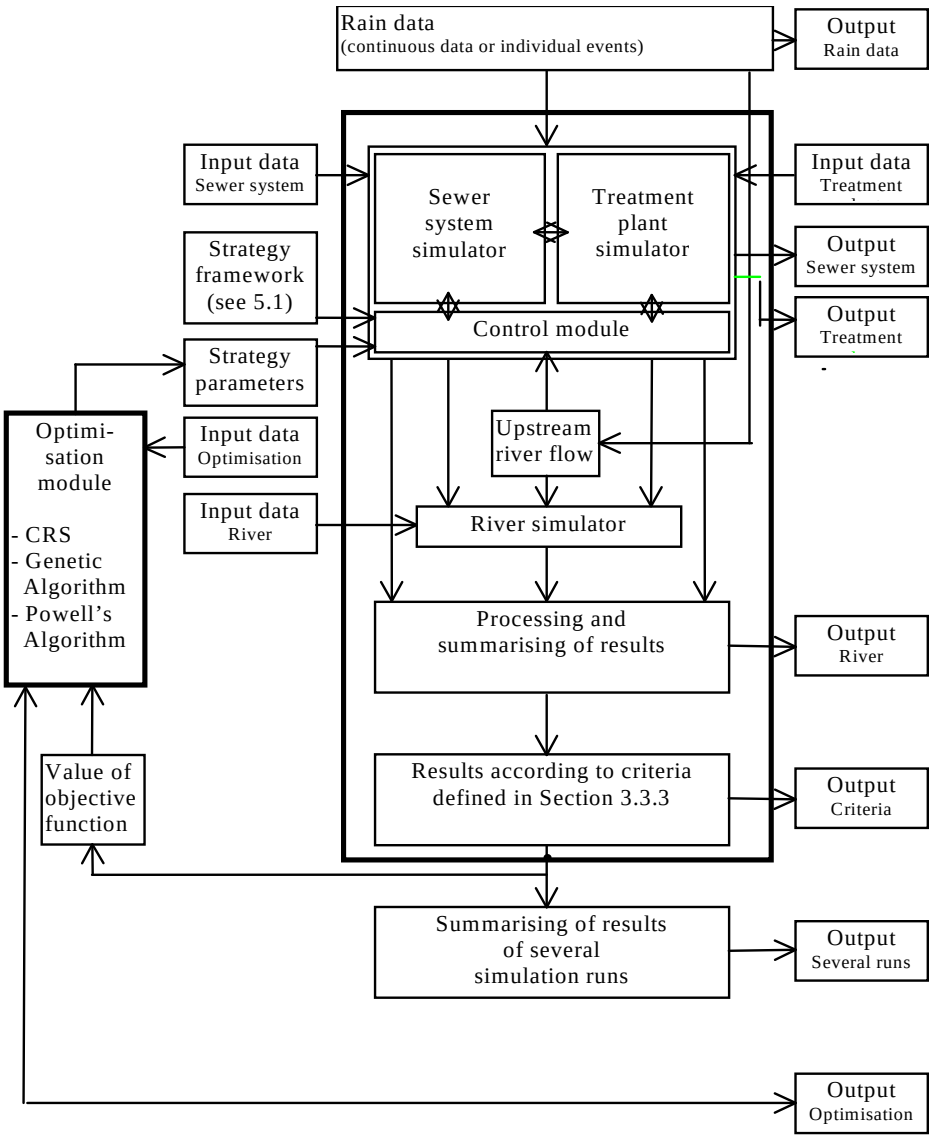


Figure 2.13: Overview of the Synopsis simulation tool (Schütze *et al.*, 2002a)

time-steps". Indeed, each submodel should be run with a time-step that allows the description of the processes. A time-step of 5 minutes appeared adequate to describe the sewer system processes (including CSO events, which typically cannot be represented with much larger time-steps). A time-step of 1 hour was chosen to simulate the WWTP, as from previous studies such a choice had appeared to be reasonable. The choice of the time-step for the river model resulted from a compromise between the accuracy requirements and faster simulations. Connections were necessary at the interfaces between the models and a synchronisation program was necessary to take into account the different time steps used in the simultaneous simulation of the sewer system and the WWTP.

These three models were connected with a library of optimisation routines. The optimisation was run in such a way that the best receiving water quality was obtained by changing pump capacities in the sewer system, emptying rates of storm tanks or maximum inflow rates to the treatment plant, etc. More details can be found in Schütze *et al.* (2002a).

Work done by Fronteau, Bauwens and Vanrolleghem

This group started with the modelling of the emissions of pollutants from combined sewer systems during storms (Bauwens *et al.*, 1994), and extended this approach to evaluate the efficiency of the combined sewer - wastewater treatment system under transient conditions (Bauwens *et al.*, 1996). The emphasis was placed on the receiving water objectives by Bauwens *et al.* (1995), Vanrolleghem *et al.* (1996a) and Fronteau *et al.* (1996). The software platforms used were Kosim (itwh, 1995), Mosifit (Vanrolleghem, 1996), and Salmon-Q (Wallingford Software, 1994). In order to illustrate the potential of an integrated approach, a series of simulation studies was performed for a particular catchment by comparing different pollution abatement scenarios. In particular, the authors evaluated the impact on river water quality of several simple variations to design and control of the sewer system and the WWTP. The evaluation criterion was based on an EQO/EQS (Environmental Quality Objective/Environmental Quality Standard) analysis of the receiving water immission characteristics (Tyson *et al.*, 1993).

Maryns and Bauwens (1997) applied an extended ASM1 model to the river system in order to have a common set of state variables in both WWTP and river model. However, the ASM model was not able to describe the behaviour of the river system adequately. These authors concluded that the extended ASM1 model was able to model the BOD concentration with reasonable accuracy, but that the observed variations in DO could not be described by the model used.

Fronteau (1999) linked existing models for sewer system, WWTP and river in a sequential way to represent two semi-hypothetical case studies (river Zenne, Brussels and rivers Molenbeek and Zwalm, Brakel, Belgium). Through the first case study, the author illustrated the usefulness of integrated modelling for the management of water quality and pointed to the problems connected to this approach (such as the problem of the incompatibility of variables, parameters and processes in the water quality modules of the different submodels) (Fronteau *et al.*, 1997). Simplified models, though unsteady, were chosen in order to represent the submodels. Software tools were developed in order to deal with data transfer between the different submodels and to allow for continuous long-term simulations with the Salmon-Q tool (Wallingford Software, 1994).

The problem of incompatibility of the variables was avoided by introducing conversion factors to translate the output variables from the sewer model into input variables for the WWTP model and to transform the latter into variables to be used in the river context. The developed sequential integrated models allowed real-time control applications to be tested (Fronteau *et al.*, 1997).

Rauch and Harremoës

Harremoës (1982) already developed a model to describe the immediate and delayed oxygen depletion in rivers. The immediate oxygen depletion originates from the utilisation of readily biodegradable organic material, while the delayed oxygen uptake is due to settled organic material and biomass. This model was later on used in studies of the IUWS system (Harremoës and Rauch, 1996; Rauch and Harremoës, 1995, 1996a). In their study on a

hypothetical catchment, existing deterministic models were linked to create an integrated model. The hydraulics of the sewer system were calculated by applying the time/area method, while for the pollutants in the runoff a constant concentration was assumed. The treatment plant model was based on the ASM1 model (Henze *et al.*, 2000), while the model of Takács *et al.* (1991) was used for the secondary clarification.

The most important conclusion from these studies is that oxygen depletion in rivers is caused by intermittent discharges from both sewer system and WWTP. Neglecting one of them in the evaluation of the environmental impact gives a wrong impression of total system behaviour. When overloading the WWTP too much, a plant break-down occurs with a dramatic decrease in oxygen concentrations in the river as a consequence (Rauch and Harremoës, 1997a). In a later study, based on the urban drainage system of Greater Copenhagen (Rauch and Harremoës, 1997b) no correlation between the minimum oxygen concentration and the volume of CSO reduction by means of RTC was found. Several reasons were given for this small effect:

- The more runoff volume is stored in detention basins, the longer the period of high hydraulic loading in the WWTP. The subsequent water pollution caused by the plant effluent is contrarily to the efforts of storing the water.
- The oxygen concentration in the river fluctuates daily due to algal growth and decay. Hence the exact time of the overflow is important, and is not taken into account by only storing the water.
- The increased flow is contributing to the dilution capacity of the river. If upstream, relatively unpolluted water is stored, the effect of a downstream CSO may be more pronounced as compared to the uncontrolled situation.
- In case of severe rain events, anaerobic conditions were found in the river and the extra volume of water stored is not changing this situation due to the large overflow volume that is still present.

Rebeka is a recent software tool described by Rauch *et al.* (2002b) that uses simplified models to describe the effect of the urban drainage system on alpine rivers. It can be used to predict both hydraulic stress (erosion) or acute water pollution (high concentration of ammonia).

The Integrated Catchment Simulator

The Danish Hydraulic Institute (DHI) and the Water Research Centre (WRc) in the UK developed an "Integrated Catchment Simulator (ICS)" (Clifforde *et al.*, 1999; Taylor *et al.*, 2000) linking together widely known commercial tools (MOUSE (for sewers), STOAT (for treatment plants) and MIKE11 (for rivers)) both in a sequential and in a simultaneous way. The ICS had the following functional requirements (Clifforde *et al.*, 1999):

- a strong graphical capacity of the user interface to provide a user-friendly working environment, including the visualisation of the modelled catchment, individual models and the model interaction points

- the model integration to be done intuitively through the user's response to simple dialogues and graphics, i.e. without the need for an in-depth understanding of the underlying data processing techniques and transfer of flow and pollution components between different models
- the system to be capable of sequential and simultaneous simulations, in order to cover the full range of applications, including hydraulic and RTC feedback in the upstream direction
- the system to allow integrated modelling at various scales (i.e. levels of detail), in order to match actual study requirements
- the system to be as open as possible, in order to enable the integration of various models within the same generic framework

This simulator is being used in integrated modelling studies as well as real-time control applications (Williams *et al.*, 2001).

Matlab/Simulink: SIMBA

Another platform created to simulate integrated models which is based on commercial existing tools is SIMBA (Alex *et al.*, 1999). This software package uses the widely used Matlab/Simulink^{TM} tools to allow for simultaneous simulations. It can be seen as a network of interlinked elements that are computed at the same time:

- PLASKI for the urban catchment
- SIMBA SEWER for the sewer system quantity and quality
- SIMBA for the WWTP
- SIMBA SEWER is used for the simulation of the river system with an adapted conversion model
- Simulink for the use of control items in any of the subsystems or across them

Alex *et al.* (1999) give several advantages and drawbacks related to the use of Matlab/Simulink, which is a general purpose simulation software, for simulation of wastewater systems. The most important are:

+ mathematical algorithms are maintained at the state of the art
+ all modern control and signal processing algorithms are available (fuzzy control, artificial neural networks (ANN), predictive control, ...)
+ open environment which is easy to extend with novel ideas or innovative designs
- no specialised solvers or optimisation routines available
- user interface is not tailored for wastewater systems

Testing control strategies in real urban wastewater systems can be done with this tool. Matlab/Simulink™ is a commercial package with many features, and due to these capacities, rather expensive. The control toolboxes mentioned above need to be paid separately. The performance of the platform is rather slow since the code is interpreted rather than compiled, although routines can be compiled to improve calculation speed (Jeppsson,

Table 2.10: Characteristics of the software packages available for integrated modelling (adapted from Rauch *et al.* (2002a))

Name of simulator	SYNOPSIS	ICS	SIMBA	WEST (this study)
Developer	Imperial College; London, UK	DHI, Hørsholm, DK; WRc, Swindon, UK	Ifak, Barleben, G.	Ghent University, B; Hemmis n.v., Kortrijk, B.
2-directional interaction between submodels	No	Yes	Yes	Yes
Truly synchronised simulation	Only Sewer System and WWTP	Yes	Yes	Yes
Simulation of control options possible	Only Sewer System and WWTP	Under development	Yes	Yes
Simulation of long time series feasible	Yes	Under development	Under development	Yes
Open simulation environment	No	No	Yes	Yes
Integrated use at a real case study reported	Semi-hypothetical	Yes	Yes	Semi-hypothetical

2002). Erbe *et al.* (2002) used this modelling platform to analyse the system in Odenthal (Germany).

Seggelke and Rosenwinkel (2002) used this tool to determine the maximum inflow to the treatment plant in order to minimise the total load of the sewer system and WWTP to the river by means of on-line simulation and optimisation.

Table 2.10 shows the main characteristics of the software packages available for integrated modelling. The properties of the software used and developed in this work are also mentioned as a basis for comparison.

Other approaches

Many other studies which can be classified as integrated modelling of the urban wastewater system can be found in literature. A lot of practical applications are reported in the proceedings of the Biennial Meetings of the Integrated Modellers User Group (IMUG), (Imug, 1998, 2000). The applications discussed are very diverse and range from master planning (Eicher, 1998; Gustafsson *et al.*, 2000), to the use of simplified models Crabtree *et al.* (1998), or detailed deterministic modelling of one or more subsystems (Raso and Malgrat, 2000; Richardson, 2000). This shows that integrated modelling is not only used in research, but also in practice, for management and planning.

Several authors have been looking at the combination of the sewer system and the treatment plant to determine the total load from the effluent and the CSOs to the receiving water (Bertrand-Krajewski *et al.*, 1997; Deyda, 1997; Durchschlag *et al.*, 1992; Fuchs *et al.*, 1997b; Guderian *et al.*, 1998; Holzer and Krebs, 1998; Kluck *et al.*, 2001; Otterpohl *et al.*, 1994). All these authors consider it important to look at the combined load discharged, when looking at several design or control options, like locations of storm tanks or volumes of storage in the system. These emission based approaches certainly have potential, but leave the possibilities of the immission based research unused.

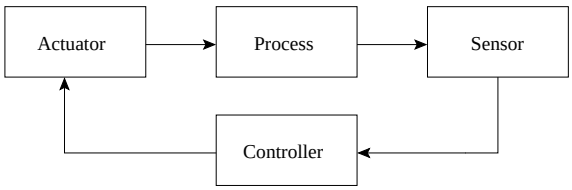


Figure 2.14: General representation of a control system

2.4 Real-time control in the integrated urban wastewater system

2.4.1 What is real-time control?

Many investments have been made in the urban wastewater systems to build sewer systems, storm tanks and WWTPs. In the past, rigid environmental standards were set according to the BATNEEC principle and systems were implemented to fulfil exactly these design guidelines (Chocat *et al.*, 2001). In traditional static (without any control action) wastewater systems, however, the performance of the system cannot be adapted to the time varying conditions after the system is taken into operation. The limited efficiency in reducing flooding, environmental pollution and health risks is very often caused by the lack of flexibility in the operation of the static urban wastewater systems under dynamic loadings. Even if the system is correctly designed, there is no guarantee that the elements are at capacity simultaneously during each single event (Schilling *et al.*, 1996). If the system is loaded with less than the design flow, much of the available capacity of the sewer system is not used. On the other hand, if a huge rain event produces flow exceeding the design flow, the system will be flooded.

The two classical tasks of wastewater management are drainage of storm runoff and transport and treatment of wastewater. These two tasks are characterised by opposite needs: the first one aims at "getting rid" of the water as soon as possible, while the second one requires the water to be retained in the system as long as possible (Schilling *et al.*, 1996). The problem of these conflicting requirements can be solved either in a static way (providing the collection and treatment systems with sufficient capacity) or in a dynamic way by using real-time control of the system.

Real-time control of the urban wastewater system can be defined as follows: "A wastewater system is controlled in real-time if process data such as water level, flow, pollutant concentration, etc. are continuously monitored in the system and, based on these measurements, regulators are operated during the actual flow and/or treatment process" (Schilling *et al.*, 1996). Three things are necessary to implement real-time control: measurement, control decision and action in the process. Three hardware parts are needed: a sensor for the measurement, a controller to calculate the control decision based on the measurement, and the actuator to adapt the situation to the control decision (e.g. change a flow rate of a pump) (Fig. 2.14).

The integrated urban wastewater system is designed to deal with the large disturbances

Table 2.11: Approaches to RTC of the components of the urban wastewater system (Schütze *et al.*, 1999)

Subsystem	**Control devices (selected examples)**	**Typical control objectives**
Sewer system	Pumps, Weirs, gates	Prevention of flooding CSO reduction Equalisation of flows
Treatment plant	Weirs, gates Return sludge rate Waste sludge rate Aeration	Maintenance of effluent standards Keeping the process going
Receiving water	Weirs, gates Aeration	Improved water quality Flood protection

frequently met in the system. Rain events, causing either a CSO or an increased inflow to the treatment plant, might be handled better if RTC is active, compared to the static case, where nothing can be changed in the process. An RTC system aims at the optimum use of the existing transport, storage and treatment facilities. RTC might also save investments (e.g. in additional storage), which would be necessary without the implementation of RTC. An overview of typical control devices and control objectives is given in Table 2.11.

If no moving regulators are involved at all (e.g. all flows are maintained only by gravity), one can define this as *static* control. The lowest level of operation can be described as *local* control. It involves regulators operating with constant set-points. One example would be a flow regulator which maintains the water level, using measurement information obtained in the vicinity. Under local control, regulators are not remotely manipulated from a certain control unit. Better operation in systems with two or more regulators can be achieved by *global* control. Here, regulators are operated conjunctively (Schütze *et al.*, 2002a). A (sewer) system is said to be under global RTC if all actuators receive the data of the other sensors in the system and adapt their action with this information. *Integrated control* of urban wastewater systems is characterised by two aspects according to Schütze *et al.* (2002a):

Integration of objectives : Objectives of control within one part of the urban wastewater system may be based on criteria measured in other subsystems (e.g. operation of pumps in the sewer system aiming at minimum oxygen concentration in the receiving water body).

Integration of information : When taking a control decision within one part of the system, information about the (present or predicted future) state of another subsystem may be used (e.g. considering treatment plant effluent concentrations when performing control in the sewer system) - hence state information is transferred across subsystem boundaries.

2.4.2 Development of control procedures

A control procedure (i.e. the time sequence of all the set points of all actuators in a RTC system) can be optimised in many different ways. *Heuristic* approaches to determine a suitable control procedure can be based on the experience of the operating staff. A set of potential procedures is specified and then improved by an iterative procedure involving a simulation model of the system. Besides simple, but laborious trial-and-error methods, also mathematical techniques have been applied successfully to the development of control procedures, in a so-called *off-line optimisation* (Dochain and Vanrolleghem, 2001). Values are determined for the parameters of control rules which are optimal with regard to the specified performance criteria (Schütze *et al.*, 2002a).

An alternative approach to determine a control procedure consists in setting up an on-line simulation model, which, at every control step, evaluates the impacts of a number of potential control actions and then actually applies that one which showed to be most beneficial in the evaluation procedure. This approach is called model based predictive control (MBPC) and was e.g. applied by Rauch and Harremoës (1999). For determining the best possible control action, on-line optimisation routines can be applied too (Schütze *et al.*, 2002c).

2.4.3 Classification of RTC-strategies

Different types of real-time control can be distinguished with different objectives: volume based RTC, pollution based RTC and immission based RTC. In volume based RTC, the control strategy is designed to minimise the volume of polluted water entering the receiving water by storing or treating it. This approach is successfully applied, for instance, by Pleau *et al.* (2001). Pollution based RTC tries to minimise the total amount of pollutants entering the receiving water by preferably storing polluted water and spilling more diluted water (Weinreich *et al.*, 1997). Finally, receiving water quality (or immission) based RTC, tries to optimise the receiving water quality directly. In this case, the minimisation of the adverse impacts in the receiving water - measured in receiving water terms - is the final goal.

Schütze (1998) classifies 60(!) papers according to the objective of the RTC and to the method of strategy development.

2.4.4 Real-time control of sewer systems

In general, for RTC of sewer systems one or more of the following objectives apply (Schütze *et al.*, 2002a):

- Prevention of flooding of properties and streets.
- Reduction of CSO discharges, in particular if storage is still available at some location within the system at the same time. Criteria conventionally chosen in the past to assess CSO spillages include the following: water volumes discharged at CSOs, frequency of overflow events, pollutant loads discharged at the CSOs, mean annual COD concentration of all overflow events.

- Uniform utilisation of storage capacity within the sewer system.
- Equalisation of peak discharges towards the treatment plant; optimum use of spare treatment plant capacity.
- Quick provision of storage capacity for subsequent rainfall events by emptying storage as quickly as possible at the end of rainfall.
- Minimisation of operation and maintenance costs. These include, for example, energy costs incurred for the operation of pumps, which would also be affected by frequent switching of the pumps.

The most commonly applied control action within a sewer system is to use flow regulators (e.g. gates, slide valves, pumps, weirs etc.) in order to attain desired flows within parts of the sewer network. In general, decisions are based on the information read by sensors concerning water levels (Hansen and Carstensen, 1997), flow rates upstream and downstream, rainfall information (Andersen *et al.*, 1997; Petruck *et al.*, 1998), residence time in tanks, forecast rainfall and flows (Andersen *et al.*, 1997; Duchesne *et al.*, 2001; Entem *et al.*, 1998; Petruck *et al.*, 1998).

Volume based control in the sewer system

The results of control actions are often evaluated with respect to water volumes. Indeed, in several studies only the total discharge volume of CSO is taken into account by the control action.

Pleau *et al.* (2001, 1996) and Field *et al.* (2000), for example, developed a robust optimal control strategy, applied on the sewer network of the Quebec Urban Community. In this system, the predicted rainfall intensities, provided by a meteorological model, are converted by a non-linear flow model into predicted hydrographs in each pipe of the sewer network. These hydrographs are then used as input flows to an input-output linear time invariant model (LTI) coupled to a Kalman filter using on-line data for increased robustness. The LTI model computes flows and accumulated volumes, keeping the computing time small enough for RTC applications. Once the state variables calculated by the LTI model are available, a cost function is minimised. The cost function is defined to meet a specific control objective: the minimisation of overflow volumes, the minimisation of stored sewage volumes and the minimisation of the cost associated with the management of the control sites. With this approach the authors achieved a sensible reduction of the total overflows maintaining the flow at the treatment plant at the target value for a long period of time. The system is implemented and working very well (Pleau *et al.*, 2002).

Entem *et al.* (1998), used an on-line control action performed with a rainfall forecast model and an enhanced version of the MOUSE software to reduce, as much as possible, the CSOs to the River Seine.

Duchesne *et al.* (2001) developed a hydraulic model which, in conjunction with rainfall intensity predictions and a runoff simulation model, was used by an optimisation algorithm to minimise sewer overflow volumes during rain events.

Pollution based control in the sewer system

Even if the general approach in sewer system RTC is often concerned with water volumes, other approaches are possible as well. Some examples of different strategies are further proposed below.

Weinreich *et al.* (1997) applied a simulation tool for pollution based real-time control (PBRTC) to the sewer system of the city of Oslo. The authors focused on the reduction of total phosphorus and nitrogen overflow loads into the receiving water by means of optimised operation of the sewer system. The principle applied in this example of PBRTC is to direct the most polluted storm water to the WWTP. The tool used for PBRTC consisted of three main-modules: a flow simulator combining a hydrodynamic flow routing model with a simple pollution transport model, a rule-interpreter, and a numerical optimisation module. According to the user's choice only one of the control modules will be activated during the simulation run. The rule-interpreter determines the operation strategy, depending on the current state of the system by pre-defined if-then-else rules. Besides water levels and flows, it is possible to incorporate the concentration and/or pollutant fluxes into rules. On the other hand, the mathematical optimisation model minimises an objective function with a linear optimisation method. Since the pollution transport process is inherently non-linear, the objective function has to be modified. The results obtained in the case study show a significant reduction of the phosphorus and nitrogen concentration in the receiving waters.

Petruck *et al.* (1998) analysed two advanced RTC strategies: a pollution based real-time control (PBRTC) and a water quality based real-time control (WQBRTC) strategy. The paper was developed in the framework of the research project "Real-time control of a combined sewer system by radar estimates of precipitation" carried out by the German government. The main aims of the project were to improve the water quality of the river by quantitatively and qualitatively reducing the discharges by CSOs and improving the WWTP efficiency.

The authors noticed that during CSOs serious damage might occur in the biotic river community if the critical bottom shear stress, DO and unionised ammonia were already at critical levels. For this reason, the authors stated that it was important to check the incident and length of critical conditions in the receiving stream. This is the aim of the WQBRTC. Notice that in the PBRTC only measurements within the sewer system are required, whereas in the WQBRTC predictions of the resulting water quality are made using both quality and volume measurements in the sewer system and river. However, the system status during rainfall events has to be predicted for the sewer system as well as for the receiving water. Therefore, a good knowledge of the system is required in order to achieve successful control. In this study the surface runoff model HYSRAD processes real-time data obtained from radar images and rain gauges and from a predictive rainfall model. The data calculated by HYSRAD are utilised by a hydrodynamic transport model (EXTRAN) which calculates the inflow and the temporal variation of flows within the control parts. The control strategy is chosen by means of a mathematical optimisation combined with a rule base. The rule base is used to define the objective function for each time step and to achieve the mathematical optimisation. The objective function incorporates the control priorities such as treatment plant performance and receiving water

conditions. Forecasting data, measured data, HYSRAD, EXTRAN and the decision finding process produce the set points that have to be transferred to the control elements. So far, only the PBRTC has been implemented, providing satisfactory results.

Carstensen *et al.* (1996) described another predictive on-line control applied to the sewer system. The authors suggested the use of "grey box" models, which constitute a combination of deterministic and stochastic models. These models are able to deduct the most important information contained in the data and point out deviations in the measured dynamics from the expected behaviour of the sewer system. The grey box models contain as many elements from the physical models that can be statistically identified, and stochastic elements are subsequently added to describe any residual variation. When the grey box models are used for sewer system control, the structure of the model is determined by the number of control points in the sewer system. In these control points storage capacity is available and regulators for the flow are present. By means of simulations it could be shown that significant performance improvements of the sewer network could be obtained with this type of models.

Other case studies

Other researches use advanced mathematical techniques to optimise the behaviour of the sewer system. Fuchs *et al.* (1997a) defined a set of fuzzy rules to optimise the coordination between three storage tanks. Willemsen *et al.* (2000) used genetic algorithms (GA) to economically optimise a sewer system with different possibilities of investment (more storage, more pumping capacity, larger pressure sewers, increase of capacity of the treatment plant).

Hajda *et al.* (1998) compare simple feedback logic, genetic algorithms and artificial neural networks for the RTC of a collection system. They show that a hybrid controller (PI combined with on-off) is superior to on-off control as such. Moreover, the genetic algorithm was able to further reduce the pumping cost in the given system. In a second stage, the artificial neural network was trained on the input-output data (that is, records of inputs to the flow routing model and the resulting strategies found by the GA). In this way, the ANN was able to quickly give a control strategy close to the optimum, without performing the iterative search necessary with the GA.

Zug *et al.* (2001) used outlets at different levels in a detention basin to optimise the flow and the quality of the released water as function of the system state. Two modes of control are possible: flood prevention (in case of heavy rainfall) and the depollution mode (for "small" rain events). The study is conducted using the Hydroworks DM and its RTC module using a calibrated and validated model of the sewer system and the detention basin.

Campisano *et al.* (2001) describes the RTC of a large wastewater tunnel in Trondheim. Two sewer models were compared: SIMBA-sewer (which uses the diffusive wave approximation of the "de Saint-Venant" equations) and FLUSS (which solves the full dynamic equation). Some differences between the two models were found in case of the simulation of real storm events. Two control strategies were used to reduce the CSO discharge (up to 63% reduction of overflow was obtained). In the first case, a fixed water level at

the WWTP inflow was maintained by means of a level sensor and a PI controller (local control). In the second case, a simple global control strategy was used, aiming at an even degree of storage in the two in-line reaches.

2.4.5 Real-time control of WWTP

In a treatment plant many different components and many different processes are involved within the overall system. Therefore, RTC of WWTP is generally considered a complex task. However, since the pollution abatement has also been directed toward nitrogen and phosphorus removal in addition to carbon removal, control operations on WWTP became a necessary task (Harremoës *et al.*, 1993).

Indeed, the numerous interactions involved in the removal process and the fact that the biological potential is taken to its limit, make the nutrient removal a sensible and vulnerable process. Besides, more restrictive effluent quality standards motivate control actions to be applied in order to avoid failure of the treatment process. The use of operational control to improve the treatment performance can also be required to deal with other issues, such as faulty design, overloads and human mistakes (Vanrolleghem, 1995).

The main aims of the control options in WWTP can be summarised as follows (Schütze *et al.*, 2002a):

- Avoidance of discharge of biomass into effluent.
- Maintenance of performance of the plant processes (“keep the plant running”).
- Maintenance of the overflow discharge and effluents standards.
- Minimisation of operation and maintenance costs.

Control of WWTP is carried out by means of four fundamental blocks (Vanrolleghem, 1995):

- Insight in the plant operation as summarised in a proper process model.
- Sensors that provide on-line data on some of the output variables of the process and disturbances acting upon it.
- Adequate control strategies which try to minimise deviations from the objectives.
- Actuators that implement the controller outputs on the plant.

Before, the weakest part of the control chain were the sensors that caused problems in calibration, fouling, reliability and sampling techniques (Harremoës *et al.*, 1993). Today, however, this may no longer be the case, as Jeppsson *et al.* (2002) state that the performance and reliability of many on-line sensors (e.g. nutrient sensors, respirometers) have improved remarkably during the last decade (if maintained properly). The most fundamental barrier for more widespread acceptance of new control strategies is that existing WWTPs are not designed for RTC.

Some sensors (DO, pH and redox potential sensors) are known for their robustness, reliability and limited demand for maintenance. These sensors, when combined with mathematical models, constitute so-called “software sensors”. The choices for the actuators of

Table 2.12: WWTP variables available for manipulation, adapted from Vanrolleghem (1995).

Manipulate variable	**Process** [1]	**Applicability**[2]
Bypass/Overflow	1, 2	∀
Equalisation / Buffering / Storm tank	1, 2	∃
Feeding point/Step point	1, 2	∃
Aeration intensity	1, 2	∀
External Carbon Source	2	∀
Internal Recycle Flow rates	2	∃
Chemical dosage	2, 3	∃
Return Activated Sludge rate	A	∀
Waste Activated Sludge rate	A	∀
Sludge storage	A	∃

[1]Process: 1:activated sludge; 2: nutrient removal; 3: sedimentation; A: all.

[2] Applicability: ∀: state of technology; ∃: applicable in certain cases.

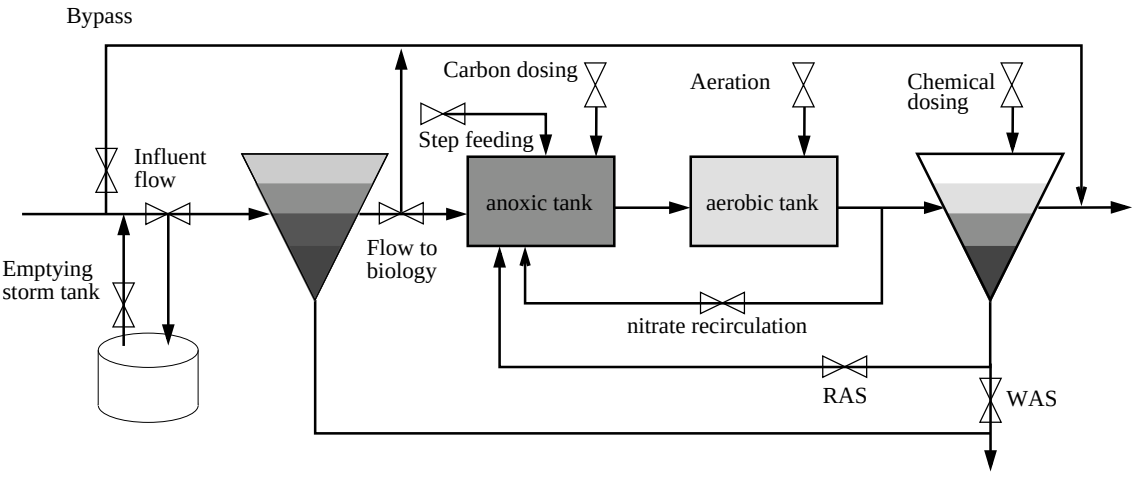


Figure 2.15: Overview of control handles in an activated sludge WWTP

the control action are limited and are, apart from some new possibilities with chemical additions (e.g. polyelectrolytes and phosphorus) or with integrated control, almost the same as thirty years ago (Vanrolleghem, 1995). Table 2.12 and Fig. 2.15 show the variables commonly used to operate WWTPs.

Control handles in WWTP control

According to Schütze *et al.* (2002a) three different control levels can be normally identified in the framework of treatment plants. At the highest level (overall level) the aim is the definition of overall operational objectives. At the second level (set point level), set points (possibly time-varying) of the individual controllers have to be determined. Finally, at the lowest level (controller level) the goal is the maintenance of set points.

With regard to the set point level control, an overview of commonly controlled settings is given (Olsson and Newell, 1999).

Maximum inflow to WWTP One of the most applied control measures is the inflow regulation at WWTP. In almost all treatment plants it is normal behaviour to bypass flow above a certain threshold directly to the receiving water (Lessard and Beck, 1991). Several studies about the threshold variation have been carried out. Lessard and Beck (1991), for instance, analysed the behaviour of their system when the maximum inflow allowed to the treatment plant was increased. In the U.K. the threshold is generally set to 3 times dry weather flow (DWF). In one of their design modifications, the authors set this value to 3.5 times DWF. The results for a rain event of short duration and high intensity showed a slight reduction in the overall suspended solids and COD mass discharged. For a long duration and low intensity storm the strategy eliminated the overflow almost entirely and improved the overall efficiency in terms of suspended solids and COD but, on the other hand, it aggravated the nitrification process. Hence, the authors concluded that the latter considerations opened up the debate on "whether all flows should be treated during an event, risking performance impairment and higher operational costs, whereas permitting overflows may prove to be (at most) no more damaging to the receiving body in terms of the pollutant mass discharges".

Dauphin *et al.* (1998) proposed, in a hypothetical case study, an influent flow control to admit a maximum of twice the dry weather peak flow. In the operation strategy twice the dry weather peak flow is admitted until the sludge blanket in the secondary clarifier reaches a security level or until a maximum time delay for sludge storage in this unit is reached, to prevent anoxic conditions. The authors concluded that neither sludge loss nor degradation through anoxic conditions might occur.

Another possibility to increase the hydraulic capacity of the WWTP is to apply aeration tank settling (ATS). In this operational mode, part of the aeration basins are used as extra settling tanks, reducing the sludge load on the actual secondary clarifier, hence reducing the risk of sludge wash-out (Nielsen *et al.*, 2000, 1996).

Carrette *et al.* (2001b) used the storm tank which is regularly present in WWTP in Flanders, as an extra secondary clarifier. In this way 6Q14 can be treated during storm conditions rather than the design capacity of 3Q14. The authors conclude that the pollution load to the receiving water is significantly reduced, while the operational costs do not increase.

Filling and emptying of storm tanks Several control strategies can be developed with storm tanks. The storm tanks are usually filled by inflows exceeding the threshold of admitted flow to the WWTP. A current practice is to fill the tank and subsequently use it as a sedimentation basin. Another possibility is to fill the tank first and, once the storm tank is full, bypass the flow to the receiving water body. Alternatively, the storm tank can be filled in the early stages of the rain event and the following flow can be addressed to biological treatment (Lessard and Beck, 1991). Stricker (2000) looked at the effect of the emptying rate of storm tanks on WWTPs with a very low F/M ratio. Provided that sufficient aeration capacity is available, the treatment plant could handle up to 7 DWF in flow rate.

Bauwens *et al.* (1996) tested the effect of a storm tank in fill-and-bypass mode on the efficiency of the combined sewer-WWTP system. The storm tank was filled when the

flow to the biological treatment exceeded 2.5 DWF and emptied when the flow fell below this value. It was found that especially the amount of suspended solids discharged could be reduced.

Aeration Maintenance of a set point for DO in the activated sludge tank is the common control objective of the aeration system. It is important to find a good balance between a sufficient concentration of DO, that is strictly necessary for removal of carbonaceous material and for the nitrification process, and excessive oxygen supply, which results in high operational costs. Details can be found in Olsson and Newell (1999).

Step feeding An interesting operational control is based on the step feed scheme. This strategy, that achieves an equalisation of the food to organisms ratio for the activated sludge, uses several inlet points to introduce the wastewater in the aeration tank. During wet weather the inlet point of the wastewater is placed near the middle or end of the tank, so that sludge may be stored at the head of the reactor. This measure reduces the suspended solids concentration in the feed to the secondary clarifier but also limits the nitrification process. Step feed control has been successfully used, e.g. by Lessard (1989) and Nyberg *et al.* (1996). Rouleau (1997) motivate the use of step feed control combined with the ratio control of the return activated sludge rate.

Return activated sludge rate (RAS) Return of activated sludge to the aeration tank is fundamental for a good operation of the activated sludge process. The maintenance of a constant mixed liquor suspended solids (MLSS) concentration represents a common method of solids control. In steady state it is possible to calculate, by means of a mass balance, the return activated sludge ratio necessary to maintain a constant MLSS concentration.

Another frequently applied method (Harremoës *et al.*, 1993) consists of relating the return activated sludge to the WWTP inflow rate by a constant factor. In this case, the sludge rate is increased with increasing flow (ratio control). However, as this disturbs the settling process, Olsson and Newell (1999) propose an alternative in making the RAS proportional with the incoming flow to the settler. This has as a consequence that the sludge load to the settler is increased.

Lessard (1989) proposed to increase the recycle rate to a predetermined value before or during the event and with this approach demonstrated an improvement of the WWTP effluent.

Waste activate sludge rate (WAS) The sludge removal rate is determined by this parameter. If a sludge age and a MLSS concentration have to be maintained constant, it is possible, in steady state, to calculate the wastage rate. By means of a mass balance, the wastage rate can be computed taking into account the MLSS concentration in the aeration tank and the MLSS concentration in the effluent and in the underflow. However, the total mass of sludge in the system is determined by the WAS. By increasing the WAS, the settling limitations may be overcome, but the biological performance may be affected at the same time.

Carbon dosage control in denitrification The denitrification rate depends on an adequate carbon concentration. If the C/N ratio of the wastewater doesn't allow complete denitrification, an external carbon source may be added to the anoxic tank. A typical control strategy for carbon dosage aims at a low nitrate level at the outlet of the anoxic tanks. However, the consequences are increased sludge production and an additional operational cost for the carbon source (Yuan *et al.*, 1996). This strategy was successfully applied on a full-scale WWTP by Devisscher *et al.* (2002).

Control of chemical dosing for phosphorus removal Chemicals may be used for the precipitation of phosphorus. The dosage rate of these chemicals could be controlled in order to obtain a sufficient but not an excessive dosage rate. These controllers need at least an estimate of the P-loading, and better an on-line phosphorus measurement (Devisscher *et al.*, 2002; Janssen *et al.*, 2000).

Polymer addition This may be used in emergency situations to avoid major settler failures. The polymers improve the formation and settleability of sludge flocs. It may be based on measurements of the sludge blanket level or the sludge settling rate (Vanderhasselt *et al.*, 1999).

Control strategies

The most usual control strategies designed for WWTP (Harremoës *et al.*, 1993; Vanrolleghem, 1995) are mentioned below.

Conventional feedback control In WWTP on-off controllers and/or PID feedback controllers are normally used. In the context of the time-varying, non-linear processes, optimal control performance cannot be expected from these controllers. However, the familiarity with concepts and properties of PID and on-off controllers has made their use very common.

Optimal feedback control Design techniques have been developed to devise the optimal controller for particular case studies. Marsili-Libelli (1989), for example, describes an optimal feedback controller design technique for linear systems or for linearised ones. The author applies this technique to design a PID controller using a linearised expression of the activated sludge kinetics. Weijers (2000) applied linear quadratic gaussian (LQG) control to a nitrogen removal plant, and found it to perform better than PI based control.

Model based predictive control (MBPC) Model based predictive control uses a model of the WWTP to determine a series of setpoints which are optimal for a given situation. Two parameters can be chosen: the control horizon and the prediction horizon (Fig. 2.16). The controller tries to minimise a predefined objective function by finding a series of setpoints for the controller output which vary during the control horizon and are constant after this

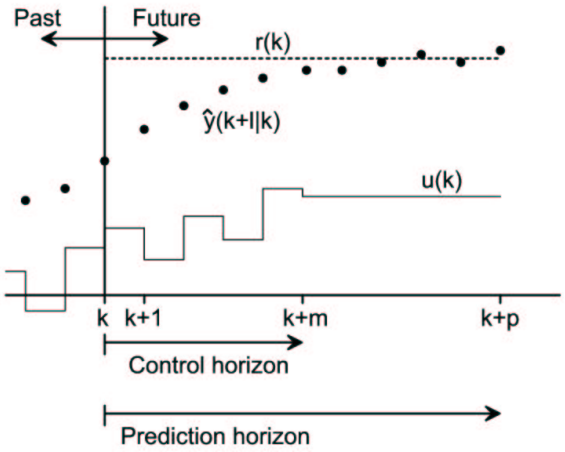


Figure 2.16: Prediction and control horizon in MBPC (Weijers, 2000)

point. The objective function has two terms: the sum of squares of the deviations between the setpoint (r) and the predicted value (y) and the sum of squares of the control actions. By choosing appropriate weights for these two terms, a balance can be found between operational costs and deviations from the setpoint. The first of the series of setpoints with the lowest value of the objective function is applied, while the optimisation procedure is re-iterated to allow the newly available data to be incorporated in the model. Weijers *et al.* (1995) applied linear MBPC to a predenitrification plant and concluded that the strategy has limitations due to model mismatch. In a second study with constraints on the controller output, the change of the controller output and the predicted states, the approach was found to be promising for a carousel type WWTP (Weijers *et al.*, 1997).

Feedforward compensation and ratio control In a feedforward control scheme the knowledge of upcoming disturbances is used to the benefit of a treatment plant's operation by preparing it to cope with for instance toxic loads, important hydraulic disturbances or increased organic loading (Vanrolleghem, 1995). Feedforward compensation is for example applied when the RAS of the WWTP is proportional to the incoming flow rate (ratio control). The goal of the control action is to maintain the sludge concentration in the aeration tank and therefore the biodegradation capacity nearly constant (Bauwens *et al.*, 1996).

MIMO control Multiple-input multiple-output (MIMO) allows the use of more than one input or output variable for the controller. Nielsen and Önnerth (1995) proved that MIMO control can improve the performance of a WWTP. In their work, both the carbon addition and the oxygen supply were used to control the effluent concentration of nitrate.

2.4.6 Real-time control of receiving waters

Even if in literature several papers regarding river control can be found (e.g. flood protection), they hardly ever take into account the river systems as recipients of urban discharges. According to Schütze *et al.* (2002a), the control options that can be applied to a receiving water are:

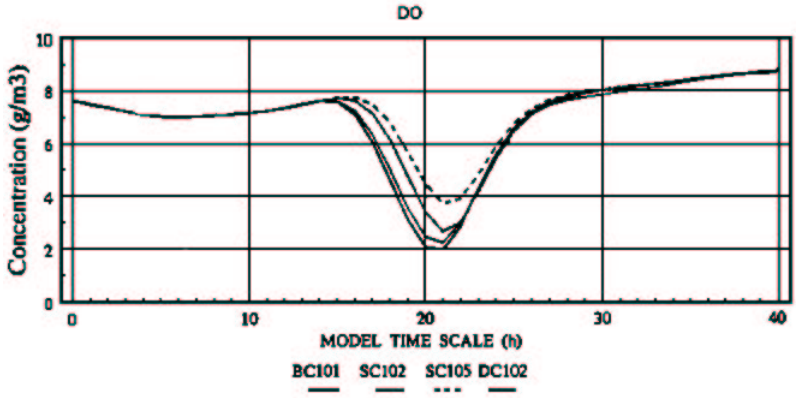


Figure 2.17: Effect of different control strategies on the DO in the river (Reda and Beck, 1999)

- Artificial aeration.
- Control of in-river flow (e.g. upstream of urban wastewater discharges).
- Control of discharge into the river from CSOs and WWTP.

On-line monitors for river water quality monitoring are available for variables as DO, pH, conductivity, temperature, oxidation-reduction potential, etc. However, these are not used for river water quality control (van Griensven *et al.*, 2000b).

Reda (1996) carried out an important study on river control. He analysed the impacts of urban effluents in the River Cam. Some gates, with a complex configuration, are present in the river in order to maintain a minimum value of the water depth. The maintenance of depth above minimum values may also be useful to promote short time pollutant dilution in the case of transient or accidental pollution events. Reda's analysis considered the gate operation with different river scenarios within two rainfall events. The author concluded that a careful operation of the gates leads to significant improvements in the water quality of the river. The water quality determinants considered were DO, BOD, ammonium-nitrogen, and both the total flux of a pollutant and its extreme concentration were taken into account. The authors concluded that the ranking of the stormwater control strategies depends on the criterion used. An illustration of the effect of different control strategies is shown in Fig. 2.17. For more details, see Reda and Beck (1999).

2.4.7 Integrated control of the urban wastewater system

RTC of wastewater systems has been a topic of research and application for over two decades (Schütze *et al.*, 2001). In the recent past, however, the three parts of the urban wastewater system (sewer system, WWTP and receiving water) have been considered as separate units in the water quality management and the aims of optimum performance were considered individually as well.

Rauch and Harremoës (1995), for example, noticed that, although the urban system is commonly recognised in literature to be composed of the three components, it was "still common practice to design and operate the components individually" as a "heritage from the historical development of municipal drainage systems". Bauwens *et al.* (1995) too

emphasised the importance of an integrated methodology for the impact assessment of the design and operation of the sewer - wastewater treatment plant system on the receiving water quality.

Similarly, Pfister *et al.* (1998) state that general engineering design practice does not take into account the interactions between combined sewer systems and wastewater treatment plant operation. According to the authors, the sewers are often designed first, using static estimates of water amount, whereas in the WWTPs, the pollution loads are generally determined in a static relation to the population equivalents. In contrast to this approach, the authors notice that on-line measurements of the inflows and the WWTP effluent can show that the treatment capacity of a plant is directly connected to the efficiency of a sewer system.

Schütze *et al.* (1999) observe that the "operational management practice of the urban wastewater system aims at optimum performance of its individual components", but that, on the other hand, "optimising the performance of each of these individual subsystems does not take into account interactions between them, nor does it ensure optimum performance of the entire system". As an example, the authors notice that conventional real-time control of sewer systems mainly aims at minimisation of overflow volumes and loads, while treatment plant operation traditionally is mainly concerned with maintaining effluent standards.

Most authors do now agree on the fact that RTC is a key aspect of successful management of the integrated urban wastewater system (Clifforde *et al.*, 1999).

The state-of-the-art of integrated control

Immission based RTC takes the resulting river water quality directly into account. For the development of such control strategies an integrated model with the three subsystems running simultaneously is essential. Indeed, with a simultaneous simulation, the current (and predicted) states of the river water can be used to determine the control actions in e.g. the sewer system. In sequential simulation on the contrary, this is not possible since the water quality is only calculated after the simulation of the other systems is completed. An integrated model can also be used when designing or upgrading a system, where it allows to quickly quantify the effect of different design options on the resulting water quality. Because of these advantages, a simultaneous simulation of the integrated urban wastewater system has been asked for since the last few years (Rauch *et al.*, 1998a; Schütze *et al.*, 1999).

One of the first significant examples of integrated control was carried out on the city of Aalborg, Denmark (Harremoës *et al.*, 1994). The authors tried to introduce RTC of the sewer system and of the WWTP, based on goals established from receiving water studies. Control actions were taken in both systems which were closely interconnected by exchanging information across the subsystem boundaries. In fact, the on-line information regarding the hydraulic capacity of the treatment plant was used as a variable in the control of the sewer system, and, on the other hand, the state variables of the sewer system were used to make predictions of the expected flow to the treatment plant.

Marsili-Libelli (1995) noticed that the operation of a wastewater treatment plant could be significantly improved if its management was coordinated with the water quality of the receiving water body. The author proposed to integrate a computer controlled wastewater treatment process into a "reach-wise flexible standard policy scheme", taking into account the water quality resulting from plant management and the upstream water quality. The control strategy can be summarised as follows: if the organic load raised without a corresponding flow increase, dilution of the incoming polluted water with treated effluent was done, otherwise, when both flow and organic load increased, sewer outflows were partially stored into a buffer tank. Bypass was used only when the capacity of the buffer tank was exceeded. The storage strategy consisted of two steps, filling and emptying the tank: part of the raw influent was stored in the buffer tank to be released later when the peak had passed. As the author noticed, one of the most interesting questions was the emptying policy once the peak load had passed. A quick emptying might create a secondary peak load that might violate the effluent quality standards. On the other hand, the need to empty the tank as soon as possible was to be taken into consideration in order to handle further overloads, as a fast emptying phase made the tank quickly available for absorbing new peaks. To reconcile these requirements a statistical analysis of peak repetition was set up in order to find a link between the BOD peak and the emptying flow.

Rauch and Harremoës (1995) outlined the main characteristics of integrated water quality management by means of deterministic models. In their study, through simulations of a simple synthetic integrated system, the authors achieved remarkable results supporting the importance of an integrated approach for water quality management. It is evident from their work, for example, that minimising CSOs does not always result in a minimum effect on the receiving body, as increasing the flow limitation in the overflow structure may lead to a substantial impact of the WWTP effluent to the recipient.

Later, Rauch and Harremoës (1999) proposed a novel approach to apply RTC to the IUWS by means of a "mixed simulation-optimisation procedure". In order to apply mathematical optimisation procedures, a vector of control parameters (such as pump rates, height of weirs, or threshold values for control actions) was used to parametrise the control of the urban wastewater system. The effects of the integrated control strategy on the overall system were quantified by an objective function to be optimised. In each time step this approach required not only the exogenous system input (e.g. rain intensity or pollutant concentrations), but also the set points of the regulators in the system. A control strategy was determined by the time sequence of the regulator set points. A non-linear model predictive control was applied. As the optimisation of the non-linear objective function was numerically problematic, the application of the most commonly used optimisation algorithms based on the gradient of the objective function was not suitable. Hence, the authors suggested the application of a genetic algorithm. The main features of such a procedure are that it does not require the calculation of derivatives of the function to be optimised and that it is, in general, a simple and robust search process (see Fig. 2.18 for the implementation scheme). Simulations of hypothetical problem sets proved the described technique to be effective in allocating all available system capacities to abatement of water pollution through RTC. Among the most interesting results, it was shown that the reduction of overflow volume was not directly linked to an increase of the oxygen concentration in the recipient.

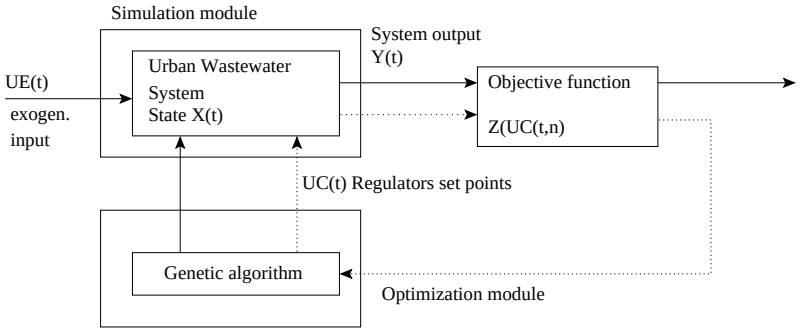


Figure 2.18: Function structure of the real-time control approach using genetic algorithms (Rauch and Harremoës, 1999)

Nielsen *et al.* (1996) used a control strategy in order to minimise the discharge effect on sensitive receiving waters during critical periods by means of on-line information. The control strategy was based on Aeration Tank Settling (ATS), which means introducing settling in the aeration tanks in order to temporarily increase the hydraulic capacity. On-line measurements in both the sewer system and WWTP were used to quantify the concentration dynamics at the control and discharge points. In this way, the control of the integrated system was optimised to retain the most polluted water proceeding from the combined sewer system in available volumes (to be discharged to the WWTP as soon as its capacity is available), and to directly discharge the less concentrated wastewater to the recipients. The authors concluded that a great potential exists for combining sensors and information technology in wastewater transport and treatment.

Mark *et al.* (1998) observed that in some operational situations a surplus capacity was available in the sewer system of Helsingborg. Consequently, RTC applications could be applied in order to utilise the storage capacity of the system with the aim of improving the WWTP performance. Hence, the authors proposed to link a deterministic model of the sewer system (MOUSE TRAP) to a model for the description of the WWTP (STOAT) so as to evaluate the performance of RTC in an integrated context. The aim of the project was to examine several control strategies in order to achieve optimum inflow conditions at the WWTP. Later, the study was extended with the MIKE software package for river water quality modelling, constituting the Integrated Catchment Simulator (ICS, see section 2.3.7) (Clifforde *et al.*, 1999; Taylor *et al.*, 2000). The modules which constitute ICS are compatible with one another and communication between them is possible allowing for transfer of data, both forward and backward, during simulations (feedforward and feedback control loops can be implemented). The practical feasibility and potential benefits of the development of global RTC strategies is currently being demonstrated on a series of large-scale pilot studies. The first results of these studies show that RTC strategies studied by using the ICS perform better than a “static” approach using the UPM methodology (Williams *et al.*, 2001).

One of the most important improvements in the field of integrated control is due to Schütze’s work (Schütze *et al.*, 1999, 2002a, 2001). After outlining the state-of-the-art in the field of RTC for IUWS, the authors systematically proposed definitions for integrated modelling. One of the main aims of the study was to demonstrate that a tool for the assessment of integrated control had been rendered available. For this reason, the authors

focused on the specific requirements that software should have in order to deal with integrated control. First of all, the simulation package should be able to simulate control actions and the related impacts with regard to the pollutants under consideration. As a second prerequisite, the simulation tool should allow for simultaneous simulation of the various submodels, as well as exchange information between them. Indeed, integrated control needs information to be exchanged across the boundaries of the subsystems. As a final remark, the authors noticed that the existing software packages hardly ever meet such requirements. The developed simulation tool SYNOPSIS has already been introduced in section 2.3.7. A control module and an optimisation module were included in the tool. Hence, the complete tool could be used for off-line optimisation of control strategies. The effects of the control strategy on the overall system were quantified by an objective function to be optimised in an off-line manner. Using rainfall data and the system description as input, the simulation software modelled the water flow and the quality processes of the IUWS. The simulation results (including the description of the impact of the RTC actions) were used to feed the optimisation module, which used them to generate a new set of control strategy parameters (several pump and flow rates in the sewer and WWTP) and triggered a new simulation run. The optimisation process ended either when a convergence criterion was fulfilled or when a maximum number of iterations was reached. The studied system is semi-hypothetical and was assembled from different existing models. The sewer system was previously defined by Härtel *et al.* (1995), the WWTP was the activated sludge plant in Norwich described by Lessard (1989), while the river was of purely hypothetical nature, but based on experience of Reda (1996). Various control scenarios were tested:

- a base case (only local control, using default values of parameters setting);
- an optimised variation of the latter case (the parameters of the control strategy were determined by optimisation, but were kept constant during the simulations);
- a simple hierarchical control (the set points of the local controllers are occasionally changed by a central control unit in order to deal with exceptional situations) using a rule base.

The results of the RTC applications were evaluated in terms of two criteria: the duration of oxygen concentration being below a certain threshold at any location in the river and the minimum DO concentration in the river during the simulated time period. According to the authors, a control strategy based on fixed (not optimised) set points produced better results than the “no control” case and further improvements were achieved for the simple hierarchical control scenario. The authors also noticed, however, that the DO-based criteria led to worse performance in terms of ammonia and stated that further studies should encompass both criteria in a carefully balanced way. Based on simulation results the authors concluded that “integrated control of the urban wastewater system can lead to its improved performance”. In a follow-up study, the authors concluded that many IUWS systems have potential for improvements by means of integrated RTC, even if the local or the global RTC strategies don’t (Schütze *et al.*, 2002b).

Recent attempts to implement RTC within the IUWS were made by Erbe and Risholt (2000), who utilised the tools PLASKI, SIMBA® sewer and SIMBA® for the simulation

of wastewater production, transport, and treatment (see Section 1.3.2). This MATLAB^{TM}/ SIMULINK based modelling system allows for simulations of RTC of the wastewater system (e.g. control the sewer system based on the operational state of the WWTP and vice versa). In fact, it was possible to implement control strategies using the SIMULINK toolboxes for neural networks and fuzzy logic as well as programming control strategies in C-code. Simulations illustrated the effect of RTC in improving the effluent water quality. It should be stressed that the latter example does not take into consideration the recipient water quality. Nevertheless, as the authors stated, "an integrated approach geared toward receiving water criteria must be included to reach sustainable management of the river basins".

2.5 Problem statement and aim of the thesis

In the previous paragraphs, a description was given of two main topics of the research performed in this PhD study. Modelling of the integrated urban wastewater system and RTC within this system. It was shown that mathematical models exist for each of the subsystems (sewer, treatment plant and receiving water). These models may be deterministic or conceptual and are able to describe the behaviour of the subsystems. More and more scientific arguments are put forward to state that it is necessary to consider the IUWS as one system, rather than separate systems, if the protection of the receiving water is to be achieved cost-effectively (Lijklema *et al.*, 1993; Rauch *et al.*, 1998a; Schilling *et al.*, 1997). The recently adopted Water Framework Directive emphasises on the fact that the system should be regarded in an integrated way on basin scale and that the good ecological and chemical status of the receiving water is the final goal.

It is clear that an integrated modelling approach is very useful in this sense: it allows for calculations of all the discharges into the receiving water (CSOs, WWTP effluents, storm water outfalls), since it is not possible (or very expensive) to directly monitor them. Integrated modelling allows to judge the effect of several management options before taking a decision. Moreover, an integrated model may also be used for the design of integrated RTC strategies, which are a promising approach when trying to meet water quality standards (Rauch and Harremoës, 1999).

Several problems need to be overcome when developing an integrated model for design and tuning of integrated RTC strategies. First, a simultaneous simulation of the complete system is necessary in order to allow upstream flow of information. Second, the state variables used in the different subsystems need to be compatible in order to have a consistent model (e.g. closed mass balances). And third, a fast simulation is required in iterative procedures like tuning of control strategies.

The specific aim of this thesis is therefore two-fold. In the first part, the three problems in integrated modelling are tackled. A procedure to reduce the calculation time of the integrated model is developed. This approach is based on both model simplification and model reduction. The model simplification focuses on the fact that in both sewer and river hydraulic modelling, the "de Saint-Venant" equations can be replaced by CSTRs in series. Moreover, an (unsuccessful) approach to replace the ASM models by neural networks is

outlined, and complemented by knowledge based model reduction. Model reduction for sewers and rivers focuses on the fact that in some cases, parts of the system need not to be modelled but can be replaced by boundary conditions. This is especially useful in the case of integrated RTC strategy design.

In the second part of the thesis, an immission based integrated control strategy is developed on a semi-hypothetical case study based on the Tielt (Belgium) situation. The immission based control strategy uses measurements of the river water quality to adapt setpoints in the sewer system and the treatment plant. The difficulties during the development and the performance of the control strategy are discussed.

Chapter 3

WEST: Modelling the integrated urban wastewater system[1]

3.1 Modelling the IUWS: benefits and practical use

The problem of modelling and simulation of the IUWS system has been found important as a result of growing environmental awareness. Compared to the modelling of well-defined (such as electrical and mechanical) systems, modelling of ill-defined systems such as WWTPs is more complex. In particular, choosing the "right" model is a difficult task.

Modelling is an inherent part of the design of sewer systems and wastewater treatment systems. At the fundamental level, a design model may be merely conceptual. The engineer reduces the complex system he is dealing with to a conceptual image of how it functions. That image then determines the design approach. Often, however, the engineer recognises that the conceptual model alone does not provide sufficient information for design and thus he constructs a physical model, such as a lab-scale reactor or a pilot plant, on which various design ideas can be tested. Given sufficient time for testing, such an approach is entirely satisfactory.

However, the engineer may find that limitations of time and money prevent exploration of all potentially feasible solutions. Consequently, he often turns to the use of mathematical models to further explore the feasible design space. He may devise empirical models, which incorporate a statistical approach to mimic the end results obtained by studies on the physical model or if his conceptual understanding expands sufficiently, he may attempt to formulate models based on mechanistic knowledge. These mechanistic models are the more powerful because they allow extrapolation of the design space to conditions beyond that experienced on the physical model. In this way, many potentially feasible solutions may be evaluated quickly and inexpensively, allowing only the most promising ones to be selected for actual testing in the physical model.

[1] Important parts of this chapter were published as: Vanhooren H., Meirlaen J., Amerlinck Y., Claeys F., Vangheluwe H. and Vanrolleghem P.A. (2002). WEST: Modelling biological wastewater treatment. *J. Hydroinformatics (Accepted)*.

To be able to use mathematical – be it empirical or mechanistic – models, a good software tool to implement and simulate the models is indispensable. Several tools are available that can be applied to the modelling and simulation of (parts of) the IUWS. Earlier software tools focused on modelling one part of the system, while currently, more and more tools become available that allow to model the IUWS completely.

The complex nature of the subsystems of the IUWS, makes mathematical modelling a challenging task. For example, wastewater treatment practice, has now progressed to the point where the removal of organic matter and nutrient removal by biological nitrification and denitrification and biological phosphorus removal, can be accomplished in a single system. The non-linear dynamics and properties of these biological processes are still not very well understood. As a consequence, a unique model cannot always be identified. This contrasts to traditional mechanical and electrical systems where the model can be uniquely derived from physical laws. Also, the calibration of the biological IUWS models is particularly hard: many expensive experiments and measurement campaigns may be required to accurately determine model parameters. Yet, even with the limitations and difficulties stated above, modelling and simulation of the IUWS is considered useful (Schütze *et al.*, 2002a). Models are excellent tools to summarise and increase the understanding of complex interactions in biological systems. More quantitatively, they can be used to predict the dynamic response of the system to various disturbances.

Despite the promising properties described above, the practical use of dynamic modelling of IUWSs is rather limited (Morgenroth *et al.*, 2000). In particular, the labour and cost intensive calibration of IUWS models is considered hard to accomplish in practical situations. New methodologies are being developed to overcome this bottleneck (Petersen *et al.*, 2001b).

Mathematical models can be used in planning and operation. Models could be used to predict dynamic responses of the system to input variations so as to develop strategies to optimise operation. This can be done either off-line or with on-line real-time simulations that are used for control and optimisation. Another possible use of models is to trouble shoot operation. Operators might be interested to use models in finding answers to practical questions. Modelling can also be used to integrate multiple processes. As mentioned above, the removal of organic matter, nitrogen and phosphorus, is accomplished in a single system nowadays. Models are promising tools to help create more understanding of the interactions between these processes. As a last point, modelling and simulation can be helpful in designing IUWSs. For instance, models can be used to evaluate data from pilot-scale reactors and to predict performance of full-scale plants.

In the first part of this chapter, the simulation software WEST will be explained. As this simulator was originally designed to model and simulate WWTPs, most of the examples given refer to this part of the IUWS. In a second part, the model base that is available for WWTPs will be extended with models for both sewer and river systems.

3.2 The WEST modelling and simulation software

Several modelling/simulation packages that can be used to describe wastewater treatment are available. Typically, four types of simulators can be distinguished. First of all, it is

possible to manually implement code in a programming language like Fortran or C++. Secondly, general-purpose simulators like Matlab/Simulink or ACSL are available. In the third place, closed dedicated simulators like Biowin, EFOR and STOAT have been developed, which are specifically designed for modelling WWTPs and in which only predefined mathematical models can be used. Finally, open dedicated simulators like GPS-X, Simba and WEST are also specifically designed for modelling WWTPs, but the user can write and use his own specific models if the models available do not fulfil his needs. For a comparison of the different WWTP simulators the reader is referred to (Copp, 2002).

The modelling and simulation package WEST (Wastewater Treatment Plant Engine for Simulation and Training) provides the modeller with a user-friendly platform to use existing models or to implement and test new models. WEST is a modelling and simulation environment for any kind of process that can be described as a structured collection of Differential and Algebraic Equations (DAEs). Currently, however, WEST is mainly applied to the modelling and simulation of wastewater treatment plants (Vangheluwe *et al.*, 1998). A dedicated modelling/simulation package such as WEST is preferred over the general purpose ones, since a general purpose modelling/simulation package typically gives too much possibilities in general. On the other hand, some specific problems are not handled thoroughly enough.

The aims of modelling and simulation of wastewater treatment are in a sense contradictory. On the modelling side, WEST is especially aimed at facilitating and optimising the implementation and reuse of knowledge in wastewater treatment models. This does, however, not necessarily result in the most efficient declaration of knowledge from a simulation point of view. Indeed, a simulator should maximise the simulation speed and accuracy of the simulations. Hence, the WEST modelling and simulation environment makes a strict distinction between a *modelling environment*, which aims to enable reuse of model knowledge and the *experimentation environment*, which aims at maximising accuracy and performance.

Next to these two user environments, the *model base* plays a central role in WEST. In this model base, models are described in MSL-USER (MSL stands for *model specification language*), 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. All reusable knowledge – such as mass balances, physical units, default parameter values and applicable ranges – is thus defined centrally and can be reused by an expert user to build new models. This indicates that WEST has an open structure in that the user is allowed to change existing models and define new ones as needed.

As depicted in Fig. 3.1, the model base is loaded and all relevant information for the modeller is extracted from it when the modelling environment is started (step 1). Using the symbolic information in the model base, the 'atomic' models available in the model base are linked to a graphical representation. A hierarchical graphical editor (*HGE*) allows for the interactive composition of complex configurations from these basic graphical building blocks. Also the input-output structures (*terminals*) of the models are extracted from the model base so as to decide whether or not two models can be linked together in the HGE.

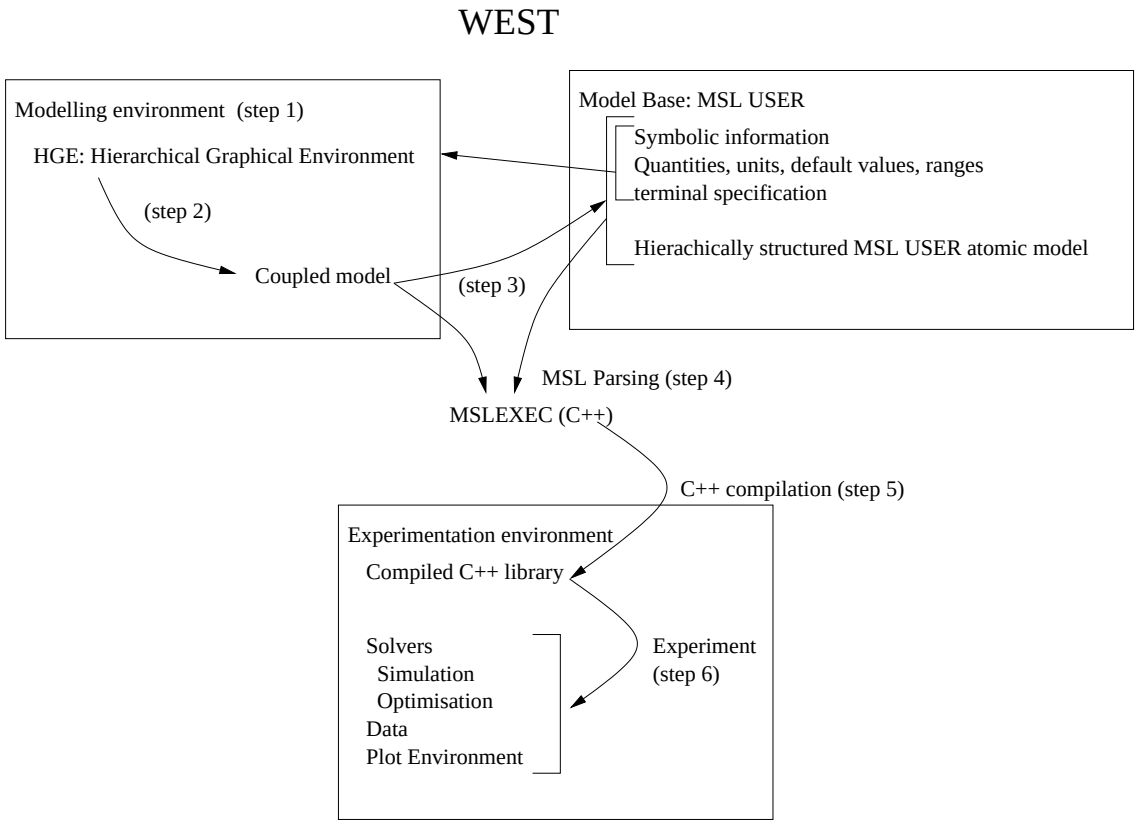


Figure 3.1: Functional WEST architecture

For instance, a model for the activated sludge process cannot directly be linked to a river model, since the set of components used in these models to describe the substrates is not the same. In case this type of coupling needs to be done, an explicit component convertor needs to be used. Next, the parameter set of the different models is loaded so that parameters of different models can be linked. For instance, the same yield coefficient can be used for all activated sludge tanks in a WWTP configuration. Finally, when a configuration has been built, the HGE starts from the information extracted from the model base and creates and outputs a *coupled model* in MSL-USER (step 2), which is automatically added to the model base for further use in new model exercises (step 3).

In a next step (step 4), the model parser generates low-level (C++) MSL-EXEC code, which after C++ compilation (step 5) can be used for execution within the experimentation environment. The parser therefore uses the coupled model together with the atomic model representations in the model base. These steps are especially oriented towards simulation performance and accuracy. Finally, the solvers within the experimentation environment generate data, which can be used for plotting, model calibration, process optimisation, output to file, etc. (step 6).

3.3 The model specification language MSL-USER

The language MSL-USER that is used in the WEST model base, is an object-oriented language, which allows for the declarative representation of the dynamics of systems.

'Declarative' means that the model (*what*) is presented without specifying *how* to solve it. As mentioned above, a compiler (MSL-parser) is provided to transform MSL-USER model representations into a low level representation (MSL-EXEC based on C++).

The MSL-USER parser is written in lex (flex), yacc (bison) and C++ and makes use of LEDA (Library of Efficient Data structures and Algorithms). MSL-USER follows the major principles of object-oriented programming in that it uses TYPES, CLASSES and OBJECTS to represent the hierarchy of the items in the model base. The relation between these representations can be visualised like a tree. Types provide a way to describe the structure of an expression in the sense that it is a template to which classes and objects add more information. Indeed, a class is derived from a type definition, further defining the properties of the template. That way, classes provide a way to describe the behaviour of values. For example, a class in MSL-USER is mostly a type to which default values have been assigned. It is clear that one type can have multiple classes derived from it. A class is a template itself for the derivation of objects that give final values to the structures defined. An object, however, cannot only be derived from a class, but also directly from a type.

Apart from being object-oriented, MSL-USER is also a multi-abstraction language. It allows one to represent abstract models of the behaviour of systems using different methods of abstraction. This includes the possibility to make use of "abstractions" such as differential and algebraic equations, state transition functions, C++ code, ... (Vangheluwe, 2000).

Other characteristics of MSL-USER are:

- Reuse of models is possible thanks to the EXTENDS inheritance mechanism. This allows for the extension of an existing model. Thus, starting from generic models, a tree of extended models can be built.
- Classification is made possible through the SPECIALISES mechanism. Hereby, it is possible to indicate that a particular type is a sub-type of another type. This not only allows for classification, but also for rigorous type-checking.

Some examples will surely clarify the explanation above. The basic types found in MSL-USER are integer, real, string, char and boolean. Based on these basic types, a number of extended type structures were built. Some type structures are the Record type, the Vector type, the Enumerated type, ... For example a vector type is used to specify vectors and matrices. A matrix can be specified as a vector of vectors. A column vector is declared as follows:

```
TYPE type_name = type[dimension;];
```

An enumerated type is a type structure consisting of a set of unique identifiers called enumerators, and is declared as:

```
TYPE type_name = ENUM {id_1, id_2, ..., id_n};
```

These basic types and structure types can now be used to create user-defined types, such as UnitType, QuantityType and RealIntervalType. The first two are defined as strings while RealIntervalType is defined as a record of two real values and two booleans, describing if the bounds are included in the interval.

```
TYPE UnitType
   "The type of physical units"
   = String;
TYPE QuantityType
   "The different physical quantities"
   = String;
TYPE RealIntervalType
   "Real Interval"
   = RECORD
   {
      lowerBound: Real;
      upperBound: Real;
      lowerIncluded: Boolean;
      upperIncluded: Boolean;
   };
```

Furthermore, existing types can be extended. For example, the Record type can be extended with extra fields. In the following example, the ExtendedType is a type extended from BasicType.

```
TYPE BasicType "Basic type"
   =
   RECORD
   {
      value: Real;
   };
TYPE ExtendedType "Extended type"
   EXTENDS BasicType WITH
   RECORD
   {
      unit: UnitType;
      quantity: QuantityType;
      interval: RealIntervalType;
   };
CLASS Concentration "A class for concentration" SPECIALISES
   ExtendedType :=
   {:
      quantity <- "Concentration";
      unit <- "g/m\ 3";
      interval <- {: lowerBound <- 0; upperBound <- PLUS_INF :}
   :};
```

The mechanism of specialisation is somewhat different. A class that is specialised from another class or type has the same signature, but the objects in the class are assigned (replaced). For example:

A class such as Concentration, can further be instantiated as an object, where a value is assigned to one of the elements of the vector:

```
OBJ S_O_Sat "Oxygen saturation concentration"
: Concentration := {:value <- 8:};
```

MSL-USER thus allows one to express *physical* knowledge such as units (m, kg, ...), quantity type (Mass, Length, ...), boundary conditions, ... The semantics of these are known by the parser which will check model consistency and, where appropriate, apply this knowledge in the translation to MSL-EXEC. Also some other object attributes are interesting to note here. When the value of a parameter or the initial condition of a variable depends on the value of other parameters, it is possible to declare this parameter or variable as *fixed*. In this case, the user cannot change its value in the experimentation environment. When, in an MSL-USER model, a parameter or variable object has the annotation *hidden* this object is not shown in the experimentation environment.

During the translation from MSL-USER to MSL-EXEC, the different abstractions used in the models created by the user will be translated into C++ representations. Algebraic equations and Differential equations (using the DERIV statement) will be recognised directly by the parser, since they are available in the MSL-USER library. Other built-in statements in MSL-USER are for example FOREACH, SUMOVER and IF-THEN-ELSE structures. Moreover, during the subsequent compilation of the generated MSL-EXEC code, some standard C libraries are automatically linked to the generated model. This way, functions that are not built-in in MSL and that are not defined in the MSL-USER function libraries can be used as long as they are available in these standard libraries. It is even possible to use user defined C++ functions.

3.3.1 Building the model base

To allow for computer-aided model building and subsequent simulation/experimentation, a *model base* must be constructed. The models in this model base will be used for modular construction (i.e. by connecting component blocks as described above) of complex models describing the behaviour of sewers, WWTPs or river systems. The steps listed below form a general method for constructing a model base for any application domain:

- Choose an appropriate level of abstraction.
- Identify relevant quantities.
- Identify input-output structures.
- Build a model class hierarchy starting from general (conservation and constraint) laws and refining these for specific cases.

In the following paragraphs, these steps will be discussed in more detail.

3.3.2 Level of abstraction

As is commonly the case, we will choose an appropriate level of abstraction, upon which Idealised Physical Models will be built. Idealised Physical Models (Broenink, 1990) represent behaviour at a certain level of abstraction. This often means using lumped parameter models (ordinary differential equations (ODEs)), even though the physical system has a spatial distribution (which would require partial differential equation (PDE) modelling), when the homogeneity assumption is a reasonable approximation.

3.3.3 Relevant quantities

Secondly, the quantities of interest must be identified. These quantities can be subsequently used to describe the *types* of entities used in modelling: constants, parameters, interface variables and state variables.

In MSL-USER, the type of physical quantities is encoded as a PhysicalQuantityType, a structure as given below:

```
TYPE PhysicalQuantityType
   "The type of any physical quantity"
   =
   RECORD
   {
      quantity : QuantityType;
      unit : UnitType;
      interval : RealIntervalType;
      value : Real;
      causality : CausalityType;
   };
```

For numerical computation purposes it is sufficient to specify whether an entity is of real, integer, boolean or string type. When modelling a particular application domain, however, more expert information is available, and it would be very helpful to the modeller if it could be stored (represented) in the model base. For example, information can be available about upper and lower bounds of variables and parameters (e.g. stating that concentration, through the definition of its interval, is always positive). Also information about the causality of a quantity (input or output) can be included, since this information is of importance when developing a-causal models. As can be seen in the PhysicalQuantityType structure, this information can easily be integrated in MSL-USER. Once represented in a model, the model parser can make use of it to determine the legitimacy of the model (e.g. checking if the dimensions of parameters that are coupled match) and to generate efficient code (e.g. by means of constraint propagation based on lower and upper bound information). The constraints integrated in MSL-USER are transferred to the symbolic part of the MSL-EXEC representation and is used to protect the user for constraint violations during simulation or user input.

Basic quantities

Using the methodology introduced earlier, the PhysicalQuantityType structure can be specialised as classes for specific quantities. Here, alike the class ‘Concentration’, the physical quantity ‘Area’ is defined:

```
CLASS Area
   "A class for area"
   SPECIALISES PhysicalQuantityType :=
   {:
      quantity <- "Area";
```

```
      unit <- "m2";
      interval <- {: lowerBound <- 0; upperBound <- PLUS_INF:};
   :};
```

Definitions of physical quantity types are used to instantiate objects of those types. The ISO 1000 standard also defines physical constants such as the universal gravity constant whose MSL-USER description is given as an object declaration below:

```
OBJ UniversalGravityConstant
   "Universal gravity constant" : PhysicalQuantityType :=
   {:
      quantity <- "G";
      unit <- "m3/(g*s2)";
      value <- 6.67259E-11;
   :};
```

It should be noted here that in the WEST environment, the units are not only used for dimensional checking during model compilation, but are also passed on to the experimentation environment where the user is presented with variable names, descriptions, values as well as their units. This way, a variable or parameter description, a default value and an interval that have been defined by the expert developing the model, are available for the user. In this way, the user is protected against erroneous parameter values and is warned when a variable evolves out of its boundaries during a simulation run.

Quantities typical for biological processes in the IUWS

Simulation of biological processes in the IUWS, incorporating phenomena such as carbon oxidation, nitrification, denitrification and phosphorus removal, must necessarily account for a large number of reactions between a large number of components (Henze *et al.*, 2000; Reichert *et al.*, 2001b). Several Activated Sludge Models (ASM 1, 2, 2d and 3) have been developed by the task group on mathematical modelling of the International Water Association (IWA), while recently the River Water Quality Models No. 1 was published. As will be described in the sequel, each of the variables in these models, denoting a component of the wastewater, indexes a column in the model stoichiometry matrix. In MSL-USER, the components of e.g. ASM1 are easily described as an enumerated type:

```
TYPE Components = ENUM {H_2O, S_S, S_O, S_NO, S_ND, S_NH, S_ALK,
                        X_I, X_S, X_BH, X_BA, X_P, X_ND};
```

Thus, the modeller refers to the components by their name, while, where necessary, the corresponding integer index is used. Though WEST's simulator uses the numerical values of the Components indexes to address matrix elements, the experimentation environment presents the symbolic name of the index to the user. This reverse mapping is performed by the model compiler when generating MSL-EXEC code. Note how H_2O is explicitly modelled as a component.

Other quantities typical for IUWS modelling are stoichiometric and kinetic parameters. Kinetic parameters characterise the rate of reaction of the conversions in the model (e.g. maximal specific growth rate, decay rate, ...); stoichiometric parameters indicate the

stoichiometric relations between the different components in the model (e.g. yield coefficient, ...). In MSL, these parameters can easily be declared as objects of a certain, more general, class specification:

```
CLASS Yield
    "A class for Yield"
    SPECIALISES PhysicalQuantityType :=
    {:
      quantity <- "Yield";
      unit <- "-";
      interval <- {: lowerBound <- 0; upperBound <- 1:};
    :};

   CLASS GrowthRate
    "GrowthRate"
    SPECIALISES PhysicalQuantityType :=
    {:
      quantity <- "GrowthRate";
      unit <- "1/d";
      interval <- {: lowerBound <- 0; upperBound <- 20:};
    :};

   CLASS SaturationCoefficient
    "Saturation coefficient"
    SPECIALISES PhysicalQuantityType :=
    {:
      quantity <- "K";
      unit <- "-";
      interval <- {: lowerBound <- 0; upperBound <- 100:};
    :};

   OBJ Y      "Yield For Heterotrophic Biomass"
      : Yield := {:value <- 0.67:};
   OBJ mu     "Maximum Specific Growth Rate For Heterotrophic Biomass"
      : GrowthRate := {:value <- 4.00:};
   OBJ K_S      "Half-velocity Constant For Heterotrophic Biomass"
      : SaturationCoefficient :={:value <- 20.00:};
```

Transferred input-output quantities: terminals

The ultimate goal is to build complex models by connecting more primitive sub-models or blocks, possibly built up of coupled models themselves. In the case of WWTP models, the sub-model types mostly correspond in a 1-to-1 relationship to physical entities such as aeration tanks, clarifiers, pumps, splitters and mixing tanks. This ensures *structural validity* of the assembled models. Note how the building blocks need not match physical objects directly but may rather correspond to abstract concepts such as processes.

To connect sub-models, these sub-models require connection *ports* or *terminals*. This implies that interaction between the sub-models is assumed to *only* occur through the con-

nections made between their terminals. When parsing a coupled model, the connections are replaced by appropriate algebraic equalities.

In WWTP models, different terminal types are used. DataTerminals represent information to be used in sensor and controller blocks. However, the main terminal type is the WWTPTerminal. In the basic model base discussed here, only flux of biochemical material is considered. Heat flow for example is not considered. This is one of the modelling assumptions mentioned in the discussion of the ASM1 model and is obvious from the WWTPTerminal definition.

The WWTPTerminal is a vector of mass fluxes for each of the components taken into consideration in the model. The size of the vector is given by the number of identifiers (the cardinality) in the enumerated type 'Components' and hence depends entirely on how many components the user includes in this type. Note how the actual Component declaration may be given after all other declarations. MSL-USER interprets the equations and declarations in a model as a set rather than as a sequence of statements. Basically, this means the order in which the declarations or equations are included in the model base is of no importance. This evidently facilitates model base development and may enhance clarity.

While the model compiler will check whether (type-)compatible terminals are connected and how many connections are allowed to/from a terminal, the graphical modelling environment will already perform a check during interactive modelling. Normally the same terminals for biochemical transport are used everywhere in a configuration. If other terminals need to be used (e.g. for modelling a river system), explicit conversion blocks converting the elements of the different component vectors need to be foreseen. Direct coupling of a river compartment model, using another set of components, to a wastewater treatment model is not possible.

3.3.4 Building a model class hierarchy starting from general laws

Introduction to the general mass conservation law

The choice to transfer mass fluxes via the terminals instead of the mostly used concentrations and flow rates has different reasons. In processes where next to water or a water suspension also gasses and carrier materials may be transferred from one unit to another, only the concentration in the water phase is measured in reality. Denoting the concentration in units of $M.L^{-3}$, the factor L^{-3} indicates only the water or the suspension and not the entire transferred volume (including gas and carrier material). This can easily be the source of errors during the model development. Also the easy formulation of mass conservation when masses rather than concentrations are used is an advantage of this choice. The mass conservation law can easily be formulated as dM/dt. This conservation can be calculated for the different components i of the WWTPTerminal, so that elemental balances for carbon and nitrogen are easily derived. The user should however still have the possibility to interact with the model through output variables like concentration and flow rather than mass fluxes. For example, a mass balance of an ideally stirred tank reactor

(CSTR) with volume $V(\mathrm{L}^3)$, components i, and terminals α, can be written as:

$$C_i = \frac{M_i}{V} \tag{3.1}$$

$$\frac{dM_i}{dt} = \sum_{\alpha} \Phi_{i_\alpha} + r_i V \tag{3.2}$$

$$\frac{dV}{dt} = \sum_{i} \left(\frac{1}{\rho_i} \sum_{\alpha} \Phi_{i_\alpha} \right) \tag{3.3}$$

In the case of an aeration tank with components dissolved at a low concentration in the water phase, the following simplifying assumption can be made:

$$\forall i \neq H_2O : \rho_i = \infty \tag{3.4}$$

stating that it is assumed that only water occupies a finite space. If the density of the suspensions is different from 1 kg/l or 10^6 g/m^3 (= ρ_{H2O}), this assumption will no longer suffice. In that case the density of the individual components needs to be known. The reaction term R_i, can be calculated by using the Petersen matrix, as explained in section 2.3.4.

In case heat transport should be modelled, the same assumptions will be used, i.e. heat flux will be transferred at the terminals.

Inheritance hierarchy

Using the general mass conservation law introduced above, models must be constructed for each type of building block. This is achieved in the form of a class *inheritance* hierarchy. Hereby, maximum *reuse* and *clarity* is achieved. Clarity is a direct result of the relationship between the inheritance hierarchy on the one hand and the different levels of specificity of the models on the other hand. In the generic model base, GenericModelType is defined:

```
TYPE GenericModelType
 =
 RECORD
 {
  comments   : String;
  interface  : SET_OF (InterfaceDeclarationType);
  parameters : SET_OF (ParameterDeclarationType);
 };
```

It shows how any model has a description (*comments*) part, an *interface* set and a *parameter* set. The interface set describes which terminals serve as an input to the model and which variables are transferred to a subsequent model via an output terminal. The parameters of the model are a set of invariant values that are given a value at the beginning of a simulation.

For basic models in the DAE formalism, PhysicalDAEModelType prescribes the structure:

```
TYPE PhysicalDAEModelType
 EXTENDS GenericModelType WITH
 RECORD
 {
  independent : SET_OF (ObjectDeclarationType);
  state       : SET_OF (PhysicalQuantityType);
  initial     : SET_OF (EquationType);
  equations   : SET_OF (EquationType);
  terminal    : SET_OF (EquationType);
 };
```

Time is mostly used as the *independent* variable. In the case of PDE modelling, multiple independent variables can be defined. Dependent (both algebraic and derived) *state* variables are defined in the *state* section. The *initial* section contains algebraic equations that will be solved only once during simulation. The result of these initial calculations can for example be used to define the initial values of derived state variables used in the *equations* section. This section contains the algebraic equations and ODEs that define the model. Equations in the *terminal* section are only calculated once at the end of the simulation run. The GenericModelType can also be extended to describe the essence of coupled models:

```
TYPE CoupledModelType
 EXTENDS GenericModelType WITH
 RECORD
 {
  sub_models : SET_OF (ModelDeclarationType);
  coupling   : SET_OF (CouplingStatementType);
 };
```

In a *coupled model*, the *sub_models* section enumerates the set of models to be coupled. In the *coupling* section, statements are included that describe how to couple these models. This can be done using two statements. The *connect* statement is used to connect the interface variables of the coupled model to the interface of one of the sub-models or to connect the interfaces of two sub-models. The *control* statement is used to indicate that a parameter of a sub-model is controlled by an interface variable of a second model. It is important to note that the MSL-USER parser will then automatically transform the controlled parameter into a new interface variable, since this model component will no longer be time-invariant and therefore, by definition, becomes a variable.

Both CoupledModelType and DAEModelType are extensions of the GenericModelType which means they inherit its structure (and add to it). The resulting top-level inheritance hierarchy is given in Fig. 3.2. In the WWTP model base hierarchy, some of the model classes are derived directly from PhysicalDAEModelType (Fig. 3.3). The ones listed directly below are models of the settler. The Takács model, for instance, is a discretised (10-layer) model of the settling process. It should be noted that the dedicated WEST-PDE parser is able to automatically discretise a class of PDE models of, for instance,

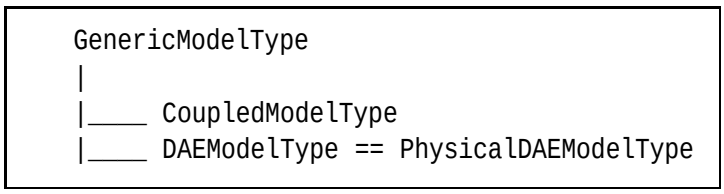


Figure 3.2: Top level inheritance hierarchy in the WEST model base

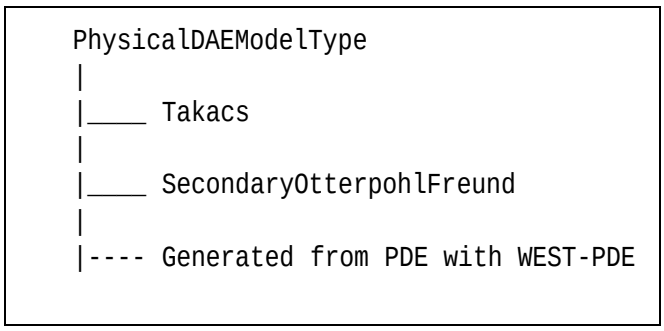


Figure 3.3: Settler models directly derived from PhysicalDAEModelType

the settling process using orthogonal collocation (Indrani and Vangheluwe, 1998). Once discretised, these models are of the ordinary PhysicalDAEModelType and fit in the hierarchy of Fig. 3.3. Sensor, controller, data filter and transformer models are also derived from PhysicalDAEModelType (Fig. 3.4). These models do not describe physical processes involving (transport of) matter and energy and hence do not adhere to physical laws. Though not subject to physical constraints, they do deal with the values of physical variables.

The shallowness of the above inheritance hierarchy reflects the diverse nature of this subset of model types used in wastewater engineering, not allowing for much reuse.

Now we will look into the development of WWTPAtomicModel, derived using the mass conservation law, from which many other model types are derived. This will illustrate the powerful reuse capabilities of the developed system. First of all, note that the matrix of the simple example (see Table 2.5 on page 25) could be implemented in MSL-USER in

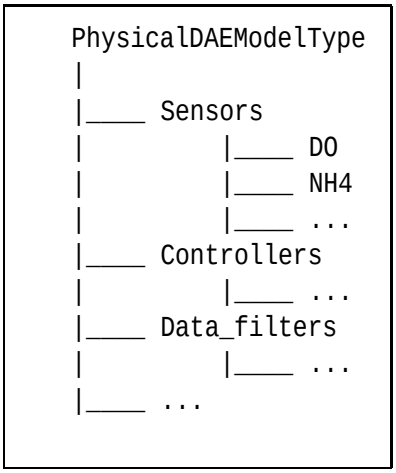


Figure 3.4: Models not describing physical processes directly derived from PhysicalDAEModelType

the following easy way:

```
TYPE Components = ENUM {H_2O, S_S, S_O, X_B};

 TYPE Reactions = ENUM {Growth, Decay};

 parameters <-
   {
    OBJ Y    "Yield"  : Yield := {:value <- 0.67:};
    OBJ mu   "Maximum Specific Growth Rate" : GrowthRate
             := {:value <- 4.00:};
    OBJ K_S  "SaturationCoeff" : SaturationCoefficient :={:value <- 20.00:};
    OBJ b    "Decay Rate" : DecayRate := {:value <- 0.40:};
   };

 initial <-
   {
    parameters.Stoichiometry[Growth][X_B] := 1;
    parameters.Stoichiometry[Growth][S_S] := - 1/(parameters.Y);
    parameters.Stoichiometry[Growth][S_O] :=
       - (1 - parameters.Y)/parameters.Y;
    parameters.Stoichiometry[Decay][X_BH] := - 1;
    parameters.Stoichiometry[Decay][S_O]  := - 1;
   };

 equations <-
   {
    state.Kinetics[Growth] := parameters.mu *
        (state.C[S_S]/(parameters.K_S+state.C[S_S])) * state.C[X_B];
    state.Kinetics[DecayOfHetero] := parameters.b*state.C[X_B];
   };
```

The basic mass balance (equation 3.2) for each of the components can also be rewritten in MSL format. First, the flux for each component i is calculated as $\sum_{\alpha} \Phi_{i_\alpha}$, where the outfluxes are by default negative values.

```
{FOREACH Comp_Index IN {1 .. NrOfComponents}:
  state.FluxPerComponent[Comp_Index] =
     (SUMOVER In_Terminal IN {SelectByType(interface,InWWTPTerminal)}:
      In_Terminal[Comp_Index])+
     (SUMOVER Out_Terminal IN {SelectByType(interface,OutWWTPTerminal)}:
      Out_Terminal[Comp_Index]);};
```

Next, the reaction (conversion) $r_i V = V \cdot \sum_j \nu_{ij} \rho_j$ is encoded in a straightforward manner as:

```
{FOREACH Comp_Index IN {1 .. NrOfComponents}:
    state.ConversionTermPerComponent[Comp_Index] =
     SUMOVER Reaction_Index IN {1 .. NrOfReactions}:
```

```
      (parameters.Stoichiometry[Reaction_Index][Comp_Index]
      *state.Kinetics[Reaction_Index])
      *state.V;};
```

Finally, the complete mass balance $\frac{dM_i}{dt} = \sum_{\alpha} \Phi_{i_\alpha} + R_i V$ is written for each component:

```
{FOREACH Comp_Index IN {1 .. NrOfComponents}:
   DERIV(state.M[Comp_Index],[independent.t]) =
    state.FluxPerComponent[Comp_Index]
    + state.ConversionTermPerComponent[Comp_Index];};
```

The rate of change of a component's mass thus consists of the net result of incoming and outgoing mass flux augmented with a reaction term due to biochemical interactions between different components. The MSL-USER compiler will expand the above few lines into the appropriate equations based on the matrix given. These equations will subsequently be manipulated to generate correct and efficient simulation code. Note that components which are transported but do not react (*i.e.* only hydraulics, no physico-chemical nor biological processes) have a column of zeroes in the stoichiometry matrix. In MSL-USER, by default, when a variable or a parameter is not given a value, the initial value is 0. Thus, if assignments to elements of the stoichiometry matrix are not made, it is a matrix of zeroes, which means no biochemical reactions take place.

Note how the use of this matrix representation is not limited to this simple example or even to the ASM1 model. Also the models ASM2, ASM2d, ASM3, ADM1 and RWQM1 developed by IWA task groups in the mean time have been implemented (Henze *et al.*, 2000; IWA Task Group for Mathematical Modelling of Anaerobic Digestion Processes, 2002; Reichert *et al.*, 2001b). The user can also easily implement mass balance models himself using this general approach. Only the component vector, the reaction vector and the stoichiometric and kinetic coefficients need to be specified.

Logically, the next level (below WWTPAtomicModel) of classification would be to distinguish between models without volume (point-model abstractions where no mass is accumulated and hence no reactions occur) and models with volume. For models with volume, the distinction must be made between models where volume is considered constant and those where volume may vary. This class hierarchy is depicted in Fig. 3.5.

3.4 The modelling environment

As mentioned above, the WEST modelling environment allows for graphical component-based modelling. A hierarchical graphical editor (HGE) was especially designed for the interactive building of complex configurations from basic building blocks. The user can entirely rebuild the physical configuration of the wastewater treatment plant in the HGE (Fig. 3.6). Each of the components (aeration basins, clarifiers, ...) are symbolically represented by an icon with one or more input and outputs (*terminals*). The program uses two types of terminals: data terminals and physical terminals. Physical terminals represent a physical connection between two components in the configuration. Data terminals on the contrary, represent a dataflow in the system. This can be a measurement signal from a

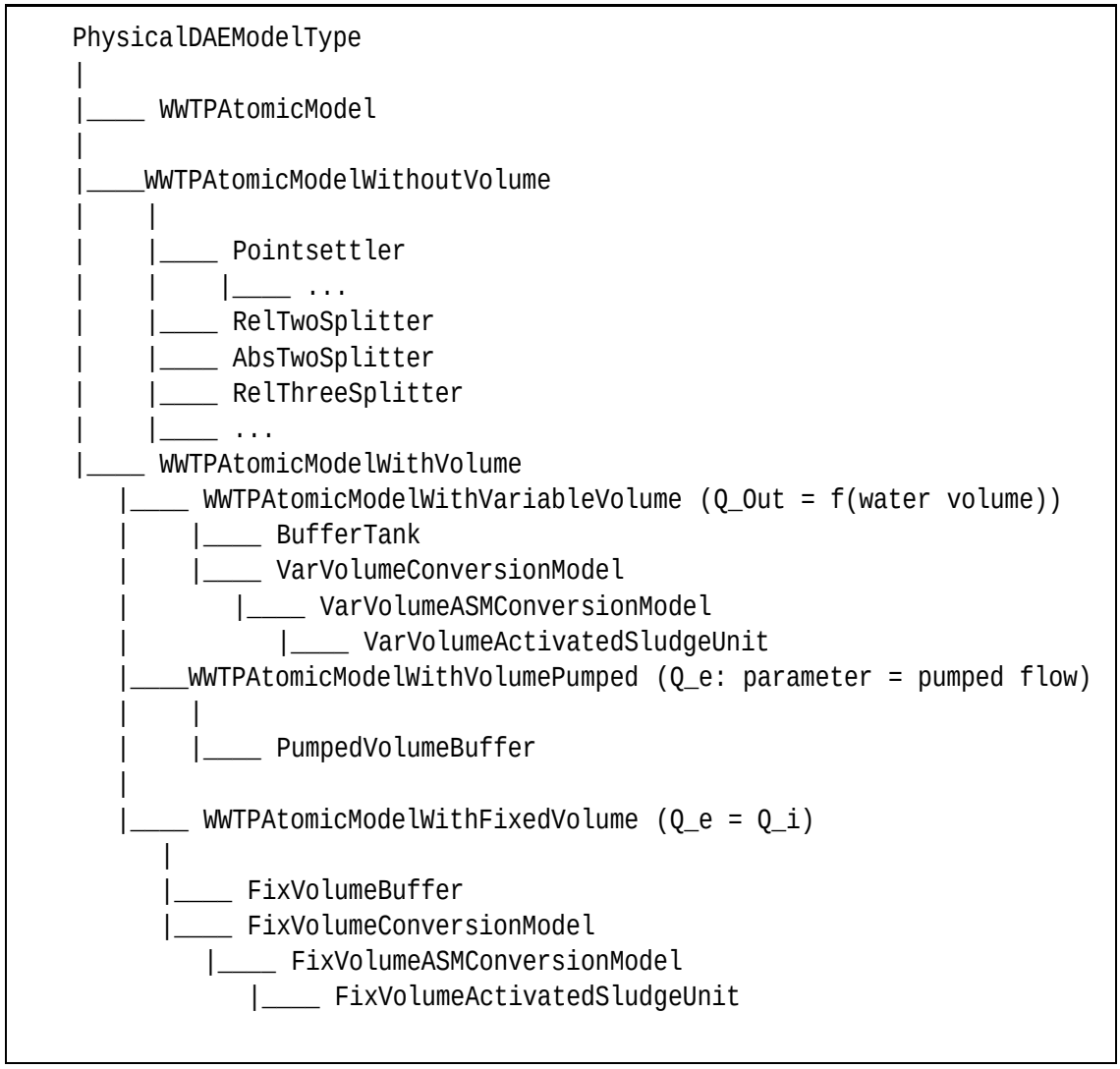


Figure 3.5: Class hierarchy of models without and with volume derived from WWTPAtomicModel

sensor to a control system, or a calculated control action from the control system to the manipulated variable in the configuration.

At this point, only a graphical representation has been made of the wastewater treatment plant to be modelled. Nothing has been specified on its behaviour. Once the configuration has been built graphically, each component of this configuration should be linked to a model from the model base. Each of these models is a structured collection of DAEs representing the time dependent behaviour of the components in question. The complete set of models together with the parameter values chosen by the users then specifies the dynamic behaviour of the system. A model base may contain multiple reasonable candidate models based on model features and user requirements. WEST leaves the final choice to the user, so model selection is mostly done manually. However, ongoing research tries to find and validate methodologies to accomplish automatic model selection based on measurements performed on the real process (Cooney and McDonalds, 1995; Dochain and Vanrolleghem, 2001; Takors *et al.*, 1997; Vanrolleghem and Van Daele, 1994).

Now from this graphical specification, together with the models chosen from the model

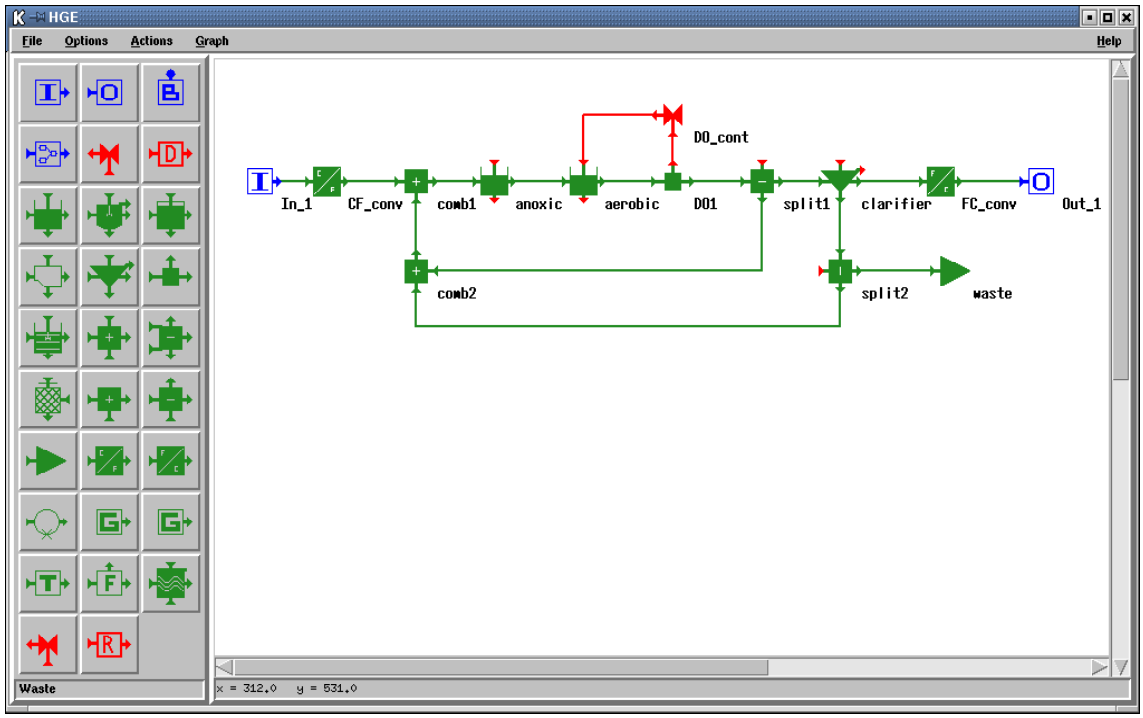


Figure 3.6: Representation of a WWTP model in the HGE (Hierarchical Graphical Editor)

base, a coupled model is produced. Some of the MSL-USER code corresponding to the coupled model represented in Fig. 3.6 is shown below.

```
CLASS simpleWWTPClass SPECIALISES CoupledModelType :=
{:
 interface <-
 {
     OBJ in_1 (* terminal = "In_1" *) "" :
        InWWTPConcTerminal := {:causality <- CIN:},
     OBJ out_1 (* terminal = "Out_1" *) "" :
        OutWWTPConcTerminal := {:causality <- COUT:},
 };
 parameters <-
 {
     OBJ Y_A "Autotrophic yield" : YieldForAutotrophicBiomass,
     OBJ Y_H "Heterotrophic yield" : YieldForHeterotrophicBiomass,
 };
 sub_models <-
 {
     OBJ CF_conv : CtoF,
     OBJ comb1 : TwoCombiner,
     OBJ anoxic : FixVolumeASU,
     OBJ clarifier : Takacs,
     ...
     OBJ DO1 : DO,
     OBJ DO_cont : PID,
```

```
    ...
};
coupling <-
{
    // parameter coupling
    sub_models.aerobic.parameters.Y_A.value := parameters.Y_A.value,
    sub_models.anoxic.parameters.Y_A.value := parameters.Y_A.value,
    sub_models.anoxic.parameters.Y_H.value := parameters.Y_H.value,
    sub_models.aerobic.parameters.Y_H.value := parameters.Y_H.value,
    ...
    // sub-model coupling
    connect(interface.in_1, sub_models.CF_conv.interface.Inflow),
    connect(sub_models.CF_conv.interface.Outflow,
       sub_models.comb1.interface.Inflow1),
    connect(sub_models.split2.interface.Outflow1,
       sub_models.comb2.interface.Inflow1),
    ...
    // control statements
    control(sub_models.DO_cont.interface.u,
       sub_models.aerobic.parameters.Kla),
};
:};
```

Each icon put on the canvas results in the instantiation of an MSL-USER object of the appropriate class in the coupled models *sub_models* section. If the user decides to define parameters of the coupled model in the HGE, they are stated in the *parameters* section. In the *coupling* section, statements are included that describe how the sub-models are connected to each other. First, the relations between the parameters of the sub-models and the user-defined parameters of the coupled model are indicated. Following this, the *connect* and *control* statements are listed. The *connect* statement is used to connect the interface variables of the coupled model to the interface of one of the sub-models or to connect the interfaces of two sub-models. The *control* statement is used to indicate that a parameter of a sub-model is controlled by an interface variable of a second model. However, parameters are invariant values to be declared at the beginning of a simulation run. In case a controller is used, the parameter serves as a manipulated variable. Therefore, it will automatically be transformed from a parameter to an input variable by the MSL-USER parser.

The graphical editor and the coupled model introduce a second level of hierarchy in WEST. Indeed, next to the hierarchical structure of the model base, aimed at maximal reuse of knowledge, also coupled models and their graphical representations can be reused. All coupled models have an interface like the sub-models from which they are composed. Consequently, the user can decide to add a coupled model to the model base and reuse it in yet another coupled model. This way, a model can be structured as a tree of coupled models and atomic models from the original model base. Again a maximal level of reusability and transfer of knowledge is obtained here. When coupling the models of the sewer system, treatment plant and receiving water, one can build and test the models separately. Afterwards, they can easily be linked in the graphical editor by reusing the

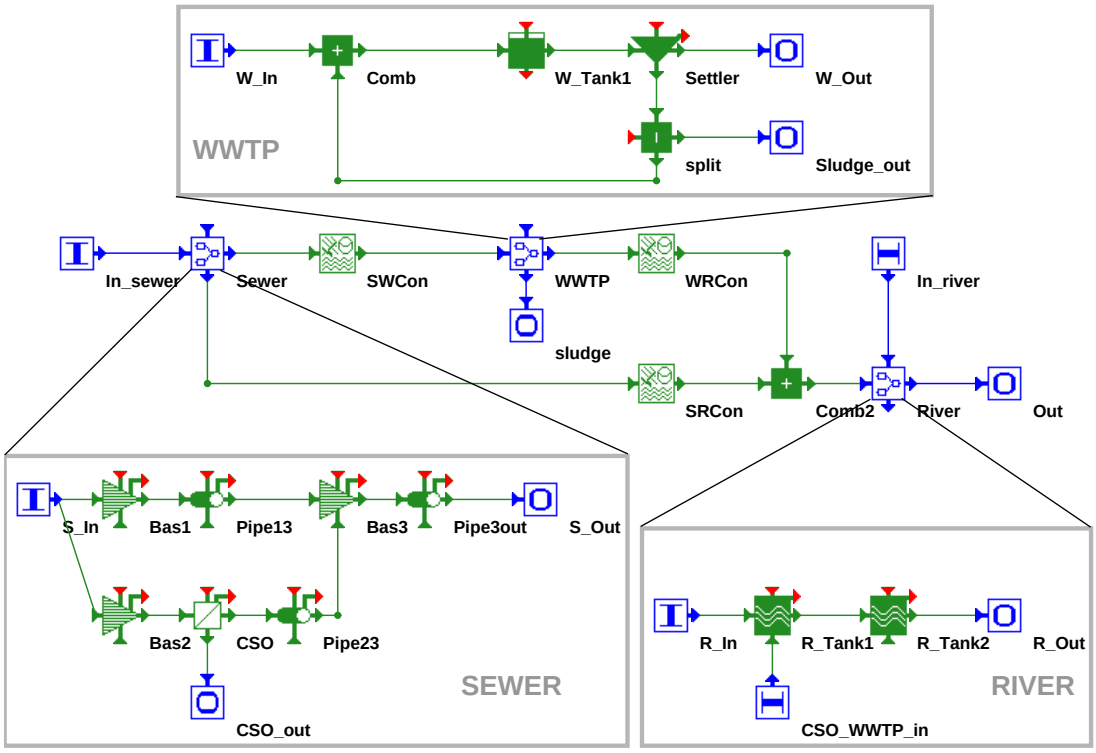


Figure 3.7: Representation of the reuse of models in the graphical editor of WEST

models created before (Fig. 3.7). Indeed, when creating large models, it is useful to first test the submodels and only afterwards connect them to create the integrated model.

3.5 Parsing from MSL-USER to MSL-EXEC

After constructing a coupled model in the HGE, the parser generates MSL-EXEC from this model for use in the experimentation environment of WEST. It therefore uses the coupled model itself along with the models stored in the model base.

During this (parsing) process, the syntax and the semantics of the MSL-USER representation are checked automatically as well as the compatibility of the nature (the units) of the variables passed on between the different sub-models. This way, some model coding errors may be detected here and not later, when simulating the model.

MSL-EXEC contains both code to describe dynamics and code to represent the symbolic information (“knowledge”). The different built-in statements are recognised by the parser and translated into their equivalent C++ formulations. The model dynamics are specified as a set of ordinary differential equations (ODEs) and algebraic equations. As the order of the equations is of no importance in MSL-USER, the correct sorting of the differential and algebraic equation has to be done by the parser. Indeed, a set of algebraic equations needs to be sorted before it can be implemented in a language with sequential semantics like C++. In order to sort the equations, dependency graphs are constructed. During the

execution of the sorting algorithm, algebraic loops are detected, since these cannot be sorted. This way, implicit sets of *n* equations in *n* unknowns may be found that can be either non-linear or linear. In case the set is non-linear, it can be solved using a symbolic solution with Gröbner bases (Davenport *et al.*, 1992). In WEST, a numerical solution using Broyden's method is implemented (Press *et al.*, 1992). In case of a linear set, an analytical solution using Cramer's rule is possible, or a numerical solution should be performed in case the analytical solution grows too large.

The symbolic information is used to display the model information in the WEST experimentation environment. For example, based on the annotations *hidden* and *fixed*, a variable or parameter will not be shown in the experimentation environment or the user will not be able to change its value. As mentioned before, a controlled parameter will automatically be transformed from a parameter to an input variable by the MSL-USER parser and will therefore no longer be visible in the parameter listing. Also the constraints on variables as integrated in the MSL-USER model base are transferred to the symbolic part of the MSL-EXEC representation and are used to protect the user from constraint violations during simulation or user input. Furthermore, default values, units and descriptions are visible in the experimentation environment.

Before the MSL-EXEC code can be used in the experimentation environment, an extra compilation step has to be performed. In this compilation step, a library file (executable code) is generated that can be loaded into the experimentation environment. This compilation step guarantees code that is optimised for simulation performance and accuracy. During this compilation, standard C libraries are linked to the generated model, enabling the user to include all functions available in these libraries in the MSL-USER models. Even user-defined C++ functions can be used and linked during parsing.

During parsing symbolic manipulation can also be performed. Symbolic manipulation is concerned with finding symbolic or exact solutions to mathematical problems. This avoids rounding errors and the need for an error analysis. Exact or symbolic computation has the disadvantage of being more compute-intensive than numerical calculation. However, as symbolic manipulation is performed only once as opposed to numerical code, which gets executed over and over again during simulation, the one-time intensive symbolic computation cost at parse time is largely compensated by the performance gain at simulation time.

The following very simple example will illustrate the usefulness of symbolic manipulation. Imagine trying to solve an equation for an unknown variable, such as: $x - 5 = 0$. An analytical solution is found if the equation can be solved explicitly for the unknown variable. In this case this is easy to see. However, an *algorithm* on a computer can be used to solve this equation numerically. The algorithm would test various values for *x*, and then stop with a solution when the equation is satisfied to some chosen tolerance. For example, the required accuracy for the numerical solution is set to 0.5. The computer would follow the algorithm until it found a solution. Given an initial guess $x = 1$, depending on the algorithm, it might come up with the following guesses: *x = 2.2, x = 3.3, x = 4.6*, and return the solution $x = 4.6$. Note that if the solution needs to be more accurate, it takes more time to solve this equation to this level of accuracy. If, through symbolic manipulation, the exact analytical solution $x = 5$ could be found immediately, an enormous gain at simulation time would be the result.

When the equations to be solved are large and complex, one has to deal with some issues about how to reach the solution in the most efficient way. Several problems can be tackled both in a numerical and a symbolic way. Getting the solution using one method rather than the other, has advantages and disadvantages. The advantages of symbolic manipulation in the case of WEST are:

- Performance, if you know a quantity analytically, you can avoid some computations and decrease the computation time.
- More accurate numerical results, because by pre-processing data with symbolic manipulations, more advanced numerical techniques can be exploited.

On the other hand, analytical solution methods do not exist for a number of problems. However, symbolic methods can still be used to derive expressions necessary for performing numerical computations – such as gradients and Jacobian and Hessian matrices. Thus, the traditional roles of numerical and symbolic computations are not distinct and many benefits arise from merging the two.

3.6 The experimentation environment

The experimentation environment depicted in Fig. 3.8 enables the user to perform experiments on compiled models. As such, it is the interface between the user and the "simulator". During simulation, the solver communicates efficiently with the model dynamics part of the MSL-EXEC model. The simulator as a whole can be asked to perform a numerical simulation. In that case the solver is used to generate a state trajectory for the MSL-EXEC model. Different numerical solvers can be chosen interactively. Since the type of system defined in wastewater treatment is normally considered to be a stiff dynamic system - i.e. the time constants for the different processes involved vary significantly - stiff solvers seem preferable. However, during the development of the COST simulation benchmark for activated sludge systems, it was shown that the numerical integrator to be preferred for simulating wastewater treatment is the WEST default 4^{th} order Runge-Kutta with variable time step size (*RK4ASC*) (Copp, 2002). Although the majority of a wastewater treatment plant can be described as a traditional continuous system, the modelling of sensors and controllers often turns it into a hybrid system, *i.e.* a combination of continuous and discrete systems. Stiff solvers, like methods based on a modified Rosenbrock formula or based on Gear's method, work very poorly for hybrid systems (Jeppsson, 2002).

The experimentation environment also queries the simulator for symbolic information. This information will be retrieved from the symbolic information part of the MSL-EXEC model. Examples of such symbolic information are the model structure and the parameter listing in Fig. 3.8. In this listing, the unit, a description and a default value of the parameter can be found together with its lower and upper bounds.

Below, different *experiment types* as implemented in the WEST environment are presented. The user thinks in terms of different *virtual experiments* with the model of a system. The following experiment types are currently implemented in WEST:

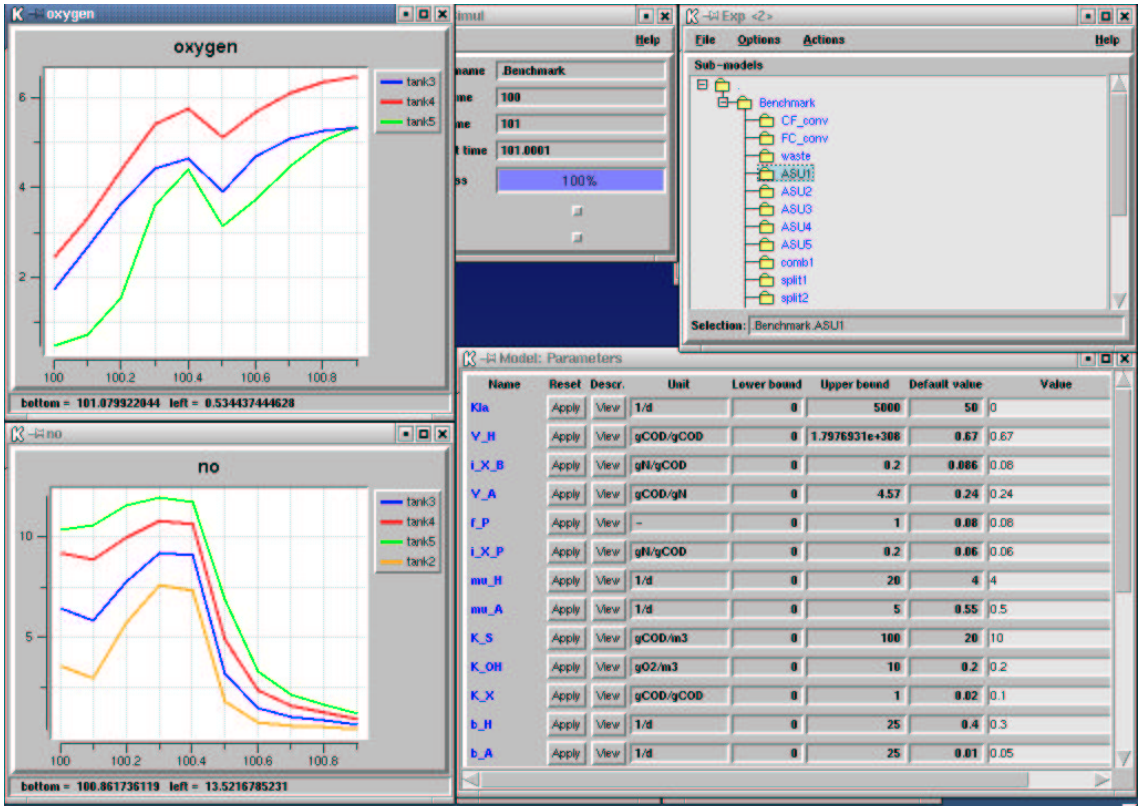


Figure 3.8: The WEST experimentation environment, showing plots and a parameter listing

Simulation experiment

Currently, there are two types of simulation experiments:

Initial value problem: state variable values are given at time t_{ini}. The simulator calculates the trajectory over $[t_{ini},t_{fin}]$. This is implemented using a set of forward integrators (e.g. RK4ASC) the user can select among.

Terminal value, end value or shooting problems: state variable values are given at t_{fin}. The simulator calculates the trajectory over $[t_{ini},t_{fin}]$. Solving the shooting problem is implemented in WEST using an optimisation algorithm whereby the varied entities are the unknown initial conditions and the goal function is the sum of absolute or squared values of differences between simulated end-value and their known/specified end-value.

Sometimes it is necessary to "synchronise" the simulator with external data. This is for example the case when the input $u(t)$ is given as a table of measurements, for instance the influent composition or a pump schedule. The integrator can determine its own integration times and when an input value is needed, interpolation is used. When the input is given as a continuous function (via a generator model), no interpolation is required.

Trajectory optimisation experiment

Certain model parameters are varied by a number of search algorithms the user can select from to minimise the *distance* between a simulated trajectory and a given (measured or

desired) trajectory. This is mostly done for (constrained) parameter estimation (model calibration), but it can also be used for controller tuning and process design optimisation. The distance measure is typically a sum of squares of differences between measured and simulated values though absolute values can also be used. The difference between measured and simulated values can be calculated at different points in time: as described above, the simulator can be forced to *synchronise* with external data or interpolation can be used. In general, the differences can be weighed to account for measurement accuracy and possible differences in the order of magnitude of the different values in the objective function. Dochain and Vanrolleghem (2001) give an overview of optimisation methods that can be used. Two methods are implemented in WEST. The method developed by Nelder and Mead (1964) (the simplex method) and the Praxis method (Brent, 1973) are implemented. Both are rather robust to local minima and quite efficient in terms of convergence. Genetic algorithms and the Shuffled Complex Evolution (SCE) algorithm (Duan *et al.*, 1992) are currently under implementation. The Hessian is calculated as indicated by Brent (1973), but does not always give good results. Therefore, the covariance matrix (confidence information) is calculated like in the Simplex method, also when the Brent method is used for the optimisation. The confidence information can then be used, for instance, to draw confidence ellipses or give parameter confidence bounds.

End value optimisation experiment

Here the optimiser is used to vary some parameters (possibly constrained) to extremise a goal function that only evaluates variables at t_{fin}, for instance total economic cost.

Sensitivity analysis experiment

The sensitivity of the model with respect to model parameter variations can be investigated. The calculation of sensitivity functions is based on the finite difference method. This method calculates the difference between two simulation experiments, a reference experiment and a perturbation experiment. The perturbation experiment is performed by perturbating a model parameter by a small factor (the perturbation factor). Dividing the difference in model outputs between these experiments by the parameter change results in the sensitivity function. To make sure that the sensitivity functions are calculated properly, a third experiment is performed, the control experiment. For this simulation experiment the parameter perturbation factor is doubled. If the resulting sensitivity function is within an allowed error band to the first sensitivity functions, it can be assumed that the non-linearity of the model or numerical inaccuracies did not influence the calculations. The error between both sensitivity functions is calculated with different criteria such as the sum of squared errors, the largest absolute difference, etc.

Sensitivity functions form the basis of optimal experimental design because they indicate where the measurements are most sensitive to the parameters. Moreover, the Fisher information matrix, which is an important cornerstone of experimental design, is calculated using sensitivity functions. This matrix is a measure for the information content of the simulated experiment.

Monte Carlo experiment

The uncertainty of the model output due to input (parameter and variable) uncertainty can be calculated in a Monte Carlo experiment. For each model input that is considered to be a random variable, a probability distribution is selected out of a predefined range of possible distributions (normal, log-normal, uniform, triangular, ...). Random samples are taken for each of the input distributions, and the set of samples ('shot') is entered into the deterministic model. The model is then solved as it would be for any deterministic analysis. The model results are stored and the process is repeated until the specified number of model iterations is completed (Cullen and Frey, 1999). From all stored model results, statistical properties (mean and standard deviation) and histograms are produced. These can subsequently be used in decision-making, *e.g.* risk analysis (Rousseau *et al.*, 2001).

User defined experiment series

The experimentation environment can also be controlled via scripting languages (Tcl scripting, Visual Basic scripting). Scripting enables the user to perform several scenarios in an automated way. It is possible to automatically perform a series of experiments using a predefined set of parameter values. Output and integrator options can be controlled interactively. Among others, the Monte Carlo simulation engine has been constructed using such relatively simple scripts.

3.7 IUWS model base

3.7.1 Problem definition

As noted in the previous section, the model base originally created for the modelling and simulation of wastewater treatment, requires all state variables to be the same in one model. In different models, different state variables can be used (e.g. ASM1, ASM2, ASM3). The components of the ASM1 are defined as:

```
TYPE Components
 '' The biological components considered in the WWTP models ''
     = ENUM {H2O, S_I, S_S, S_O, S_NO, S_ND, S_NH, S_ALK,
             X_I, X_S, X_BH, X_BA, X_P, X_ND}
```

Due to the way the model base is built, these variables cannot be combined within one model of a treatment plant. This limitation does not cause large problems as long as one only looks at the behaviour of the biological treatment, since in most cases, only one type of sludge is present in an installation. Before model compilation, one chooses the set of state variables to be used in the whole installation.

When creating an integrated model, these limitations become more problematic, since as Fronteau *et al.* (1997) noted, the state variables used in the traditionally used models of

the subsystems, are not the same. This means that within the given model base structure, it would not be possible to describe the behaviour of the sewer system, the treatment plant and the river within one integrated model.

Different approaches can be followed to overcome this problem. As a quick and dirty solution, the model base may be copied, all model names changed, and the same models used next to each other. One can easily see that this leads to a very large model base as more types of models are used. Also, this is a very inefficient reuse of models since the same code is used in different places. This is also likely to cause problems in the maintenance of the model base. If one wants to rewrite some part of the code, the same lines have to be changed on several places, making it prone to errors or differences between the several submodels. Another disadvantage of this approach is the amount of work needed if one wants to add an extra model type.

3.7.2 The C-preprocessor and the model base

In order to overcome the problems mentioned in the copy and change approach, it was decided to make use of the capabilities of the C-preprocessor. The C-preprocessor is already used with the msl-code to connect the different files of the model base. A part of the topfile of the model base as described in the previous section looks as:

```
#ifndef WWTP_MSL
#define WWTP_MSL

#include "generic.msl"
#include "wwtp.quantity.msl"
#include "wwtp.general.msl"
#include "wwtp.base.msl"

#endif
```

The C-preprocessor commands start with a # and only perform textual operations. For example, the `#include` statement, copies the named file into the top file of the model base. This mechanism is used extensively throughout the model base and allows to separate different models in different files. Another possibility of the C-preprocessor is the `ifdef/ifndef` mechanism. In this way the preprocessor checks whether a certain variable has been defined previously or not. If the condition is true, the code following the command is also executed, while if it is false, the code is skipped until an `#endif` statement is reached. This mechanism is used in the MSL model base, to prevent double inclusion of the same file (by two `#include` statements for the same file). This would lead to syntax errors by having the same types or classes defined twice, which is obviously not allowed. If the file is processed for the first time, it is checked whether a certain variable is already defined (`#ifndef WWTP_MSL`). Typically the name of the processed file in capitals is used in this test. If it has not been defined before, it is defined the first time (`#define WWTP_MSL`) and all the other files are included. If by mistake, this file would be processed a second time, the `#ifndef` command would result in a false result, skipping all includes till the `#endif` command.

The C-preprocessor has many more possibilities than the one described here, like macros, conditional compilation or line control (see e.g. Kelley and Pohl (1998) for more details). The macro possibilities of the preprocessor are the basis of the solution presented here to the efficient reuse of models within one large model base structure.

For instance, the macro definition can be used to concatenate strings in the code.

```
#define par(A) WWTP_ASM1##A
```

This macro defines that any part of the code that matches the `par(NAME)` structure will be replaced by `WWTP_ASM1NAME`. The MSL-code:

```
CLASS par(TwoCombiner) SPECIALISES ...
```

will expand to the following code after the preprocessor run:

```
CLASS WWTP_ASM1TwoCombiner SPECIALISES ...
```

This mechanism will be used extensively in the creation of the IUWS model base.

3.7.3 Reuse of models in the IUWS model base

When creating any model base within MSL, it is advantageous to reuse models as much as possible, since this will minimise the frequency of errors, while the creation of new models can be done faster, since parts of the programming and checking of the code has already been done. The reuse of code will also result in a smaller model base that can managed better. The possibilities of the reuse depend on the number of properties that can be modelled the same way throughout the different subsystems in the IUWS model base. Due to the hierarchy, the models can be reused until a certain level, after which separation of the properties and the behaviour will be necessary. For example, a CSTR has the same mass balance equations (change in mass equals transport + reactions), independent of the subsystem. However, the reactions taking place in this CSTR will be different and depending on the subsystem. Other examples of models that can be reused are combiners, splitters, sensors, etc…

When creating a model base of the IUWS, with reuse of models, it was decided to use the previously described concatenation possibilities of the C-preprocessor. Since this preprocessing step is already used in the existing model bases, it did not require any software changes.

When models with different components would be reused without any precautions, models could be defined more than once with the same name. Since it is not allowed to have two models with the same name, all models must get a new name every time the model is reused. Therefore, the code was changed to allow for automatic renaming by means of the concatenating macro of the preprocessor described above. The top file of the IUWS model base looks as follows:

```
#ifdef IUWS
   #include "generic.msl"
   #include "iuw.quantity.msl"
   #include "iuws.general.msl"

   #define par(A) Sewer##A
      #define SEWER
         #include "iuws.base.msl"
         #include "iuws.sewer.msl"
      #undef SEWER
   #undef par

   #define WWTP
      #define par(A) WWTP_ASM1##A
         #define ASM1
            #include "iuws.base.msl"
            #include "iuws.wwtp.msl"
            #include "iuws.wwtp.asm1.msl"
         #undef ASM1
      #undef par

      #define par(A) WWTP_ASM2##A
         #define ASM2
            #include "iuws.base.msl"
            #include "iuws.wwtp.msl"
            #include "iuws.wwtp.asm2.msl"
         #undef ASM2
      #undef par

   #undef WWTP

   #define par(A) RWQM1##A
      #define RWQM1
         #include "iuws.base.msl"
         #include "iuws.river.msl"
         #include "iuws.river.rm1.msl"
      #undef RWQM1
   #undef par

   #include "iuws.connectors.msl"
   #include "iuws.base.controllers.msl"
   #include "iuws.base.timers.msl"
   #include "iuws.base.data_modules.msl"
#endif //IUWS
```

The following pattern can be recognised: all generally reusable models are grouped into iuws.base.msl. These are models high in the hierarchy which are not very specific for any submodel in general. These include general mass balances for CSTRs, sensors, controllers, etc. The next level of reuse of models is located in the iuws.<submodel>.msl file.

In this part, models which are specific for one subsystem are defined. For example, for the wastewater treatment plant models, the clarifiers are defined in the file iuws.wwtp.msl. These are specific for the WWTP-subsystem, but the models are still independent of the biological conversion model used for the activated sludge. As a last specification, the very specific (with respect to subsystem or biological conversion type chosen) models are defined, for which the most clear examples are the conversion models such as e.g. the ASM1 or the RWQM1. On the other hand, specific structures like overflows are defined in the sewer part. Note that the concatenation macro `par(X)` is redefined every time a new model category is started.

In this way, the model parts that are reused are separated in files and new models can be added without much editing to the existing file. This is useful if one wants for instance, to include a submodel of the RWQM1. In this case, the components and reactions have to be defined, together with the stoichiometry matrix and the kinetics vector. Only these very specific elements need to be added to the model base by means of a proper definition of the `par(A)` macro and an `#include` statement.

An initial substantial rewrite of the model base was necessary in order to make this approach possible. However, once done, no further modification was necessary. In the first place, the models needed to be organised in a file structure in such a way that the reuse was possible in a clear and easily extendible way. This was illustrated by the structure of the iuws.msl file before. Second, the models to be reused had to be renamed automatically and uniquely. Part of the iuws.base.msl file looks now like:

```
CLASS par(AtomicModelWithVariableVolume)
EXTENDS par(AtomicModelWithVolume) WITH
 {: ... :}
```

From this example it is clear that every reference to a model name has to be changed into a macro call, which was defined in the iuws.msl file on page 89. After preprocessing this part of the code with the given iuws.msl file, the result is the following:

```
CLASS SEWERAtomicModelWithVariableVolume
EXTENDS SEWERAtomicModelWithVariableVolume WITH
{: ... :}

CLASS WWTP_ASM1AtomicModelWithVariableVolume
EXTENDS WWTP_ASM1AtomicModelWithVariableVolume WITH
{: ... :}

CLASS WWTP_ASM2AtomicModelWithVariableVolume
EXTENDS WWTPASM2AtomicModelWithVariableVolume WITH
{: ... :}

CLASS RWQM1AtomicModelWithVariableVolume
EXTENDS RWQM1AtomicModelWithVariableVolume WITH
{: ... :}
```

As one can see, the models automatically get, by means of the preprocessor, a unique name , and it is immediately clear to which category the model belongs. This makes the model selection easier, if one has to select models in the HGE later on.

Not only the model names have to be changed, but also some definitions, and the references to those later on in the model base. For instance, the dimension of the vector in which the state variables are stored, is depending on the model. Therefore, these vectors have to be redefined for every category, in the following way:

```
CLASS par(MassVector) = Mass[par(NrOfComponents);];
CLASS par(MassFluxVector) = MassFlux[par(NrOfComponents);];
CLASS par(ConcentrationVector) = Concentration[par(NrOfComponents);];
```

In this way, four classes are defined in the different calls of this file: a `SEWERMassVector`, `WWTP_ASM1MassVector`, `WWTP_ASM2MassVector` and a `RWQM1MassVector`. The same needs to be done for all terminals which are also depending on the number of state variables in every model. If a model has an object which belongs to this class, the right name has to be used as well, this for all objects, i.e. interfaces, parameters and states.

```
OBJ Inflow (* terminal = "in_1" *) "Inflow" :
   par(InTerminal) := {: causality <- "CIN" :};
OBJ C "Vector containing concentrations for all the components" :
   par(ConcentrationVector);
```

So far, only the names of models and classes have been adapted, but the use of the names in the component vector has also consequences for the way the equations are written. In section 3.3.3 on page 71 the definition of the components vector was already introduced. However, in case of the IUWS-model base, the names in the vector are dependent on the category of the model in which they are used.

```
TYPE par(Components)
"
 The biological components considered in the WWTP_AMS1 models
"
 =  ENUM {par(H2O), par(S_I), par(S_S), par(S_O), par(S_NO), par(S_ND),
 par(S_NH), par(S_ALK), par(X_I), par(X_S), par(X_BH), par(X_BA),
 par(X_P), par(X_ND)};
```

which means that also in the equation section changes have to be made. Every reference to one of the components needs to be adapted with the appropriate macro structure. It is important to note that *every* occurrence has to be changed, not only those in the reused files. Also, the references in the category specific files have to be changed, since otherwise the compiler detects some names which were not defined in the model base before and hence, generates an error. The names have to be unique due to the way the `ENUM` statement works. The elements of such an `ENUM` statement are replaced by the compiler with number. If for one submodel `S_S` is number 3 and for the other submodel `S_S` is number 4, errors during the simulation will occur, since the wrong element in the vector will be selected. By also appending the category to the names of the derived states, unique names are used and this type of errors cannot occur. An example of the code is:

```
state.Kinetics[par(AerobicGrowthOfHeterotrophsWithNH4)]
    = parameters.mu_H_Aer_T*state.C[par(X_H)]
       * (state.C[par(S_S)] / (parameters.K_H_S_Aer+state.C[par(S_S)]))
       * (state.C[par(S_O)] / (parameters.K_H_O_Aer+state.C[par(S_O)]))
       * (state.C[par(S_NH4)]/(parameters.K_H_N_Aer+state.C[par(S_NH4)]))
       * (state.C[par(S_HPO4)]
       / (parameters.K_H_HPO4_Aer+state.C[par(S_HPO4)]));
```

Luckily, since the pattern of the items to be changed is reasonably well described, some of these substitutions can be automated with a scripting language using regular expressions. Nevertheless, the transformation from the WWTP model base to the IUWS model base was a large task which required a substantial effort. The parser helped to find missed changes.

A last remark needs to be made, regarding the use of the preprocessor for model reuse and generating unique names. The mechanism of protecting files as described in section 3.7.2 (`#ifndef FILE_NAME`), cannot be used anymore for the files needing multiple processing, since they need to be included more than once. This means that the creator/maintainer of the IUWS model base, has to be extra careful in avoiding multiple inclusion of files.

In order to enhance the overview in this fairly complex model base, a html parser has been written too. This parser transforms any model base into a set of html files and two overview files. The first overview file gives the so-called file-structure of the model base, simply indicating which file is included where. In this way the file tree of the model base is created and can be used to quickly find a file or part of the code. A second overview file contains the class hierarchy. In this way, the user can easily see the model hierarchy a certain model depends on. Together with these overview files some html colouring for easier reading is done, but most importantly, tags are placed on every type or class used. This means that if one has a certain object of a given class, one can immediately find out the properties of this class. This is very useful in order to understand the properties at any point in the model base.

3.7.4 The Kosim model base

Kosim

Kosim is a commercially available software package for the simulation of sewer systems (itwh, 2000). It is officially recommended as a consent tool for design of sewer systems by several German states. Rainfall-runoff simulation in Kosim distinguishes between impervious, pervious and natural catchment areas. For impervious areas, wetting, depression and evaporation losses are considered. Infiltration for permeable areas is simulated using Horton's approach, which has been adapted for use in long-term simulations (Paulsen, 1986). Flow routing on subcatchments is modelled by Nash cascades (see section 2.3.2 on page 17). Flow between the subcatchments is modelled by translation or by translation and retention. All pollutants are considered to be conservative and transported with the water. Different structures are implemented:

- simple overflow
- on-line bypass tank
- off-line bypass tank
- on-line pass-through tank
- off-line pass-trough tank

For the connection between catchments either a translation, or a translation with retention can be used. In the first case, a pure plug flow is modelled, while in the second case,

wave attenuation is taken into account by routing the water through a series of tanks. The number of tanks used is a function of the parameters such as the roughness, the slope and the length of the connection pipe.

Two approaches were followed when implementing the Kosim modelling approach in WEST. The first was to translate the discrete equations as described in the Kosim manual into continuous equations that can be solved by WEST. This was e.g. the case with the Horton equation for infiltration in pervious areas. Kosim implements a discretised form while the differential equation was implemented into WEST. The second was to implement the different functions calculated by Kosim directly. The implemented functions are the relationships between the water depth and the throughflow, overflow and volume.

From discrete to continuous equations

Kosim simulates the behaviour of the sewer system by solving discrete equations with a fixed time-step of 5 min. The response of a catchment on a rain event is analytically calculated as:

$$Q_{out} = \sum_{i=1}^{L} N_{wt-i+1} \cdot A_E \cdot E_i \tag{3.5}$$

where

Q_{out} The outflow rate of the catchment
N_w The effective rainfall
A_E The area of the catchment
E_i Ordinate of the unit hydrograph response curve
L The number of terms in the unit hydrograph response curve

By some mathematical transformations, this equation can be written in a form that can be calculated recursively, and hence, very fast, without the need for numerical integration. Due to the fact that a finite number of terms of the unit hydrograph response curve is used, some water would be lost if this equation is applied as such. However, correction terms are used to make sure the mass balance is closed for every catchment.

Within the WEST simulation software, so far only continuous equations can be implemented. Therefore, the equations found in the user manual of Kosim were translated into continuous equations that could be implemented in WEST. The general concept of a catchment implementation in WEST is shown in Fig. 3.9.

It can be seen that different elements were needed to implement a standard Kosim basin with 3 tanks. The input element was used to read the rain data from a file. The evaporation generator was used to calculate the evaporation. The runoff calculator calculates the amount of netto runoff after subtraction of the losses (wetting, depression and evaporation losses). In the next element, three linear reservoirs are implemented. The equations relating the outflow to the volume can be written as:

$$Q_{out} = \frac{1}{K} V \tag{3.6}$$

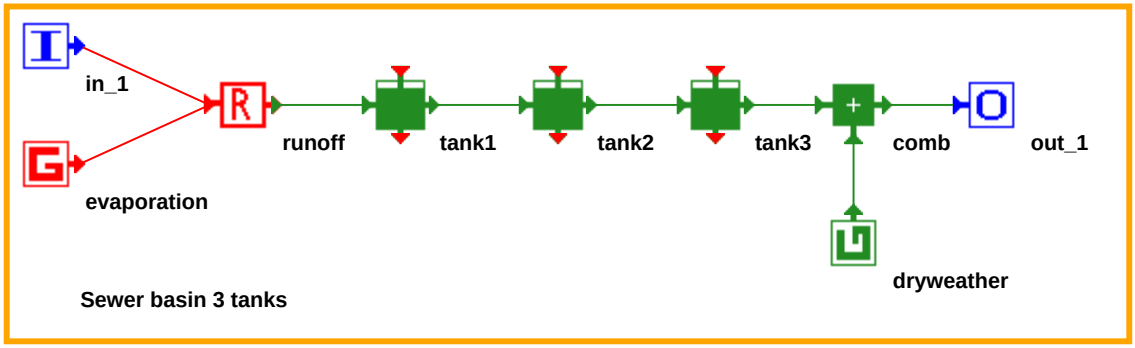


Figure 3.9: WEST implementation of a catchment with 3 subbasins

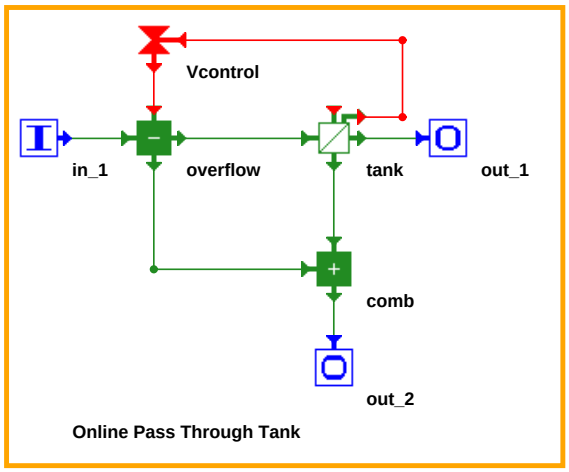


Figure 3.10: WEST implementation of an on-line pass through tank

where K is the storage constant, determining how fast the three tanks-in-series react to a change in the input of the first tank.

To describe a Kosim on-line pass-through tank, several WEST elements (Fig. 3.9) were used. The first overflow determines the amount of water that goes into the tank if the tank is filled. From the tank, the flow rate going to the next part of the sewer system is limited and the remainder of the flow is overflowed as well.

The equations described in the Kosim manual were used to implement the different elements in WEST. For the generation of dry weather flow, the Kosim concept of daily and weekly patterns was implemented within WEST without much problems. An example of this is given in Fig. 3.11. Implementing the linear reservoirs too did not present any problem as the equations were clearly described. However, the implementation of the evaporation and runoff calculation models was not entirely successful.

Several problems were encountered, but the main problem was the lack of clear documentation of how the evaporation is exactly calculated within Kosim. Also, the value of the linear reservoir storage constant had to be adapted from the Kosim value in order to make the simulated flow rate correspond to the flow rate predicted by Kosim. Still an exact match was never reached. An illustrative example of the results obtained for a small storm event are shown in Fig. 3.12. It can be seen that the two models give different

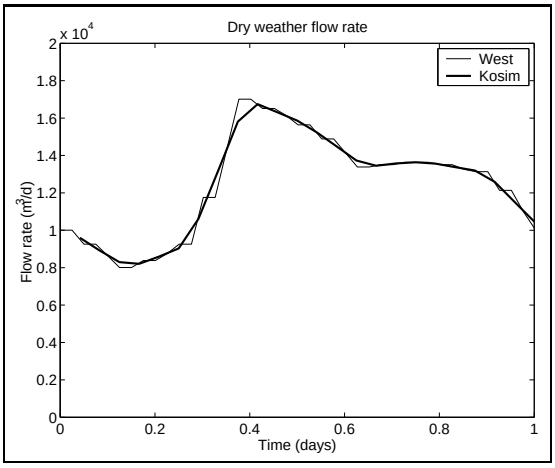


Figure 3.11: Dry weather flow generated by WEST and by Kosim

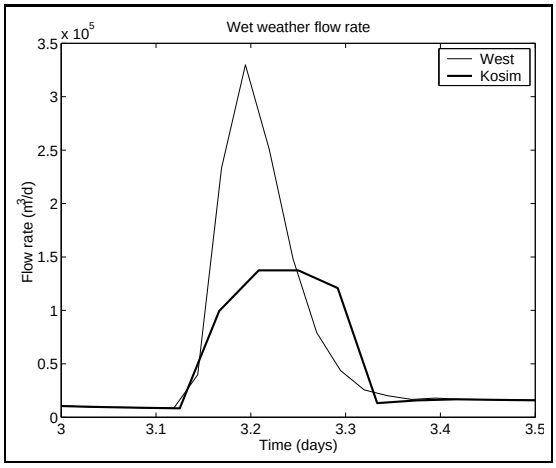


Figure 3.12: Wet weather flow generated by WEST and by Kosim

results for the wet weather flow. In this case, the flow predicted by the WEST model had a larger peak value, but a shorter tail than the corresponding Kosim model.

In order to be able to model the sewer system within WEST, it was decided to leave this approach and implement the Q-h relationships taken directly from the Kosim software.

Implementation of Q-h relationships

Since the previous approach was not completely successful, a pragmatic approach was followed, in order to be able to simulate the sewer system within WEST. Rather than trying to implement the concept of Kosim and to reuse existing models, the different equations of the Kosim model were implemented as look-up tables.

For every element (storm tank or CSO), Kosim generates a series of look-up tables as a function of the parameter values specified by the user. In these tables, the volume or overflow rate are defined as a function of the water height in that element. Since a Kosim model of the catchment of Tielt was available, these look-up tables could be used in a look-up table model within WEST. This approach was successful as is shown in Fig. 3.13, which shows the comparison of the overflow volumes predicted by the Kosim model, and the corresponding values predicted by the WEST model. Also, an example is given of the simulated COD concentration in the sewer system for WEST and Kosim (Fig. 3.14). It was concluded that the WEST implementation of the Kosim equations was successful for the types of elements needed for this study.

It should however be noted that, due to the continuous solution of these equations, together with a rather inefficient look-up table implementation, the simulation time of WEST was much longer than the corresponding time within Kosim. Moreover, only the elements used in the integrated case study of chapter 8 were implemented in this way.

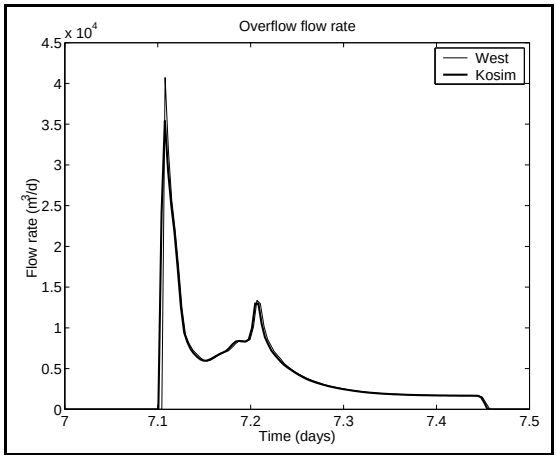


Figure 3.13: Comparison of the implementation by look-up tables in WEST with the Kosim predictions for an off-line bypass tank: flow rate

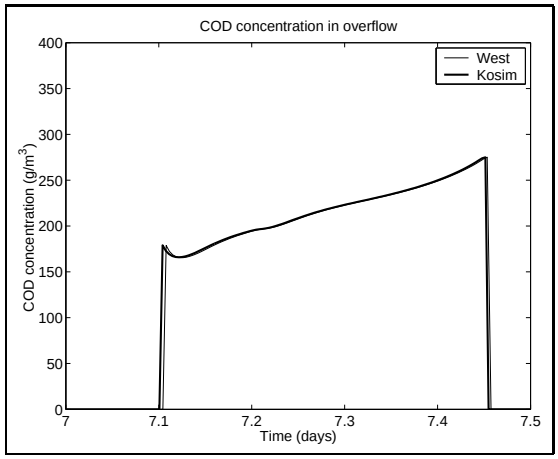


Figure 3.14: Comparison of the implementation by look-up tables in WEST with the Kosim predictions for an off-line bypass tank: COD

3.7.5 River water quality modelling

As the RWQM1 (Reichert *et al.*, 2001b) describes the conversions taking place in the river with a Peterson matrix similar to the ASM model, this model could straightforwardly be implemented into the WEST model base. Also, the implementation of submodels of the RWQM1 could be done without any problem. In this way, a range of river models was implemented in the WEST model base and could be used in modelling the IUWS.

3.8 Conclusions

The mathematical modelling of IUWSs can be used during the design and optimisation phase. WEST is a general modelling and simulation environment and can, together with the developed model base, be used for this task. The model base is written in MSL-USER in which symbolic information can be included in the code. In the graphical modelling environment, the physical layout of the system can be rebuilt, and each building block can be linked to a specific model from the model base. The graphical information is then combined with the information in the model base to produce MSL-EXEC-code, which can be compiled with a C++-compiler to generate fast, executable code. In the experimentation environment, the user can design and run different experiments with this model such as simulations or optimisations.

The main advantages of the use of this software are the following. First, the modelling and simulation environment are strictly separated since these have different objectives (i.e. flexibility and model reuse vs. accuracy and performance). The MSL-USER language is a high level language which is easy to learn and use, while information about realistic upper and lower values and units of parameters and variables can be implemented. Furthermore, an extensive model base for the modelling of WWTPs is already available. The parser uses symbolic manipulation to create numerically efficient code. Finally, the experimentation environment can be easily used to perform different types of experiments

with the models. The user can extend these experiments by scripting.

WEST was originally developed to model WWTPs. By changing the general structure of the WWTP model base, models with different state variables can now be used easily. Moreover, models for the sewer system and the rivers have been added. In this way, a simultaneous simulation of the IUWS is now possible with WEST.

Chapter 4

Model simplification and reduction in the integrated urban wastewater system

4.1 Introduction

The urban wastewater system (sewer system and wastewater treatment plant) has a major impact on the water quality of the receiving water (urban rivers or lakes). During rain events, the sewer system might spill diluted, but untreated water in the receiving water via combined sewer overflows. The WWTP on the other hand, continuously discharges effluent which contains, depending on the treatment efficiency of the plant, more or less pollutants. In contrast to the sewer discharge in the river, the effluent always contains some pollutants and has, consequently, a continuous impact which is probably not negligible.

To minimise this impact in a given situation, several approaches can be used. One can for instance, build extra storage volume or use bigger sewer pipes. Usually this type of solution is very expensive and is only feasible if sufficient space is available. Another option is the use of real-time control on the sewer system or the treatment plant. Typically this type of solutions requires less investment costs and tries to make optimal use of the facilities already present in the catchment (Schilling, 1989).

Mathematical models are useful in the design and tuning of such control strategies, since the possibilities to evaluate a strategy in practice are usually very limited. When using a mathematical model of the system under study, different sensors (level, flow, DO, ammonia, pH) and/or actuators (pumps, weirs) can be selected and evaluated before investing in expensive equipment. Moreover, different control laws (P, PI, On-Off, fuzzy) can be easily tried and the parameters of the selected control law can be tuned without risk of disturbing the system.

Three problems are encountered when developing an integrated model that is to be used for developing an integrated control strategy or for system optimisation. First, the state-of-the-art models use different variables to describe the aquatic system (e.g. BOD, COD or TOC to describe organic pollution). Second, the hydraulic equations, which describe

flow propagation in sewer pipes and rivers (the “de Saint-Venant” equations) are non-linear partial differential equations. These require complex numerical algorithms to solve, making the models slow and thus difficult to use for optimisation studies. Third, the state-of-the-art models are typically implemented in different software packages, making simultaneous simulations difficult to achieve, since communication typically requires file transfer from upstream to downstream. Moreover, the flow of information about the downstream state to the upstream models, which is necessary for an integrated control action is even more complicated or even impossible.

This chapter outlines the general concept on how these problems were solved in this work. Two main ideas are presented to gain calculation time: model simplifications with mechanistic surrogate models (section 4.2) and model reduction (section 4.3). The problem of the different state variables is tackled by the development of consistent connectors with closed elemental balances (section 4.4). Finally, the problem of the different software packages is solved by implementing all models into the WEST® modelling and simulation environment. The approach on extending the model base for the IUWS was already explained in section 3.7.

4.2 Model simplification: Mechanistic surrogate models

The individual components of the IUWS (sewer, treatment plant and river) are often modelled using complex mechanistic models. For example, flow routing in sewer pipes or rivers is described by the “de Saint-Venant” equations, which are based on the conservation of mass and momentum. These partial differential equations have to be solved using advanced numerical integration algorithms with a high computational burden, which makes the model impractical for use in long-term simulations or in optimisation problems. However, this complex mechanistic model is able to accurately predict flood wave propagation in open channels. However, design and tuning of control strategies are both examples of optimisation problems, which typically require a lot of simulations in order to find a (sub)optimal solution. Hence, shorter simulation times are required in order to find a solution within a reasonable time. The use of mechanistic surrogate models as an alternative for complex mechanistic models is proposed here.

The complex mechanistic models (with the “de Saint-Venant” equations) as described above may be substituted by faster models. The term “surrogate” models is used for the latter, as they form a surrogate (an approximate substitute) for the “real thing”, i.e. the complex mechanistic model that is approximating reality better. Surrogate models are faster and less but still sufficiently accurate, and require more data to be calibrated. The possibilities of replacing actual field data by virtual data generated with a complex mechanistic model for calibration of the surrogate model are explained.

As with any model, two types of approaches are possible, the empirical (black box) and the mechanistic (white box) approach. Mechanistic surrogate models are introduced here as simplified models that still contain some physical knowledge. This is different from the black box approach (like in regression models or neural networks) where the knowledge about the system is not represented in the model structure. First, the general concept on

how to go from reality to a mechanistic surrogate model is proposed and subsequently applied to the integrated urban wastewater system.

4.2.1 The concept: from reality to mechanistic surrogate models.

When modelling a system, there are typically three sources of information that can be used (Spriet and Vansteenkiste, 1982). The first one is the goal of the modelling exercise, the second one is the prior knowledge about the system under study, and the third one is the set of available data. In this work, the goal of the model building, whether it is the complex or the surrogate model, is the same in both cases and is not further discussed. However, concerning the amounts of data and prior knowledge used during the model building, differences do exist.

When there is a lot of knowledge available (like e.g. in physical systems), only a relatively small amount of data is needed to calibrate the few unknown parameters of the model (this is illustrated by the small data arrow in Fig. 4.1A). Indeed, many parameters have a physical meaning and even a known value (e.g. the gravity constant g). The collection of real-life data may be assisted by optimal experimental design (OED) (Petersen *et al.*, 2001a) in which the complex mechanistic model to be calibrated is being used. This means that numerical techniques are applied to the complex model in order to find the experimental conditions which provide a large amount of information to calibrate the parameters of the model.

When using a simplified model, in which less information ("knowledge") is contained in the equations, more data are needed to compensate for the lack of information from the knowledge side (large data arrow in Fig. 4.1B). Many parameters no longer have a strict physical meaning, as they are the result of "lumping". Rather than trying to recalculate them from the lumping equations, it is preferred to use data to empirically find them. However, collecting data is an expensive and time-consuming task (Vanrolleghem *et al.*, 1999). Hence, collecting enough data to reliably calibrate a surrogate model may be an enormous or even impossible task. On the other hand, complex mechanistic models can be calibrated with a reasonable amount of effort, which is proven by numerous articles in literature in a wide range of fields. These mechanistic models are accurate, but require too much calculation time for iterative use such as in tuning of control strategies.

The proposed solution to this problem is shown in Fig. 4.1C. Instead of trying to collect all the data necessary to calibrate the surrogate model from reality, one can also generate "data" by using the complex mechanistic model. After calibration of the complex model (with relatively few data), simulation results yield virtual data that can be used to calibrate the surrogate model. This can be seen as "pumping" the knowledge summarised in the complex mechanistic model into the surrogate model by means of these virtual data. These data generating simulations with the complex mechanistic model can be designed with the aid of OED. This means that the mechanistic surrogate model is used to design virtual experiments which have to be done with the complex mechanistic surrogate model. The experiments and data collections that can be done with the complex mechanistic model are much broader and more flexible, when compared to the OED on

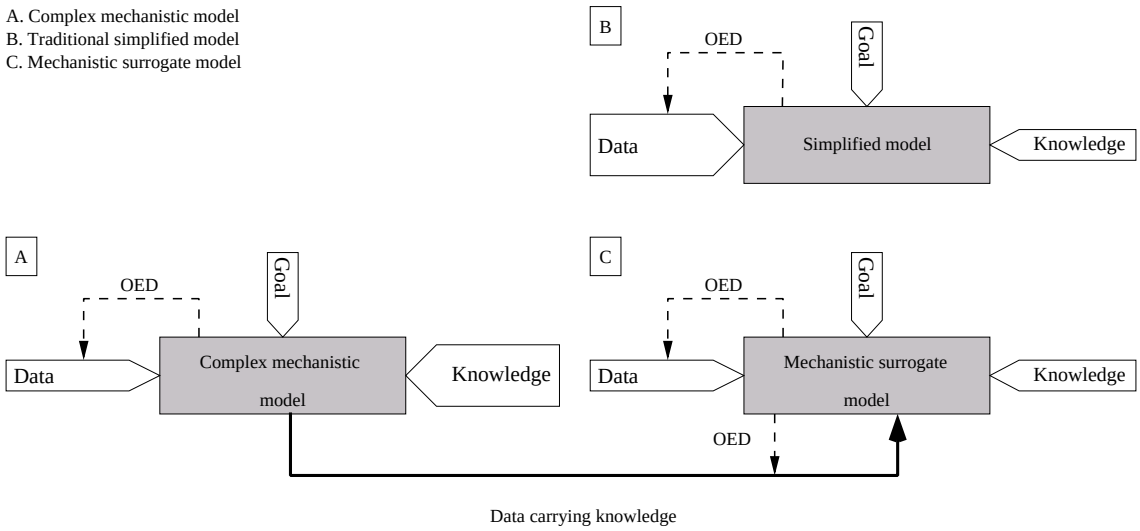


Figure 4.1: The use of virtual data in the creation of surrogate models

reality. Hence, the number of degrees of freedom is much higher and only limited by the creativity of the user and by the validity of the complex mechanistic model.

Once this surrogate model is calibrated, it can be used within a procedure to design a control strategy and optimise its parameters. To improve the reliability of the predictions by the surrogate model one can, before its implementation in practice, check the solution suggested by optimisation with the surrogate model, with the predictions for that solution obtained with the more accurate complex model. When this last test is passed successfully, the solution can be applied to reality.

The suggested procedure to go from reality to a surrogate model can be summarised as follows.

1. Determine the system under study, its boundaries and the problem to be solved.
2. Collect data on the system to calibrate the complex mechanistic model. This data collection may be assisted by optimal experimental design (OED) on reality by using the complex model to be calibrated.
3. Calibrate and validate the complex mechanistic model.
4. Generate data for the calibration of the mechanistic surrogate model. This data collection may be assisted by OED on the complex mechanistic model by using the mechanistic surrogate model.
5. Calibrate and validate the mechanistic surrogate model.

4.2.2 From catchment to an integrated surrogate model of the urban wastewater system

Fig. 4.2 shows the application of the very general previous concept on the urban wastewater system. Typical examples of complex mechanistic models of the different sub-

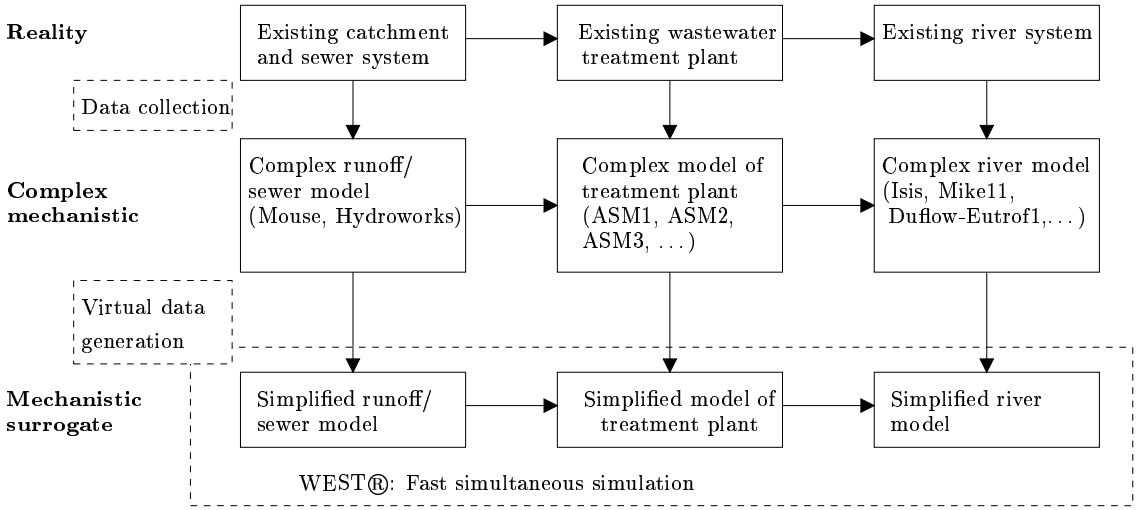


Figure 4.2: The creation of mechanistic surrogate models in the urban water system

systems are given. In both the sewer models (HYDROWORKS, MOUSE, HYSTEM-EXTRAM, SWMM, ...) and the river models (DUFLOW-EUTROF1, ISIS, MIKE11, ...) flow propagation is described using the "de Saint-Venant" equations. These partial differential equations can be simplified in certain cases (see section 2.3.2), but they still require advanced numerical integration and, hence, a long calculation time. Therefore, alternatives for these models are suggested.

Vaes and Berlamont (1999) used physically based conceptual models to assess combined sewer overflows. Comparing the emission results of a reservoir model with a hydrodynamic model, showed that both models predict the overflow emissions (in terms of water volumes) equally well, taking into account the uncertainties in the input data. Most importantly, the calculation times reported for the reservoir model are a factor 10^4 smaller. Fronteau (1999) compared the conceptual sewer model Kosim (Paulsen, 1986) with the complex mechanistic Hydroworks model (Wallingford Software, UK). Kosim describes runoff and flow propagation in the sewer system of each subcatchment by means of a Nash-cascade and a transportation time. When comparing this to the complex mechanistic models in which most of the pipes are calculated in detail, the simulation time of the Kosim surrogate model is much shorter. The long-term simulations of Kosim and Hydroworks gave similar results in Fronteau's work, but Kosim was significantly faster.

Flow routing in rivers can be approximated by a series of tanks with variable volume (Beck and Young, 1975). Moreover, when these tanks are also used to describe the transport of solutes in the river, the model is also able to describe dispersion in a reasonably accurate way (Reda, 1996). When, in addition, a biological conversion model is used to predict the conversion taking place in the river, a series of continuously stirred tanks can be easily used for modelling the dynamics of river water quality. The procedure of calibrating the flow propagating properties of a series of tanks on data generated by the "de Saint-Venant" equations will be illustrated in chapter 6 in a case study performed on the river Zwalm (Belgium).

It has to be noted that due to the large uncertainties in river water quality modelling, it might be sufficient to only apply this procedure for the hydraulic part of the model. The

water quality model can be directly calibrated on the collected field data. It is thought that the water quality data generated by the complex mechanistic model are too uncertain to use as calibration data for the surrogate quality model.

In chapter 5 the possibilities of generating data with the ASM models are illustrated. These data will be used to train an artificial neural network which could be used as a fast alternative to the large number of differential equations needed when applying the ASM models.

4.3 Model reduction through boundary relocation

4.3.1 Model reduction for controller tuning

The problem with integrated models is that, despite the choice for already simplified – surrogate– models, they still do not allow sufficiently fast calculations to easily perform control optimisation studies. Model reduction with minimal deterioration of the accuracy is an additional way to develop a fast calculating model. Four approaches are investigated here to create a so-called control model that can be used to design, optimise and tune a control strategy:

1. Relocating the upstream system boundaries of the controlled system to those points just upstream of the most upstream control action.
2. Relocating the downstream system boundaries on the basis of the location of the most downstream sensors used in the control strategy.
3. Reducing model complexity further on the basis of an analysis of the sensitivity of the control actions on submodel elimination.
4. Relocating the time boundaries to exclude some periods at the beginning and the end of the optimisation.

The first acceleration focuses on the fact that in both the sewer system and the river system under study, relatively large parts of the system are located upstream of the most upstream control action. This means that, whatever the control action is, the model output for these parts will always be identical. Hence, it is not necessary to recalculate these parts of the system in a control optimisation study. The system boundaries for the controlled system can be relocated and influent files might be generated at these new system boundaries to feed the simulation. It is important to notice that they only have to be generated once and can be reused afterwards for all control system evaluations. Consequently, important time savings can be achieved. To a certain extent this relocation of the system boundaries can be automated by using the dependency-structure between the model variables that is constructed during model analysis (Vangheluwe *et al.*, 1998).

A second reduction focuses on the fact that it may not be necessary to calculate the flow or the conversions of water quality components (ammonia, biomass, COD, ...) occurring

in some part of the receiving water since the inclusion of these conversions would not have an impact on the way the controller calculates its control actions. For instance, when the controller aims at preventing flooding, the height of the water at some location in the river might be measured and used as an input for the controller acting on some pumps or weirs. The behaviour of the river downstream of this level sensor will not influence the controller and can therefore be left out when tuning the control strategy. In general, the part downstream of the last sensor that is used as a control input can be left out of the control model.

Another example is a controller that aims to minimise the peak ammonia concentration in the river. One can imagine that this concentration most probably occurs at those locations where either sewer overflow or treatment plant effluent are mixed with the receiving water. For this example, two things can be taken advantage of. First, there is no time delay (assuming immediate mixing) between the discharge of the pollutant and the effect in the river and, hence, a measurement of ammonia at the mixing point can be considered sufficient as an input to calculate the control actions more upstream in the system. This is in contrast with a situation where one, for instance, focuses on the minimum oxygen concentration in the river, which will be located at some distance downstream of the place of discharge since the oxygen consumption may take considerable time. Moreover, the location of the highest peak of ammonia is fixed (the critical mixing point) and can, hence, be measured with an ammonia sensor located at that site. When looking at the minimum oxygen concentration, however, the place where the minimum occurs will depend on different factors such as the flow rate, biomass concentration in the river, biodegradability of the organic pollution, etc. In conclusion, for simulation of an ammonia controller it is sufficient to model a system ending at the critical mixing point where the ammonia sensor is located.

Third, to support a further reduction of the model complexity, it can be evaluated whether the control actions are sensitive to the elimination of a certain submodel from the overall model. This is basically a more specific application of the ideas presented by Rauch *et al.* (1998a) concerning the fact that in most cases the purpose of water quality management does not need to consider all aspects of the river system. Other hints on submodel selection are given in Reichert *et al.* (2001b). One could, for instance, replace the two step nitrification process by a one step process (and eliminate nitrite as an intermediate), and ignore the influence of algae and consumers.

As a last approach to the model reduction, it might be useful to relocate the time boundaries of the system. For instance, if the controller is only active in one part of the state space and it is sure that for a given time period the system is not in this part, one can leave this period out of the simulated period. For instance, if the period under study contains a dry period at the start, a controller designed to act in wet weather conditions will not have any influence until the first rain event occurs. Therefore, one could simulate the first dry period only once and start with the control simulations a short time before the first rain event. It is also possible to cut off the last part of the simulation if that is again a dry period. However, one cannot stop directly after the last rain event, since one has to be sure that the effect of the control actions on the receiving water has completely been calculated before ending the simulation. Again, it must be certain that the system is not in the part of the state space where the control strategy is active and that it will not come

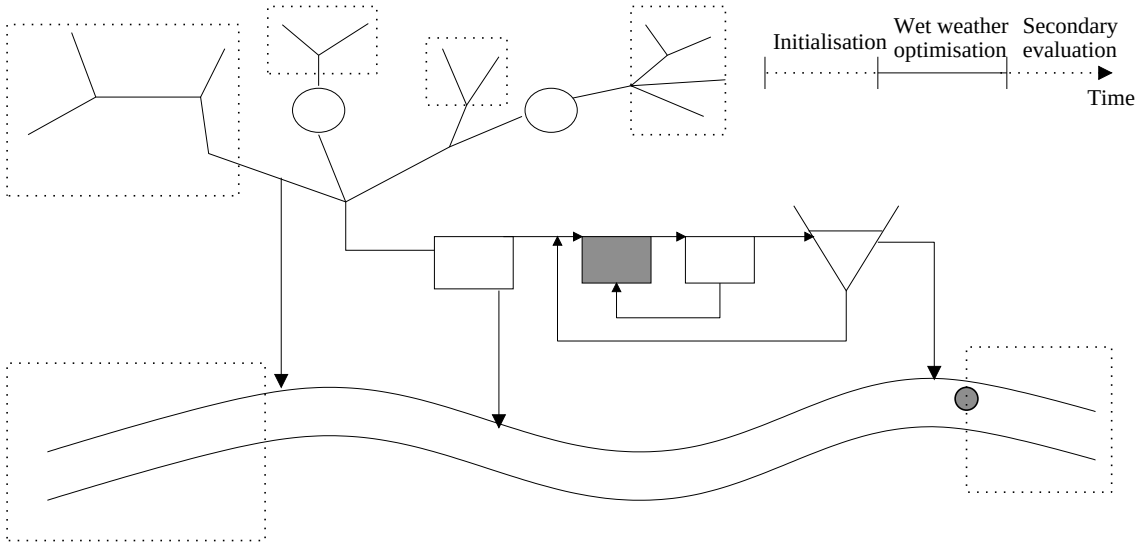


Figure 4.3: The model of the integrated urban wastewater system with location of the sensors (closed circles) and control action (large open circles). The parts that can be eliminated to construct the control model are indicated with dashed boxes.

back into that part anymore during the remainder of the simulation (which could e.g. be the case when a storm tank gets emptied too fast).

The different steps of these model reductions are conceptually presented in Fig. 4.3. The upstream parts of the sewer system may be eliminated since the control actions under study can never influence the behaviour of those parts. The upstream river part may be eliminated since no input influenced by the control strategy enters this part of the river. The part of the river downstream of the last sensor may be eliminated since the control actions will not be affected by what happens there. Further on, conversion processes might be left out of the river control model, in case they do not influence the control actions. The time during which the wet weather optimisation will be performed depends on situations during which the controller is active. While the initialisation period is relatively easy to determine, the secondary objective evaluation period (see section 4.3.2) is more complicated, as discussed above.

4.3.2 Secondary objective evaluation

Any optimisation study in environmental management is multi-criteria in nature, i.e. one has to take more than one objective into account when evaluating management or control strategies. Here, the objective(s) used as direct input to the controller is (are) termed the primary objective(s). These are typically the on-line measurements of the water quality variables that one wants to improve in a feedback control way. If these variables become critical, the controller starts to act in order to try and improve this measured variable. The secondary objectives, on the other hand, are all other objectives one is interested in, but which do not influence the controller. These might be unmeasured water quality variables, but also operating costs or operator acceptability (e.g. related to the complexity of the control system). With increasing stake holder involvement even public acceptability

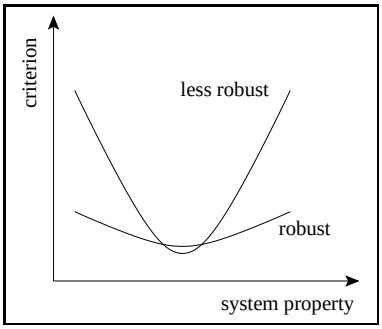


Figure 4.4: Criterion values for a robust and a less robust strategy

might become an issue. Also the robustness of the controller is an important secondary objective.

Here, robustness is a measure of how well a controller works in situations which are different from those it was tuned for. When evaluating a control strategy, it would be of great interest to have a criterion that can indicate the range of application of the studied control strategy. In other words, it would be useful to have a measure of the sensitivity of the tuned strategy towards some system parameters. Vanrolleghem and Gillot (2002) proposed a global sensitivity analysis in which parameters that are uncertain or variable are evaluated. The relative sensitivity of the evaluated control strategies towards a system change for a given water quality criterion is calculated as follows (Vanrolleghem and Gillot, 2002):

$$S_i = \frac{\partial CriterionValue}{\partial \theta_i} \cdot \frac{\Delta \theta_i}{CriterionValue}$$

in which $\Delta\theta$ represents the range over which one can expect a parameter to vary in the given system (Rousseau *et al.*, 2001). The robustness index (RI) for a certain criterion summarises the sensitivities towards different disturbances:

$$RI = 1 \Big/ \sqrt{\frac{1}{p}\sum_{i=1}^{p} S_i^2}$$

If RI is maximised, the control strategy will perform more or less similarly in different conditions. This is illustrated in Fig. 4.4, where the criterion values of two control strategies are shown. For the control strategy that is less robust, the criterion value increases when the system properties change. For the robust control strategy, the criterion value is more stable for different system properties. Even if the minimum value is lower for the less robust strategy, the robust strategy is still preferred since it will perform better in other situations.

The tuning of a control strategy focuses on reaching the primary objective, for instance minimise the peak ammonia concentration. Obviously, the actions generated by the control strategy also have an influence on the secondary objectives. It is therefore important to verify that the defined and tuned strategy, while improving on the primary objective, is not making things (a lot) worse on the secondary objectives. If the control strategy requires the addition of chemicals in the treatment plant, costs will have to be looked at.

If, in another case, a storm tank needs to be built in a residential area, public acceptability might be a problem.

By evaluating the performance of the control strategies with respect to the secondary objectives, the full effect of the control strategy on the river system (in its broad sense) is verified, and some proposed control strategies might be rejected completely on the basis of the results of this secondary objective evaluation. Less severe than a complete rejection, the results obtained with the full model may also suggest a further optimisation of the control strategy's characteristics (set points, tuning parameters) due to the simplifications made in the control model. The advantage is of course that these characteristics have already been given values that are probably close to the optimum for the complete model.

Compared with other authors (Rauch and Harremoës, 1999; Schütze *et al.*, 1999), the approach presented in this work is based on the combination of complex and simplified models, while truly integrated control becomes possible due to the implementation of the simplified and reduced model within a single software package, WEST® Hence, information about the state of the river can be used within the controllers acting on the sewer system and treatment plant.

4.4 Connecting models with different state variables

When creating a model base for the integrated urban wastewater system, different types of models are used, with different state variables, and different concepts. In order to be able to create an integrated model, the different models need to be connected. As Fronteau *et al.* (1997) showed, this is not a straightforward task and needs to be carefully handled in order to obtain reasonable results. This connection may be easily done in some cases, in other cases a more theoretical concept might be necessary to obtain good results.

4.4.1 Elemental balances

Elemental and charge balances are one of the basic concepts of the ASM3(C) (Henze *et al.*, 2000) (see also section 2.3.4) and the RWQM1 (Reichert *et al.*, 2001b). An elemental balance is kept when during any conversion reaction, the number of moles of the element is the same at the left side and the right side of the reaction. The concept used in this work is based on mass and elemental balances. The basic idea about the connection between two types of models is that no mass should be lost or created. This mass can be expressed in terms of COD, but also in terms of elemental masses of carbon, nitrogen, oxygen, hydrogen, phosphorus and charge. A basic requirement for this to be calculated is that the chemical compositions of every state variable are known. In the RWQM1, the state variables describing organic matter are composed of 5 elements: carbon (C), oxygen (O), nitrogen (N), hydrogen (H), and phosphorus (P). Furthermore, these elemental compositions are assumed to be constant in time for each model application. The mass fractions for organic matter are denoted as $\alpha_C, \alpha_H, \alpha_O, \alpha_N, \alpha_P$ for C, H, O, N and P, where a mass fraction represents the fraction of the total mass of organic substance contributed by a particular chemical element. All other elements are put together in α_X, which is in

the framework of this explanation put to zero. Hence, the sum of the other mass fractions is equal to one:

$$\alpha_C + \alpha_H + \alpha_O + \alpha_N + \alpha_P = 1 \tag{4.1}$$

The chemical formula of organic matter may be written as follows (for 1 g of organic matter):

$$C_{\alpha_C/12} H_{\alpha_H} O_{\alpha_O/16} N_{\alpha_N/14} P_{\alpha_P/31} \tag{4.2}$$

Using the conservation principles for the five elements and for charge, the mineralisation process might be written as:

$$C_{\alpha_C/12} H_{\alpha_H} O_{\alpha_O/16} N_{\alpha_N/14} P_{\alpha_P/31} + \left(\frac{\alpha_C}{12} + \frac{\alpha_H}{4} - \frac{\alpha_O}{32} - \frac{3\alpha_N}{56} + \frac{5\alpha_P}{124}\right) O_2 + \left(\frac{\alpha_N}{14} - \frac{2\alpha_P}{31}\right) H^+ \rightarrow \left(\frac{\alpha_H}{2} - \frac{3\alpha_N}{28} - \frac{3\alpha_P}{62}\right) H_2O + \frac{\alpha_C}{12} CO_2 + \frac{\alpha_N}{14} NH_4^+ + \frac{\alpha_P}{31} HPO_4^{2-} \tag{4.3}$$

From this formula, the relationship between the mass of organic matter and COD can be deducted as follows:

$$COD = 32 \left(\frac{\alpha_C}{12} + \frac{\alpha_H}{4} - \frac{\alpha_O}{32} - \frac{3\alpha_N}{56} + \frac{5\alpha_P}{32}\right) OM \tag{4.4}$$

The mass fractions of N and P per unit of COD, which are usually used as parameters in the activated sludge models, are then given as:

$$i_N = \frac{\alpha_N}{32 \left(\frac{\alpha_C}{12} + \frac{\alpha_H}{4} - \frac{\alpha_O}{32} - \frac{3\alpha_N}{56} + \frac{5\alpha_P}{32}\right)} \tag{4.5}$$

$$i_P = \frac{\alpha_P}{32 \left(\frac{\alpha_C}{12} + \frac{\alpha_H}{4} - \frac{\alpha_O}{32} - \frac{3\alpha_N}{56} + \frac{5\alpha_P}{32}\right)} \tag{4.6}$$

In this way, the relationship between the traditionally COD based ASM-models and the new mass fraction based RWQM1 can be easily made. These relationships will be extensively used when creating a connector model between the ASM1 and RWQM1.

These elemental balances are found important as they impose a rigid check on model equations and implementations. Six extra equations (5 elemental balances and a charge balance) can be used in the construction of the stoichiometric matrix. The elemental balance for every process and every element considered can be written as:

$$\sum_i \nu_{ji} \cdot i_{k,i} = 0 \qquad \forall \text{ components } i \tag{4.7}$$

where

ν_{ji} stoichiometric coefficient for component i in process j
$i_{k,i}$ Element from the composition matrix of component i for element k ($k \in \{C, N, O, H, P, charge\}$)

In this way, six equations may be constructed, and six elements in the stoichiometry matrix may be calculated from these balances.

Moreover, mass balances are one of the basic principles in all types of models, and it is hence important to adhere to these principles. This can also be seen from the evolution of the ASM-models, where the ASM2 and ASM3 models have closed mass balances as well (Henze *et al.*, 2000). Another advantage is that the measurement of Total Organic Carbon (TOC), can easily be incorporated in the data used for model calibration, which is probably not always the case when using ASM1 or ASM2(d).

4.4.2 Connecting ASM1 and RWQM1

The principles of mass conservation are also useful when defining a connector model between different subsystems. As an example, a connector will be developed between the state variables of the ASM1-model and the RWQM1-model. This connector has the advantage that both models are COD based, which makes the conversion between a WWTP-model and a river model more straightforward than it would have been with the more traditional water quality models which are usually BOD based (Rauch *et al.*, 1998b).

A comparison between the state variables of the two models is given in Table 4.1. A small *riv* is added to the states of the river model, to be able to easily distinguish between the components of the two models in the later discussion. The table shows that some state variables are the same in the two models. Some others, like S_{NO} are split into two variables in the RWQM1-model. A third category can be found in the state variables of the ASM1 which are not present in the RWQM1, like S_{ND}, but are implicitly present in the organic material. The fourth category includes the new variables of the RWQM1, which are not present in the ASM1. It is clear that these different classes will be important when developing a connector between these two models.

As a starting point for the mass conservation laws, the conversion of COD is discussed. The soluble COD (both the degradable and the inert fractions) are considered to remain unchanged in passing from the ASM1-model to the RWQM1-model. The particulate COD is a bit more complex due to the different conditions in WWTPs and receiving water. The slowly biodegradable substrate (X_S) and the inert particulate COD (X_I) will probably also keep their properties in the receiving water. Since X_P is not present in the RWQM1 it is added to the $rivX_I$, since the properties of these two substances are the same in the two models.

The conversion of the bacteria is less straightforward. Due to the different conditions in the WWTP and the river, it might be that part of the heterotrophic biomass, which was active in the treatment plant, becomes inactive in the river, due to a lack of substrates for example. Let the fraction of the heterotrophic biomass that remains active in the river be f_H. The part that becomes inactive, can be further divided in an inert (f_I) and a biodegradable part ($1 - f_I$).

The same reasoning can be applied to the autotrophic biomass, with one difference, i.e. the active biomass is split into the two groups of nitrifying bacteria of the RWQM1. Let

Table 4.1: Comparison of the state variables of the ASM1 and the RWQM1

ASM1		RWQM1	
S_S	Easily degradable org. material	$rivS_S$	Dissolved org. substances
S_I	Inert soluble org. material	$rivS_I$	Inert dissolved org. substances
S_O	Dissolved oxygen	$rivS_O$	Dissolved oxygen
X_I	Inert particulate org. material	$rivX_I$	Inert particulate org. material
X_S	Slowly biodegradable org. material	$rivX_S$	Particulate org. material
X_{BH}	Heterotrophic biomass	$rivX_H$	Heterotrophic organisms
S_{NO}	Nitrite and nitrate nitrogen	$rivS_{NO2}$	Nitrite-nitrogen
		$rivS_{NO3}$	Nitrate-nitrogen
S_{NH}	Ammonia and ammonium nitrogen	$rivS_{NH3}$	Ammonia nitrogen
		$rivS_{NH4}$	Ammonium nitrogen
S_{ALK}	Alkalinity	$rivS_{CO2}$	Sum of carbon dioxide and H_2CO_3
		$rivS_{HCO3}$	Bicarbonate
		$rivS_{CO3}$	Dissolved CO_3^{2-}
		$rivS_H$	Hydrogen ions
		$rivS_{OH}$	OH^- ions
X_{BA}	Autotrophic biomass	$rivX_{N1}$	Organisms oxidising ammonia to nitrite
		$rivX_{N2}$	Organisms oxidising nitrite to nitrate
S_{ND}	Dissolved org. nitrogen	-	not present
X_P	Inert partic. from biomass decay	-	not present
X_{ND}	Particulate org. nitrogen	-	not present
-	not present	$rivS_{HPO4}$	Inorg. dissolved phosphate: HPO_4^{2-}
-	not present	$rivS_{H2PO4}$	Inorg. dissolved phosphate: $H_2PO_4^-$
-	not present	$rivS_{Ca}$	Dissolved Ca^{2+} ions
-	not present	$rivX_{ALG}$	Algae and macrophytes
-	not present	$rivX_{CON}$	Consumers
-	not present	$rivX_P$	Phosphate adsorbed to particles
-	not present	$rivX_{II}$	Particulate inorg. material

f_{N1} be the fraction of X_{BA} that becomes $rivX_{N1}$, while f_{N2} is the fraction of X_{BA} that is considered to be $rivX_{N2}$. It is clear that $f_{N1} + f_{N2} \leq 1$. In most cases, f_{N1} will be larger than f_{N2} since the yield of the first step nitrifiers ($rivX_{N1}$) is larger than the yield for the second step nitrifiers ($rivX_{N2}$). According to Focht and Verstraete (1977), the ratio is about 3. The remaining fraction of X_{BA} is again divided between $rivX_S$ and $rivX_I$. A schematic overview of the divisions of the particulate COD is given in Fig. 4.5.

Some parameters have to be known in order to complete the mass balances for this connector. The pH is needed to convert the alkalinity to the different molecules adding to the total alkalinity in the river model.

$$[ALK] = [HCO_3^-] + 2[CO_3^{2-}] + [OH^-] - [H^+] \tag{4.8}$$

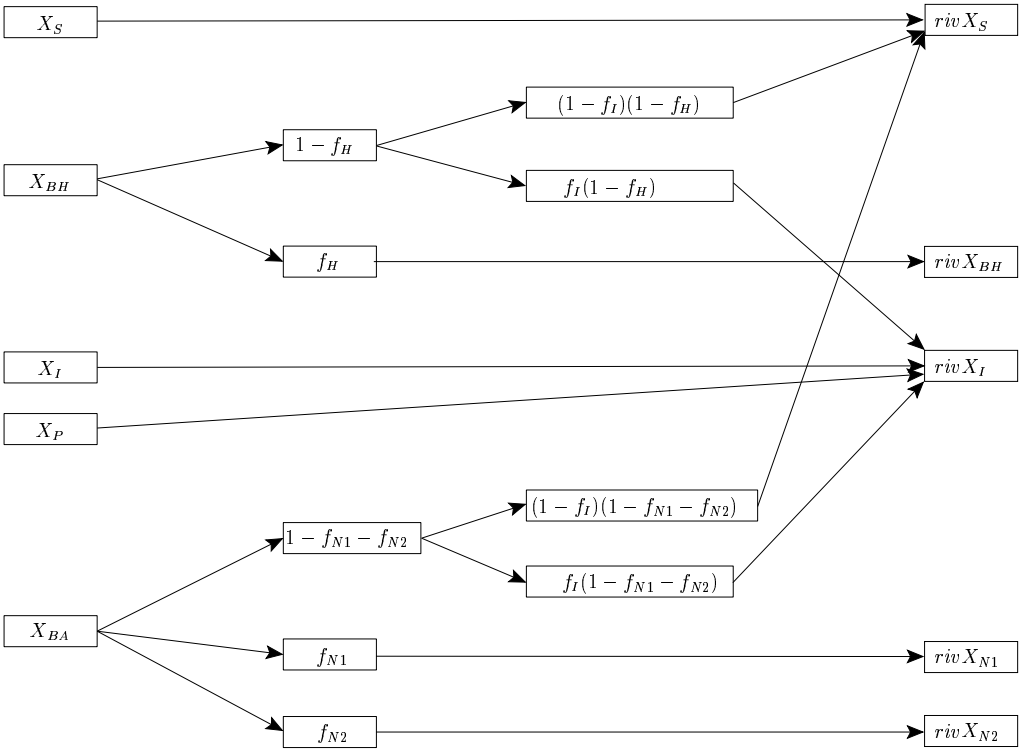


Figure 4.5: Fate of the particulate COD when passing from the WWTP to the receiving water

Together with the dissociation constant of water, k_w, and the two dissociation constants of carbonic acid, k_{a1} and k_{a2}, the concentration of the different molecules can be found if the pH is known. For example, the relation between the pH, ka1, ka2 and the concentration of carbonic acid, bicarbonate and carbonate can be written as:

$$k_{a1} = \frac{[H^+][HCO_3^-]}{[H_2CO_3]} \tag{4.9}$$

$$k_{a2} = \frac{[H^+][CO_3^{2-}]}{[HCO_3^-]} \tag{4.10}$$

$$k_w = [H^+][OH^-] \tag{4.11}$$

$$pH = -\log_{10}([H+]) \tag{4.12}$$

Equations 4.8 to 4.12 form a set of equations that can be solved. It is, starting from the above equations, possible to calculate the concentrations of the different components of the RWQM1.

The pH is also necessary to calculate the equilibrium between ammonia ($rivS_{NH3}$) and ammonium ($rivS_{NH4}$) in the river, given a total concentration S_{NH4} and the dissociation constant. The same can be done for the equilibrium between $rivS_{HPO4}$ and $rivS_{H2PO4}$, but the total inorganic phosphorus concentration is a given parameter, rather than a state variable of the ASM1. It is clear that this will be different when developing a connector between the ASM2(d) and the RWQM1, since in the ASM2(d) soluble phosphorus is present as a state variable.

Table 4.2: The parameters needed for the connector between the ASM1 and the RWQM1

f_H	fraction of heterotrophs that remains active in the river
f_{N1}	fraction of first step nitrifiers that remains active in the river
f_{N2}	fraction of second step nitrifiers that remains active in the river
f_I	fraction of the inactive biomass that becomes inert
pH	the pH of the effluent
$rivS_{NO2}, in$	the nitrite concentration in the effluent
$rivS_{HPO4}, in + rivS_{H2PO4}, in$	the dissolved inorganic phosphorus concentration
$rivX_{ALG}, in$	the algae concentration in the effluent
$rivX_{CON}, in$	the consumer concentration in the effluent
$rivX_P, in$	the concentration of phosphate attached to particles
$rivX_{II}$	the particulate inorganic material concentration in the effluent

Another parameter which is necessary for this connector is the nitrite or nitrate concentration, in order to distinguish between these two forms of oxidised nitrogen in the RWQM1. Currently, the nitrite concentration in the effluent from the WWTP is modelled as a fixed parameter ($rivS_{NO2}, in$). The nitrate concentration is calculated as the difference between S_{NO} and $rivS_{NO2}, in$. Furthermore, the concentrations of algae, consumers, phosphate attached to particles and particulate inorganic material are other parameters of the connector. An overview of the parameters needed for the connector model is given in Table 4.2.

In order to close elemental balances it is necessary that the elemental compositions of all the states of the ASM1 are known. Although this introduces a lot of unknown parameters that are difficult to determine, this principle is found more and more important (Reichert *et al.*, 2001b) and is hence used in this concept. For the elemental balances to hold, the sum of the elements in the ASM1 must be equal to the sum of the elements in the RWQM1:

$$\forall j \in \{C,H,O,N,P\}: \qquad \sum_{k}^{ASM1} i_{j,k}(S,X)_k = \sum_{k}^{RWQM1} i_{j,k}(rivS,rivX)_k \tag{4.13}$$

where

$(S,X)_k$ all the states of the ASM1 in g COD/m^3
$(rivS,rivX)_k$ all the states of the RWQM1 in g COD/m^3
$i_{j,k}$ fraction of element j in state k in g j/g COD k

If the compositions of the different organic states are not chosen in a special way, this balance will not hold automatically. This is due to the fact that some, for example, autotrophs are transformed into $rivX_S$, which has not the same elemental composition as X_{BA}. In this conversion step, some elements might be released, while others are taken up. Therefore, correction terms are introduced to compensate for the difference in mass of a certain element when the other equations are applied. The correction terms are chosen to be the inorganic representatives of the different elements. These are $rivS_{CO2} + rivS_{HCO3} + rivS_{CO3}$ for carbon, $rivS_O$ for oxygen, $rivS_H$ for hydrogen, $rivS_{NH4} + rivS_{NH3}$ for nitrogen and $rivS_{HPO4} + rivS_{H2PO4}$ for phosphorus.

The way to fulfil the correction in equation 4.13 is to write the resulting concentration of these correction terms at the side of the RWQM1 as:

$$correction\,term = \sum_{k}^{ASM1} i_{j,k}(S,X)_k - \sum_{k}^{RWQM1/correction} i_{j,k}(rivS,rivX)_k \tag{4.14}$$

where the sum of the RWQM1 states is made except for the balancing state. For the nitrogen balance this expands to:

$$\begin{aligned} rivS_{NH4} + rivS_{NH3} = & \sum_{k}^{ASM1} i_{N,k}(S,X)_k \\ & - \sum_{k}^{RWQM1/rivS_{NH4}+rivS_{NH3}} i_{N,k}(rivS,rivX)_k \end{aligned} \tag{4.15}$$

or more explicitly:

$$\begin{aligned} rivS_{NH4} + rivS_{NH3} = & S_{NH} + i_{N,S_S}S_S + S_{ND} \\ & + i_{N,S_I}S_I + i_{N,X_S}X_S + i_{N,X_I}X_I + X_{ND} \\ & + i_{N,X_{BH}}X_{BH} + i_{N,X_BA}X_{BA} + i_{N,X_P}X_P \\ & - i_{N,rivS_S}rivS_S - i_{N,rivS_I}rivS_I \\ & - i_{N,rivX_H}rivX_H - i_{N,rivX_{N1}}rivX_{N1} \\ & - i_{N,rivX_{N2}}rivX_{N2} - i_{N,rivX_{ALG}}rivX_{ALG} - i_{N,rivX_{CON}}rivX_{CON} \\ & - i_{N,rivX_S}rivX_S - i_{N,rivX_I}rivX_I \end{aligned} \tag{4.16}$$

It should be born in mind that in the ASM1, different components have no nitrogen associated with them, like S_I, S_S, X_I and X_S. It should therefore be noted that the different $i_{N,k}$ terms are zero by default, but can be changed when experimental data show that the assumptions of the ASM1 are not valid. It can be noted that the concentration of $rivS_{NH4} + rivS_{NH3}$ is equal to the sum of all nitrogen coming from the ASM1 – the nitrogen present in the other terms of the RWQM1. Similar equations can be written down for the other balance terms. There is some risk of the balance terms becoming negative if the elemental compositions of the different state variables are not chosen properly. During simulation, this situation should be accounted for, while the user is getting a warning that something was wrong in balancing some elements. This is also an extra check to find errors in e.g. parameter values or model implementations.

In this part, the development of a connector model between state variables of the ASM1 and the RWQM1 has been outlined. After an introduction about elemental balances, the state variables of the two models are compared. It was explained how the corresponding states were connected to each other, using a general understanding of the system behaviour at the boundaries, together with elemental balances. In this way, both a logical and consistent connector model has been created, which can be easily extended or used for other types of models, (e.g. connecting an ASM2d model with a simplified version of the RWQM1).

4.5 Conclusions

Modelling the integrated urban wastewater for design and optimisation of control strategies, is focused on delivering a relatively fast control model. Two approaches to gain calculation time were outlined and illustrated in this paper. First, the use of mechanistic surrogate models is suggested to be a promising approach to replace the complex equations with simplified ones, e.g. replace the partial differential equations of "de Saint-Venant" with a tanks-in-series model. A new procedure to build and calibrate surrogate models with the aid of complex models has been outlined. This procedure solves the problem of the amount of field data required to calibrate simplified surrogate models. Indeed, a calibrated complex mechanistic model is used to generate virtual data, which are subsequently used to calibrate a fast surrogate model. The surrogate model used in this study can predict the hydraulic behaviour, is easier to implement and can be used in combination with a biological conversion model. Hence, the use of surrogate models within optimisation problems seems to be promising.

Second, model reduction through boundary relocation has been introduced. By relocating the upstream and downstream system boundaries, parts of the model can be left out when tuning the control strategies. The parts upstream of the first controlled actuator and downstream of the last measurement point can be left out. Further, if the controller under study is not influencing the states of the model in some periods, these periods might be left out of the optimisation study. Moreover, when carefully looking at the time period under study, some further reductions (e.g. of certain conversion processes) might be possible as well.

After tuning the controllers for the primary objectives with the control model, the effect of the control strategies on the secondary objectives of the system under study must be checked in order to be more confident about the performance of the controllers. Based on these secondary objective evaluation simulations, the control strategy can be adopted, adapted or even rejected. Next to the secondary objectives, the robustness of the proposed controller should be checked. In this way a measure of the performance of the controller in different conditions is obtained and can be used in judging the controller.

In a last paragraph, a concept of connecting models with different components to each other is developed. A consistent approach based on mass and elemental balances is proposed. As an example, the connection between the ASM1 and the RWQM1 model was elaborated.

Chapter 5

Simplification and reduction of WWTP models

5.1 Simplification of the ASM2d model

As outlined in the previous chapter, simulation time might slow down the optimisation of control strategies. To dynamically model activated sludge systems, a lot of differential equations are used, which may lead to a relatively slow calculation, especially in optimisation studies (parameter estimation or control tuning), as well as in quantifying uncertainties (Bixio *et al.*, 2001a). Two techniques are used in this chapter: replacing the ASM models by neural networks and knowledge based reduction of these ASM models. The knowledge based reduction focuses on elimination of equations that are of no or minor influence to the simulation results of the components of interest.

Before trying neural networks on the complete ASM2d model, the possibilities of these techniques were tested on a simple model. If successful for a simple example, the complete ASM2d model could be tackled.

5.2 Neural networks and ASM2d

There already exists some literature on the use of artificial neural networks in combination with activated sludge models. Côté *et al.* (1995) use neural networks to improve the predictions made by the ASM1 model. This means that a neural network is trained in parallel with the ASM1 and learns to compensate for the mismatches between the data and the full model predictions. It is clear that such an approach will improve predictions but won't improve calculation time because the full model is still used. Hence, it is not really relevant for the task at hand.

Another approach used by Zhao and McAvoy (1996) is to compensate the lack of dynamic data by using a neural network. In this work, the ASM1 model is calibrated on steady state data, without accounting for the influence of pH, temperature and MLSS. These three parameters are used as input for the ANN model together with the influent and previous

errors. Again the ANN learns to compensate for errors introduced by the ASM1. This is interesting because fewer data are needed to fully calibrate the ASM1, but it is an approach that cannot be used in this study, since there is no reduced simulation time. On the contrary, the implementation and calculation of the ANN will even increase the simulation time.

An interesting approach was followed by Zhao *et al.* (1999, 1997). In these papers the authors use a simplified mechanistic model to describe the removal of phosphorus from a sequencing batch reactor. The simplified model contains only five states and six processes, which is an important reduction compared to the 19 states and 21 processes of the full ASM2d model. This simple model can be calibrated on data of one batch experiment but does not have any extrapolation capacities. Consequently, the simulation of other experiments, which were not used for calibration, is not possible. In order to overcome these problems, this simplified model is run in parallel with a neural network which is trained on the errors between the simplified and full ASM2d model. The MLSS, temperature and pH are added to the ANN inputs in order to extend the extrapolation capacities to other experiments with different MLSS or pH. The need for the MLSS as an input to the neural network is no problem when using this hybrid model (simplified + ANN) for batch experiments where the MLSS can be measured. However, this requirement makes this technique not suited for the long-term prediction of a wastewater treatment plant behaviour because no data on the MLSS are available.

Recently, Lee *et al.* (2002) described the hybrid neural network modelling of a full-scale industrial WWTP. Four different types of models were compared: a simplified mechanistic model based on the ASM1 (Henze *et al.*, 2000) with adaptations for cyanide toxicity. The second model was a neural network model, which was trained with 8 input nodes and 5 hidden nodes. The third model was a serial hybrid neural network model, where the neural network was used to estimate the parameters of the mechanistic model. The fourth model was a parallel hybrid neural model. In this case the neural network was trained to compensate for the errors made by the mechanistic model. The authors conclude that the parallel hybrid neural model gives the best results.

Smets *et al.* (2001) have rewritten the ASM model into a state space format with linear approximation of the non-linear kinetic terms. The state space was split into different parts, for each of which the parameters of the linear time invariant model have to be identified. The data generated with the full ASM model are used to identify the unknown linear terms. In order to limit the amount of identifications to be performed, an interpolation method was introduced. With this interpolation, only the the parameters at the corners of the state space need to be identified, while for the intermediate classes an interpolation of the parameters of the corners results in sufficiently accurate predictions compared to the complete ASM1 model.

5.3 Neural network for bioconversion prediction

5.3.1 Modelling approach: grey box models

The approach followed uses “grey box” models (Van Can, 1997). In this approach physical laws (like conservation of mass) are built in the model (“white box knowledge”). Other

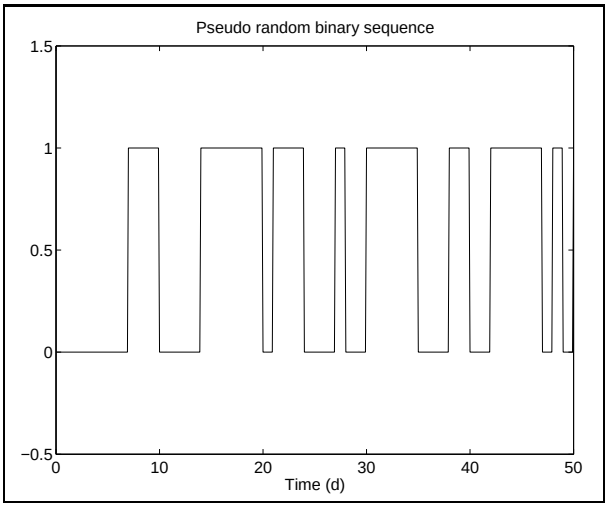


Figure 5.1: The signal of the PRBS sequence

relationships are modelled with a data based approach ("black-box") by means of neural networks. In this way, the advantages of both deterministic modelling and modelling by neural networks are combined.

The aim of the model was to create a simple grey model structure. The mass balance of this grey box model is

$$\frac{dM}{dt} = influx - outflux + conversion \tag{5.1}$$

The goal was to describe the conversion with an ANN while keeping the transport terms in the mass balance as a white box part. This part is well-known because it is related to the discharges, which are known accurately. In the conversion there are a lot of unknown or badly known parameters and therefore this term is not fully based on mechanistic knowledge anyway. Moreover, the conversion term is the most complicated part, asking for most calculations.

A neural network needs to be trained, which requires a large training data set. The deterministic model was used to generate this set. In order to have a sufficient coverage of the state space, a special influent data file was used. The influent was generated with the aid of pseudo random binary sequences (PRBS). This PRBS gives a signal that switches between two values (0 and 1). The time of switching is randomly chosen and the result has a uniform frequency distribution (Fig. 5.1).

In reality the input data of a treatment plant never changes between zero and a certain maximum number, but the changing frequency of this PRBS is suited for training a neural network. In order to obtain a more realistic influent sequence, this PRBS was used to trigger a random number selection. A random number is selected, but the time of changing to another value is determined by the PRBS. In this way two ways of randomisation are obtained: the value and the length that each value is kept constant (Fig. 5.2).

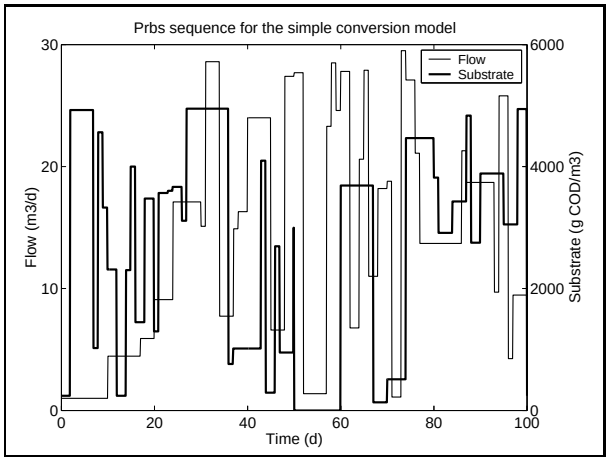


Figure 5.2: The PRBS transformed to an influent for the biological conversion reactor

5.3.2 Training a simple biological conversion model

The training of the neural network started with a case study of a simple "one biomass - one substrate" reactor model. The following equations were used:

$$\frac{dX}{dt} = -\frac{Q_{in}}{V}X + \mu_{\max}\frac{S}{K+S}X - bX \tag{5.2}$$

$$\frac{dS}{dt} = \frac{Q_{in}}{V}(S_{in} - S) - \frac{\mu_{\max}}{Y}\frac{S}{K+S}X \tag{5.3}$$

with the following values for the parameters:

Y Yield, 0.67 (g biomass/ g substrate)
μ_{max} Maximum growth rate, 4 (d^{-1})
K Affinity constant, 20 (g/m^3)
b decay constant, 0.4 (d^{-1})
V volume of the reactor, 10 (m^3);

The incoming discharge varied between 1 and 30 m^3/d, while the influent substrate concentration fluctuated between 0 and 5000 g/m^3, no biomass was present in the influent. These high substrate concentrations were used to excitate the ANN model during the training phase. The influent training set was created with the aid of 2 PRBS sequences (Fig. 5.2).

Only two processes take place in this reactor, growth of biomass with consumption of substrate and decay of the biomass.

The training set is formed by running a dynamic simulation with this model. The output file contained the influent discharge and substrate concentration, the concentration of biomass and substrate in the reactor and the conversion rates of both substances every 15 minutes. Because of possible variations of the conversion rates within one time step, the theoretical average conversion rates for each time step were calculated as:

$$conv(X(t)) = \frac{X(t+1) - X(t)}{\Delta t} + Q_{in}(t)X(t) \tag{5.4}$$

This is the conversion rate on time t that gives the observed biomass concentration on time $t+1$ when using an Euler integration algorithm. The neural network was trained to predict these theoretical conversion rates, i.e. the network predicts the conversion rates and compensates the errors introduced by using a larger time step. When using a neural network to solve part of the differential equations it is necessary to use a fixed step algorithm, because the network predicts in the same time steps as the data used for training it.

Using the neural network toolbox of Matlab™(version 5.3) a feedforward neural network was created and trained with the previous output file.

The input of a neuron can be written as:

$$\text{input}(\textit{neuron}\,j) = \Sigma(w_{ij} * u_i) + b_j \tag{5.5}$$

and output of a neuron can be written as:

$$\text{output}(\textit{neuron}\,j) = f(\text{input}(\textit{neuron}\,j)) = f(\Sigma(w_{ij} * u_i) + b_j) \tag{5.6}$$

where

b_j Bias of neuron j
f The activation function of the neuron
u_i Input i
w_{ij} The weight of neuron i on hidden neuron j

Different training algorithms (trainlm, trainbr, trainbfg) available in the Matlab toolbox were used, together with different network structures (feedforward and recurrent networks) and different numbers of hidden neurons (1-50). Also the number of previous values that had influence on the network output was varied (from no history influence till 5 time steps back influence), while also different pre- and postprocessing methods (to zero mean and standard deviation 1 and to the interval [-1 1]) were used. The network finally used had three hidden neurons and only the previous values of the inputs had an influence on the network output (memory size of 1). The network is shown schematically in Fig. 5.3. The hidden layer of the network had a *tansig* transfer function, while the output layer had a linear transfer function. A *tansig* function has the following form:

$$tansig(x) = \frac{2}{1+e^{-2x}} - 1 \tag{5.7}$$

which is an S-shaped function which has a left asymptote at -1 and a right asymptote at +1. The linear transfer function just passes through the value, i.e. input = output.

There is an important difference between the way the neural network is used in the training phase and during simulation. This is illustrated in Fig. 5.4 and Fig. 5.5 and explained below.

Fig. 5.4 shows how the training algorithm uses the input data to minimise the error between the desired and produced outputs (dashed box). This is done by comparing the output of the network (conversion rates on each time instance) for a given set of inputs

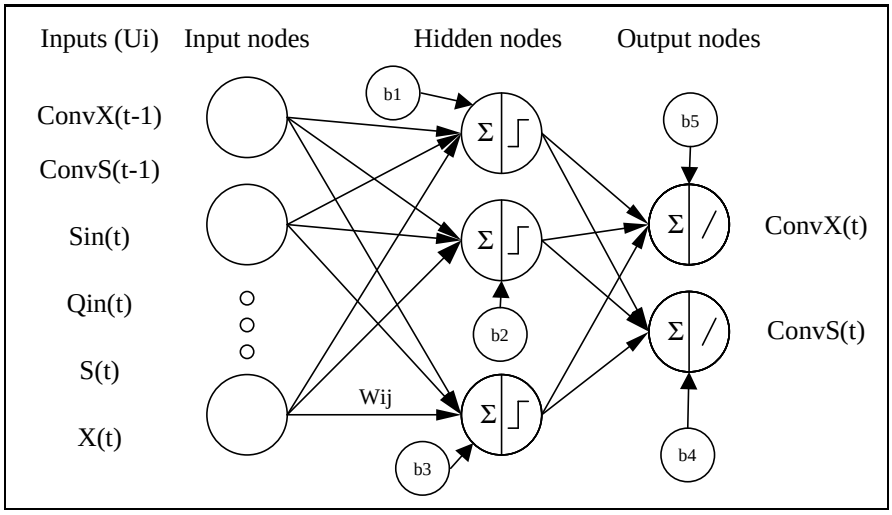


Figure 5.3: Schematic representation of the network used in the simple model (Wij = weight of the i-th input to the j-th hidden neuron, b is the bias of the specific neuron)

with the desired output (theoretical conversion rates). The weights and biases of the network are adapted in order to minimise the difference between the desired and the predicted outputs. The different training algorithms have different rules on how to adapt the weights of the network and are not discussed here in detail, but can be found in the Matlab help files.

After this minimisation, the simulation with the grey box model is done in two steps. First, an input series is fed to the network, creating an output series of conversion rates for each time step. This series of conversion rates is then used by an Euler integration algorithm, leading to a time series of biomass and substrates. The prediction by the network and the integration are independent of each other, while also the prediction of the conversion rate on $(t+1)$ is independent of the prediction of the conversion rate on t.

This is in contrast with the use in simulations where the conversion rate of one time step is used to calculate the substrate and biomass concentration on the next time step. These calculated values are used as input for the neural network on the next time step. This is illustrated in Fig. 5.5. The important difference with the training phase is, hence, that the results of the ANN (both the predicted conversion rates and the predicted concentrations) are used as input for the network.

This difference has an influence on the results of the predictions by the neural network. Fig. 5.6 and Fig. 5.7 show the result of the one step ahead prediction of the conversion rates for biomass and substrate. Fig. 5.8 and Fig. 5.9 show the resulting predicted concentrations of both biomass and substrate. While the biomass is predicted reasonably close, the predicted substrate concentration deviates from the reference. The explanation can be seen in Fig. 5.10, showing that the ANN predictions are close, but have a more or less constant offset. Integrating this offset over a certain time period, leads to the deviating substrate concentration shown in Fig. 5.9.

The simulation results for the long term simulation showed that the network is unstable in modelling the conversion of both substrate and biomass and that the predictions of biomass and substrate concentrations are not acceptable (Fig. 5.11). Notice that in

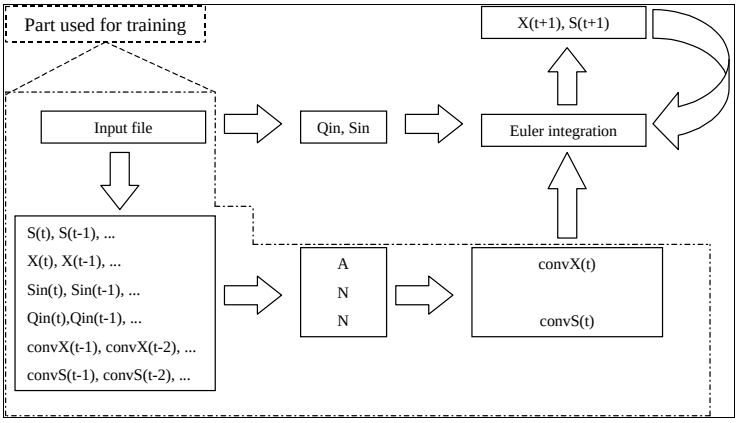


Figure 5.4: Schematic representation of simulation with neural network during training phase (one step ahead prediction)

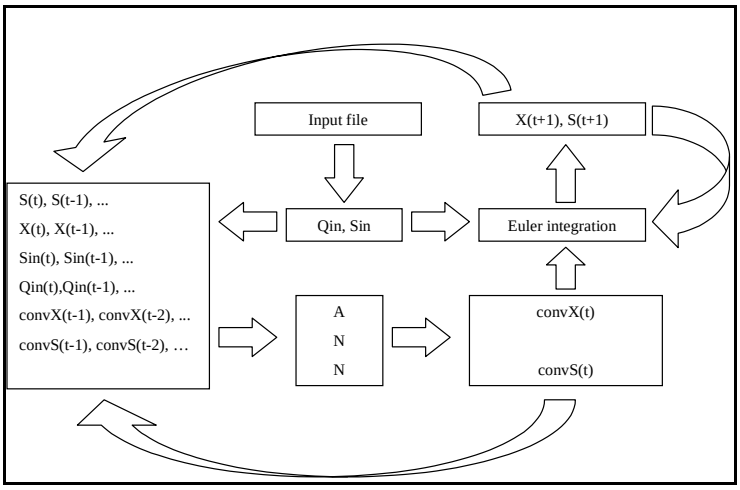


Figure 5.5: Schematic representation of simulation with neural network during validation phase (open loop simulation)

this study already a safety measure against negative values of the state variable after integration was introduced. It consists of replacing this negative value by a very small value if the calculated concentration becomes negative. Otherwise frequent negative concentration would be encountered, which, in addition to being physically impossible, also would bring the inputs of the network outside the range covered during the training phase. However, as Fig. 5.11 shows, the solution used here is far from optimal and only keeps concentrations positive, but not acceptable. The reason why the ANN, during the training phase, was able to reasonably predict the conversion rates and the biomass and substrate concentrations is that the (wrongly) predicted conversion rates were not used in the next time step. Indeed, the ANN is in this case always fed with “correct” inputs.

5.3.3 Conclusions from the simple biological conversion model

One step ahead prediction of the conversion rates was possible with a reasonable accuracy. However, integration of the small error between the predicted and the real conversion rate

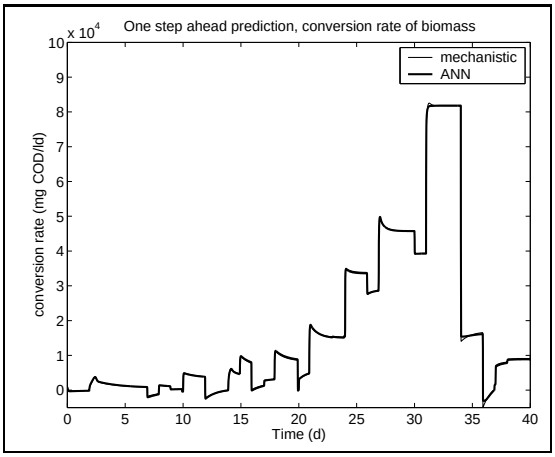


Figure 5.6: One step ahead prediction of the conversion rate of biomass

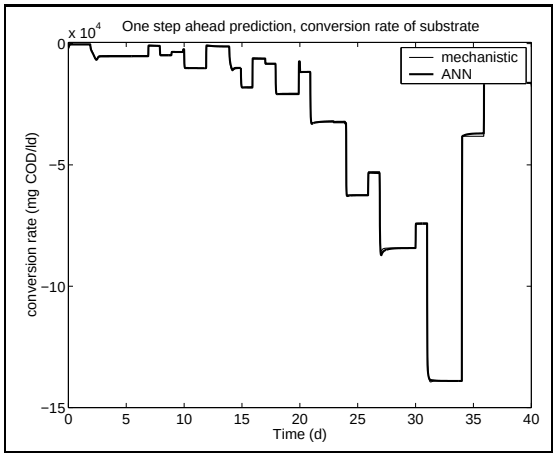


Figure 5.7: One step ahead prediction of the conversion rate of substrate

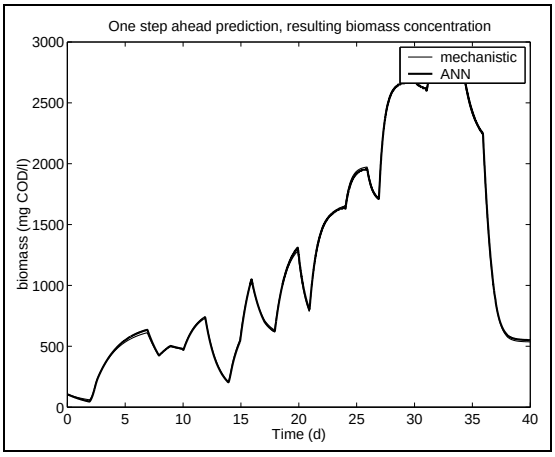


Figure 5.8: One step ahead prediction of the biomass concentration

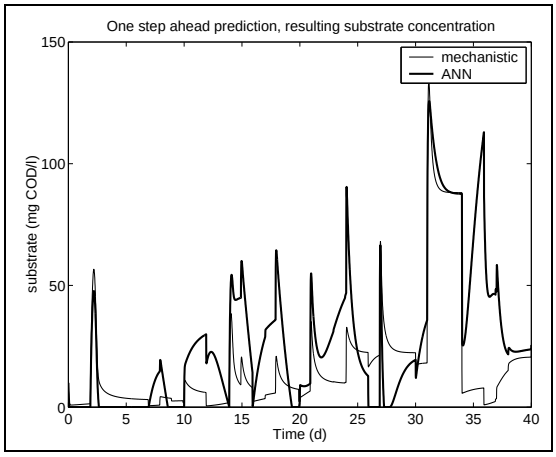


Figure 5.9: One step ahead prediction of the substrate concentration

for more than one step leads to erroneous results.

From the figures it is clear that a network can be trained to predict the conversion rates very closely, though not always perfectly. However, when there is a constant small error between the real and the predicted conversion rate, this results in an ever-increasing difference after integration. The problem encountered in this study is due to the fact that the training algorithms used (like backpropagation) are not suited for elimination of the errors induced by integration. Such errors are not detected during the optimisation of the network, because during optimisation no integration takes place. This is a restriction on the use of existing training algorithms with grey box models as proposed above.

A possible solution to the problem of predicting long time series with neural networks is the backpropagation through time algorithm, which learns by also using the outputs of the model as inputs in the next time step. As this algorithm is not present in the Matlab neural network toolbox used in this study (Matlab version 5.3), it couldn't be used. To solve the problem of the ever-increasing error induced by integration of a constant small error, either the training algorithm should be adapted to deal with this, or alternatively the network input should consist of variables, which are directly predicted by the ANN. This

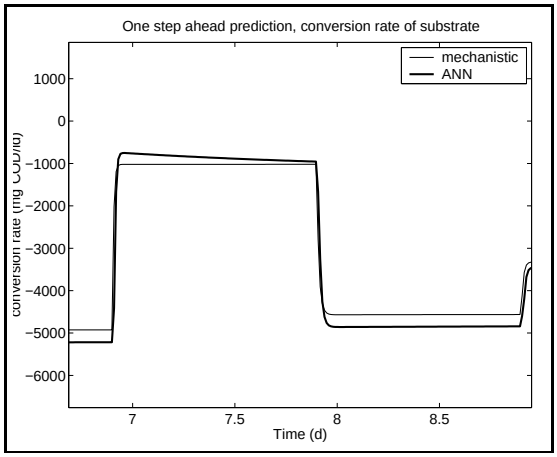


Figure 5.10: One step ahead prediction of the conversion rate of substrate

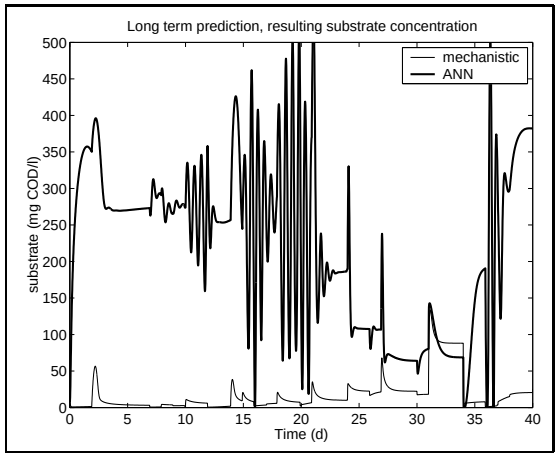


Figure 5.11: Prediction of the substrate concentration during long term simulation

would mean in this case that only Qin, Sin and convX and convS are used as input for the neural network, and no longer make use of the current (predicted) concentrations of substrate and biomass. This last solution does not guarantee in any way a better result after integration. However, it does prevent the error after integration to be fed back into the ANN input. This last option was also tried on the simple case, but the results were not satisfactory either. This seems logical because the current concentration of a state has a very important influence on its conversion rate. Hence, when this information is not available, it is more difficult for the network to extract the relevant information.

5.4 Reduction of mechanistic WWTP models

5.4.1 The Tielt WWTP

The ultimate objective of this part is to create a reduced model of the WWTP of Tielt. The treatment plant of Tielt is an extended aeration plant with biological phosphorus removal. The plant has an anaerobic tank (1000 m^3), two aeration basins (total volume of 5938 m^3), two secondary clarifiers (2152 m^3 each, diameter = 28m) and a storm tank (also 2152 m^3). This WWTP is an activated sludge plant with both biological nitrogen and phosphorus removal.

5.4.2 Implementation of the Tielt model into WEST

The treatment plant has been modelled using the ASM2d model (Henze *et al.*, 2000) for the activated sludge conversion part, while the settling model of Takács *et al.* (1991) was used to describe the behaviour of the clarifier. Intensive measurement campaigns have been carried out to allow the calibration of the most important parameters (Carrette *et al.*, 2001a). The influent fractionation (i.e. the division of the incoming COD in the

Table 5.1: Overview of the models used in the model of the Tielt WWTP

Model block	**Explanation**
Inflow	Input for the incoming wastewater: Q, COD, TKN, S_NO, TP.
denitrification_in	Input for the % denitrification from the input file
b_aut_in	Input for the decay coefficient of the autotrophs from the input file
temp_in	Input for the temperature from the input file
Qwaste_in	Input for the sludge residence time from the input file
Qunderflow_in	Input block that reads the underflow in the settler from the input file
Fraction	Fractionator which splits the influent into the ASM2d components
cfconv	Converter which transforms the influent in concentration/flow to fluxes, used in all the other models
twocomb	Twocombiner which combines the influent with the underflow from the settler
asu1	First activated sludge tank, always anaerobic, Kla is always put to zero
asu2	Second activated sludge tank, intermittently aerated, Kla 120 or 0
asu3	Identical to asu2, but aeration is in opposite phase from the second tank
splitter	Divides the mixed liquor in a waste stream and an inflow to the settler
waste	Block to connect the waste stream
Settler	Secondary settler with controlled underflow, either point or Takács settler
fcconv	Converter, which transforms the overflow of the settler from fluxes to concentrations/flows
Outflow	Output for effluent
denitrification	Pass-through controller, only reads a value from the input file and is linked to the Kla controllers of the second and third tank
Klatank2	Controller, which determines on the basis of the percent denitrification if the aeration is on or not. This tank starts with an anoxic phase
Klatank3	Idem of Klatank2, except that the two hour cycle is started with an aerated period
b_aut_cont	Pass-through controller that controls the b_aut parameter of the ASU models to the value in the input file.
Temp_cont	Idem as the b_aut_cont, except that now the Temp parameter is controlled.
Q_underflowcontrol	Pass-through controller, connects the underflow of the input file with the Q_u parameter of the settler models
Qwastecontrol	Controller determining the amount of waste mixed liquor according to the SRT

states used in the ASM2d model) was the factor most influencing the predicted effluent concentrations. The original model consisted of 11 different submodels.

The general structure of the plant model is shown in Fig. 5.12. An overview of the different submodels is given in Table 5.1.

The activated sludge model consists of three tanks in series, one is completely anaerobic (ASU1), while the other two are intermittently aerated. After the third activated sludge tank, a splitter is installed which controls the sludge-wasting rate. The mixed liquor is passed to the settler the overflow of which goes to the effluent, while its underflow is returned to the entrance of the plant and combined with the influent.

Fractionator

The influent at the treatment plant is analysed on a regular basis for COD, total Kjeldahl nitrogen (TKN), total phosphorus (TP) and total suspended solids (TSS). These influent

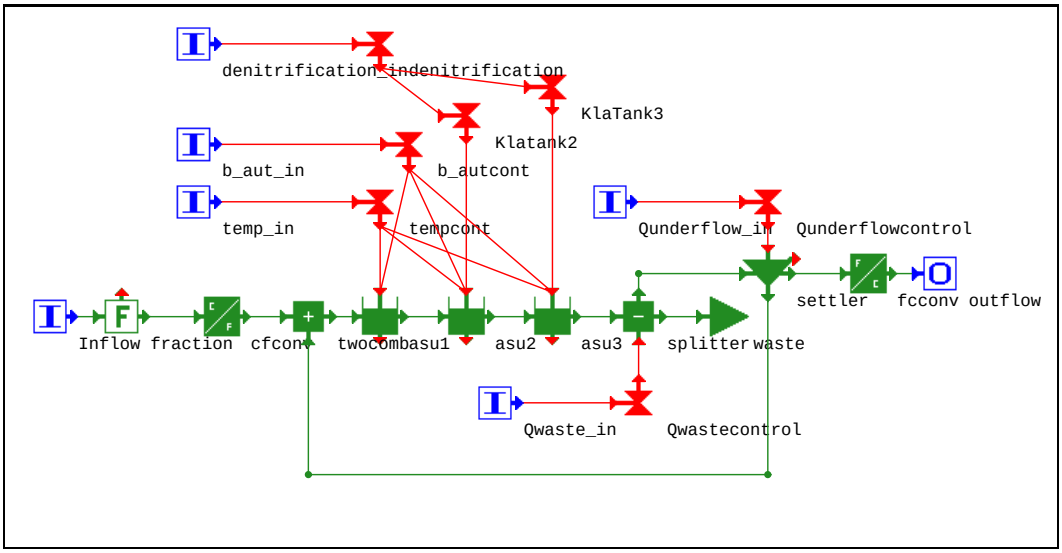


Figure 5.12: Graphical representation of the Tielt WWTP model as implemented in WEST

data cannot be used directly to feed the ASM2d model. Therefore, the so-called influent fractionation has to be determined. The influent fractionation splits the measured variables of the influent into the components of the ASM2d. A procedure to estimate the different fractions of the ASM1 was described in Roeleveld and Kruit (1998).

Several experiments have been carried out to determine the different COD fractions in the influent of the WWTP of Tielt (Carrette *et al.*, 2001a). The total COD is split into the different COD fractions with fixed parts for each COD component present in the ASM2d. Fractions are 0.07 for S_I, 0.04 for S_A, 0.15 for S_F, 0.17 for X_I and 0.57 for X_S respectively. All biomass COD fractions are assumed to be zero. It is clear that this is a simplification, since Krebs *et al.* (1999b) showed that the composition of the wastewater, and hence the different COD fractions vary within a single rain event. In this model, the fractions were kept constant for the whole simulation period, since there was not enough information about the dynamic variations.

The connector was based on the ideas presented in section 4.4. The mass balances were closed for COD, TKN and TP. The COD was divided with fixed fractions that sum to 1, so that the COD-balance is always closed. The soluble ammonia nitrogen and soluble phosphorus were used as correction terms to close these balances. For each of the organic components the nitrogen and phosphorus contents were specified. With these numbers, the soluble ammonium and phosphate is calculated as the total incoming nitrogen or phosphate minus the nitrogen or phosphate present in the COD fractions. If this calculated amount is negative, the output concentration is put to zero. All other outputs (like oxygen and oxidised nitrogen) are fixed to very small values.

Kla-controller

The Kla-controller divides the day in cycles of two hours and compares if the current simulation time is within a certain part of this two-hour cycle. This is done with the $fmod(x,y)$ function. This function gives the number remaining after an integer division

of its two arguments. In this case the simulation time multiplied by 24 (to transform it from day units into hours) is divided by 2. So, if the current simulation time is 3.1 days, then 24 * 3.1 = 74.4 is divided by 2 which leaves 0.4. This number is compared to the fraction of denitrification of this two hourly cycle and the output is assigned to the according value (Kla = 0 or Kla 120 d^{-1} in this case). The second tank has an anoxic period at the beginning of each two-hour cycle, while the third tank has an anoxic period at the end of each two-hour cycle. With a denitrification of 35 %, this means that there is a period in the middle of each cycle during which both tanks are aerated.

Qwastecontroller

The Qwastecontroller reads the sludge residence time (SRT) as input from the influent file. Wasting was modelled as if the waste sludge was removed from the bioreactors. In this way, the amount of mixed liquor to waste can be calculated as (assuming the sludge concentrations in all bioreactors are identical):

$$\theta_X = \frac{V_{tot} \cdot X}{Q_w \cdot X} = \frac{V_{tot}}{Q_w} \tag{5.8}$$

$$\Rightarrow Q_w = \frac{V_{tot}}{\theta_X} \tag{5.9}$$

where

V_{tot} Total volume of bioreactors
Q_w The flow rate of the waste sludge
θ_X The sludge residence time
X The sludge concentration in the bioreactors

Hence, the amount of mixed liquor to waste is calculated as the total volume of the three activated sludge tanks, divided by the SRT. The sludge present in the settler is not accounted for, while it is also implicitly assumed that the sludge concentration in the three activated sludge tanks is the same. From simulation results it is shown that this is not exactly the case, but this Qwastecontroller is used anyway.

Other controllers

All other controllers are pass-through controllers, which means that they get input from the influent file and that their output is exactly the same value. The controllers are necessary because it is only with a controller component that one can link the output of a submodel to a parameter of another model.

Other models

All other models used in the overall model are taken from the standard WEST model base (converters, activated sludge units and settler models), except for the adaptations needed for model reductions which will be commented upon further on.

5.4.3 The Tielt model and ANN

Because the simple model used in the previous paragraph may have been an unrealistic case, it was decided to try to predict the conversion rates of the ASM2d with an ANN anyway. To accomplish this, the training influent set was used to run a simulation with the full model, in order to generate a training set for the neural network. Because the models in WEST use fluxes instead of concentrations to describe transport between the different components, it was decided to try and train the network with the incoming fluxes, the concentrations and the conversion rates of the different substances. The mass balance can then be written as:

$$\frac{dM}{dt} = Flux_{in} - Flux_{out} + conversion \tag{5.10}$$

As in section 5.3.1 the conversion rates need to be predicted by the ANN. Because the conversion of a substance does not depend on all the concentrations of the other substances, it was decided to perform a dependency analysis, i.e. to determine on which factor the conversion of a component is dependent, and only use the ones that are influential to predict the conversion rate of that component. Unfortunately, for this complex model, even the one step ahead prediction could not be achieved with a reasonable accuracy.

It was concluded that the training algorithms present at the time of this project, were not able to train a network in such a way that it can make long term predictions without deviating too much from reality. The big difference with successful applications of ANN in control systems is that these control algorithms regularly get updated information on the process. Hence, it uses correct information to calculate the best control action, while during long term simulations, the output of the neural network is the only source of (erroneous) information about the state of the process coming into the network.

5.4.4 Reduction and simplifications of the ASM2d model and the Takács model

Model reduction is frequently applied to overcome some practical problems. Jeppsson and Olsson (1993) used model reduction to improve the identifiability of the activated sludge model and to use the model in control strategies (Jeppsson, 1996). Also, Janssen *et al.* (2000) applied model reduction to a model of a full-scale industrial WWTP in order to reduce the simulation time during controller tuning. Because neural network model reduction did not seem feasible with the tools currently available, knowledge based reduction techniques were used to improve calculation time. Five different scenarios were tried.

The first case was the full case: this means the complete ASM2d model was used together with a Takács settler model.

In a second case the Takács settler model was replaced by a pointsettler model. A pointsettler is a settler model with no residence time in which the incoming flow is divided into a concentrated underflow and a (nearly) solid-free effluent which contains only a small fraction of non-settleable solids.

Table 5.2: Different scenarios to simplify the ASM2d model

Scenario	Explanation
fulltielt	the full ASM2d model together with the Takács settler
fulltieltpoint	the full ASM2d model together with a pointsettler
simpleTakács	removing "useless" states as S_I, S_{ALK}, S_{N2}, X_{MeOH} and X_MeP from the full ASM2d model, still using a Takács settler
fullDO	removing oxygen dynamics from the model and replacing it with a switching function which is one during aeration and zero when aeration is off, with a Takács settler
tieltallsimple	combination of all previous simplifications, i.e. pointsettler, no useless states and no oxygen dynamics

In a third case some "useless" states were eliminated from the model. For instance, the nitrogen gas was removed, since this state is only used to close mass balances, but is not important for the performance of the model. From the simulation results, it was found that the alkalinity was never a limiting factor. The switching term was always very close to one, and was removed from the equations. The inert soluble COD component (S_I) is used for closing mass balances too, but is not important when the COD concentration of the effluent is not considered. Hence, S_I was removed as well. Finally, the components X_{MeOH} and X_{MeP} states were also removed from the model, since they were only considered to be present in very low concentrations in the full model, and have hence no serious impact on the sludge concentration.

In a fourth case, the oxygen dynamics were replaced by an on/off function. This is implemented as:

$$\frac{S_O}{K_{S_O}+S_O} = \begin{cases} 1 & \text{if aeration is on} \\ 0 & \text{if aeration is off} \end{cases} \tag{5.11}$$

$$\frac{K_{S_O}}{K_{S_O}+S_O} = \begin{cases} 0 & \text{if aeration is on} \\ 1 & \text{if aeration is off} \end{cases} \tag{5.12}$$

In the fifth case all above model reductions were used together. An overview of the different model simplifications is given in Table 5.2.

The different model reduction strategies were evaluated on calculation time and agreement with the full model. The more simplifications were applied the faster the calculations became, but at the same time the larger the difference between the full and simplified model turned out. A calculation time of 30 minutes for 100 simulated days was achieved, well within the requirement of the later use, while the full model took 50 minutes to simulate these 100 days (Table 5.3). These calculations were performed on a Pentium II 350 MHz processor with 64MB of RAM. All the different scenarios used the Runge-Kutta variable stepsize integration algorithm (Press *et al.*, 1992) with following parameters: accuracy 10^{-6}, initial step size 10^{-6}, minimum stepsize 10^{-4}, maximum step size 1. The time scale is put in days.

One way to compare these simulation results is to look at the graphs of all components in

Table 5.3: Comparison of the different scenarios with the fulltielt scenario

Scenario	simulation time 100 days (min)	correlation for ammonia	correlation for nitrate	correlation for phosphate
fulltielt	50	1.00	1.00	1.00
fulltieltpoint	42	0.99	0.99	0.99
simpleTakacs	* (112.5)	0.96	0.97	0.98
fullDO	42	0.54	0.56	0.63
tieltallsimple	31	0.47	0.51	0.71

* The simpleTakacs scenario encountered stability problems during simulation (negative oxygen concentrations). Therefore the minimum stepsize had to be decreased to 10^{-5}. With this adaptation, results were more stable but the simulation time was much longer as indicated between brackets.

the effluent and see if they match. Because this is not useful in this chapter a correlation analysis of the three most important effluent concentrations (ammonia, nitrate, phosphate) is made and illustrated with some graphs. The results are shown in Table 5.3, together with the simulation time needed for a simulation of 100 days.

The different scenarios show a varying correlation for the effluent concentrations of these three variables. The simulation results of the *fulltieltpoint* and the *simpleTakacs* models have excellent correlation with the *fulltielt* model. The removal of the oxygen dynamics seemed to have a negative effect on the correlation as is shown by the lower correlation coefficient for the *fullDO* and the *tieltallsimple*. Care should be taken when looking at the correlation analysis because with the variable step size method, the output times are never exactly the same, and a little time shift may cause a decrease in the observed correlation.

Another way to compare the results of the different simulations is to evaluate at the mean values, the standard deviations and the maximum values. These are shown in Tables 5.6, 5.4 and 5.5. When comparing means or correlations one should also take care of the fact that in many model applications the extremes are more important than the mean effluent concentrations.

A parity plot shows the results of two simulations plotted against each other and allows to judge, next to the correlations, whether the values are the same on the same moment by looking at the deviations of the diagonal. It can be seen in Fig. 5.13, that the correlation is reasonable (grouped data points), but that there is a large deviation from the diagonal, indicating a different mean value. In Fig. 5.14, a good parity plot of the nitrate concentration for the *fulltielt* and the *simpleTakacs* models is shown, indicating a good correlation and data points close to the diagonal of the plot.

Other figures illustrate the problem of comparing simulation results. In Fig. 5.15 it is easy to see that the two concentrations of phosphate in the effluent are clearly different. This is also clear from the correlation coefficient and the mean values for phosphate in the fullDO case. When comparing the ammonia concentrations for the same scenario (Fig. 5.16), it could be agreed that these results match enough to be acceptable. These two figures illustrate the fact that when the results are reasonable for one variable, they are not necessarily correct for other variables. It is hence important to look at all important variables and to look at a number of measures of agreement, like the correlation coefficient

Table 5.4: Comparison of the means of the nutrients in the effluent. (Numbers between brackets indicate percentage difference compared with the detailed simulation)

Scenario	mean NH_4-N (mg/l)	mean NO_3-N (mg/l)	mean PO_4-P (mg/l)
fulltielt	1.1 (100)	3.0 (100)	0.40 (100)
fulltieltpoint	1.1 (99)	3.1 (103)	0.40 (100)
fullDO	0.8 (72)	2.5 (85)	2.30 (577)
simpleTakacs	0.8 (70)	3.0 (100)	0.39 (98)
tieltallsimple	0.6 (53)	2.3 (77)	0.36 (89)

Table 5.5: Comparison of the standard deviations of the nutrients in the effluent. (Numbers between brackets indicate percentage difference compared with the detailed simulation)

Scenario	std NH_4-N (mg/l)	std NO_3-N (mg/l)	std PO_4-P (mg/l)
fulltielt	1.7 (100)	2.8 (100)	0.89 (100)
fulltieltpoint	1.7 (100)	2.8 (101)	0.84 (94)
fullDO	1.2 (72)	2.6 (95)	1.88 (211)
simpleTakacs	1.3 (75)	2.9 (103)	0.89 (100)
tieltallsimple	0.9 (52)	2.5 (90)	0.74 (83)

Table 5.6: Comparison of the maximum of the nutrients in the effluent. (Numbers between brackets indicate percentage difference compared with the detailed simulation)

Scenario	max NH_4-N (mg/l)	max NO_3-N (mg/l)	max PO_4-P (mg/l)
fulltielt	12.3 (100)	12.4 (100)	5.40 (100)
fulltieltpoint	12.6 (102)	12.6 (102)	5.50 (101)
fullDO	9.4 (76)	13.1 (106)	8.90 (163)
simpleTakacs	10.5 (86)	14.0 (113)	5.50 (101)
tieltallsimple	7.5 (61)	11.9 (96)	6.60 (121)

and the mean value.

The comparison of the nitrate concentrations in Fig. 5.17 shows a good agreement between the two simulations in this period. In Fig. 5.18 the same concentrations are shown for a different period and it can be seen that there are relatively large differences between the two simulation results. The correlation analysis shows a 70% correlation between the two output curves. The mean values indicate that there is an average difference of 0.7 mg/l between the two scenarios. Expert judgement is needed to decide whether this is acceptable or not.

An additional check consists of comparing the histograms of the different variables. As illustrated in 5.19, it is not easy to find differences between the different simulations with this method either. However, it again gives some useful information on the extreme behaviour. As can be seen from this figure, the tieltallsimple and the simpleTakács scenario show higher probabilities for low ammonia concentrations, and vice versa. The fullDO model has a clearly different distribution for the phosphate concentrations (Fig. 5.19right).

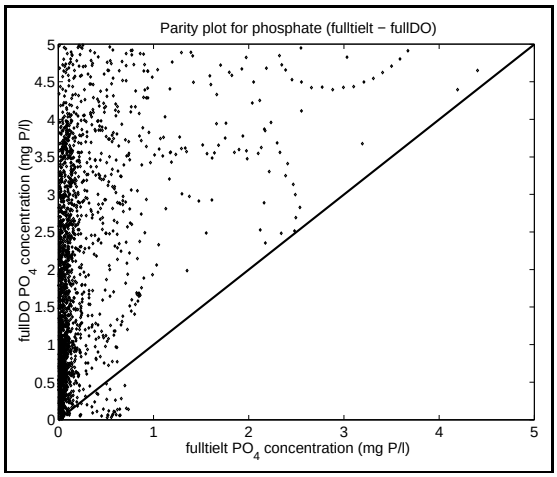


Figure 5.13: Parity plot of phosphate for the fulltielt-fullDO models

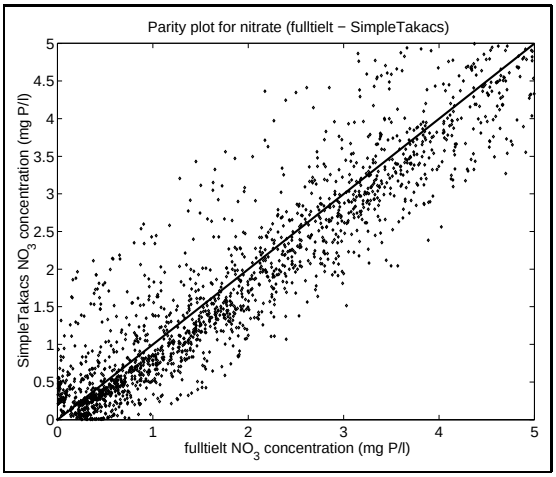


Figure 5.14: Parity plot for nitrate for the fulltielt-Simple Takács

Because an acute impact may be dependent on a combination of different conditions, it is important that the two models behave the same in the same conditions and not only statistically.

Summarising, it is not easy to decide on accepting or rejecting the different simplifications or whether the gain in calculation time ($\pm$ 40%) is sufficient to accept some errors introduced by these simplifications. Other combinations such as a pointsettler together with the simple models but including oxygen dynamics might also give good results. Advanced statistical techniques are necessary to scientifically discriminate between the different model results.

5.5 Discussion

The goal of this chapter was to obtain a model that was able to simulate the behaviour of a treatment plant with biological phosphorus removal. The model reduction techniques described in literature are applied to the ASM1 model. However, the reduced models are used mainly in controller optimisation or MBPC studies. The model used in this study had to be incorporated into an integrated model. Therefore, it should be able to simulate relatively long time series without input about the measured model states, while most of the techniques described above only use short time predictions which get updated by measured data.

The two techniques used, application of grey box models with ANN and knowledge based reduction have been applied before in controller optimisation of WWTPs (see e.g. (Lukasse, 1999)). However, in this case, the models were fed with measurement data in order to give the ANN correct inputs. In this way, an accumulation of errors could be avoided, which was not the case in this study.

Several other model reductions for ASM models are described in literature, see e.g. Weijers (2000). However, these reduced models are not used as a substitute for the ASM

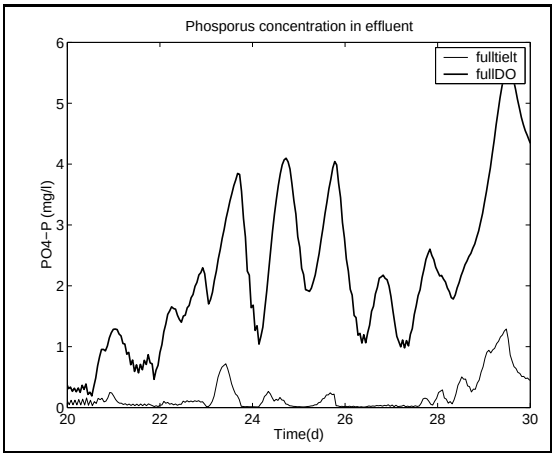


Figure 5.15: Phosphate concentration in the effluent for the fulltielt and the fullDO case

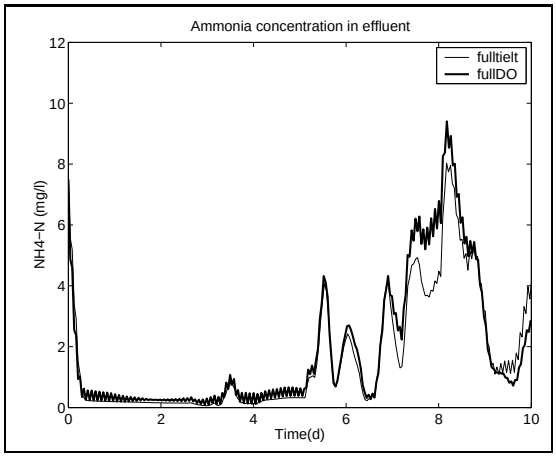


Figure 5.16: Ammonium concentration in the effluent for the fulltielt and the fullDO case

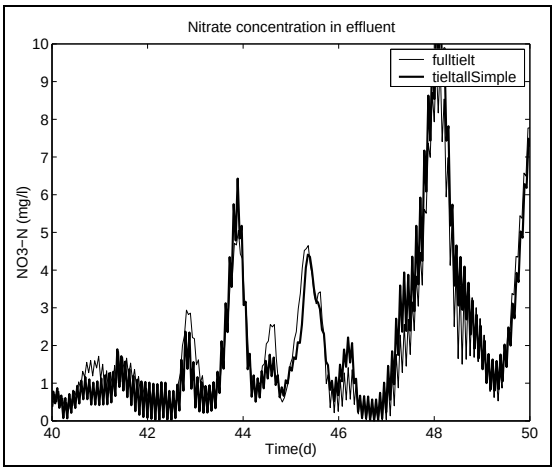


Figure 5.17: Nitrate concentration in the effluent for the fulltielt and the tieltallsimple case

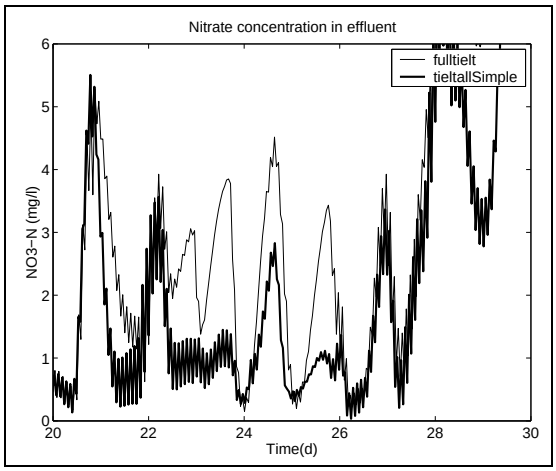


Figure 5.18: Nitrate concentration in the effluent for the fulltielt and the tieltallsimple case

models, but they are used to facilitate the design of controllers or in MBPC. Therefore, these could not be used in this project.

5.6 Conclusions

The use of grey box modelling techniques seemed a promising approach at the start of this study, because the best of both the mechanistic and black box techniques might be incorporated in one model. However, using neural networks to cover the black box part, did not work at all, because no training algorithm was applicable to cover long term predictions, while the algorithms were not suited either to eliminate the errors induced by integration of the grey box mass balance.

When applying model reductions by eliminating certain states or processes, it is difficult to discriminate between the different model results. There are different ways of comparing time series, none of which allows for a clear discrimination between acceptable

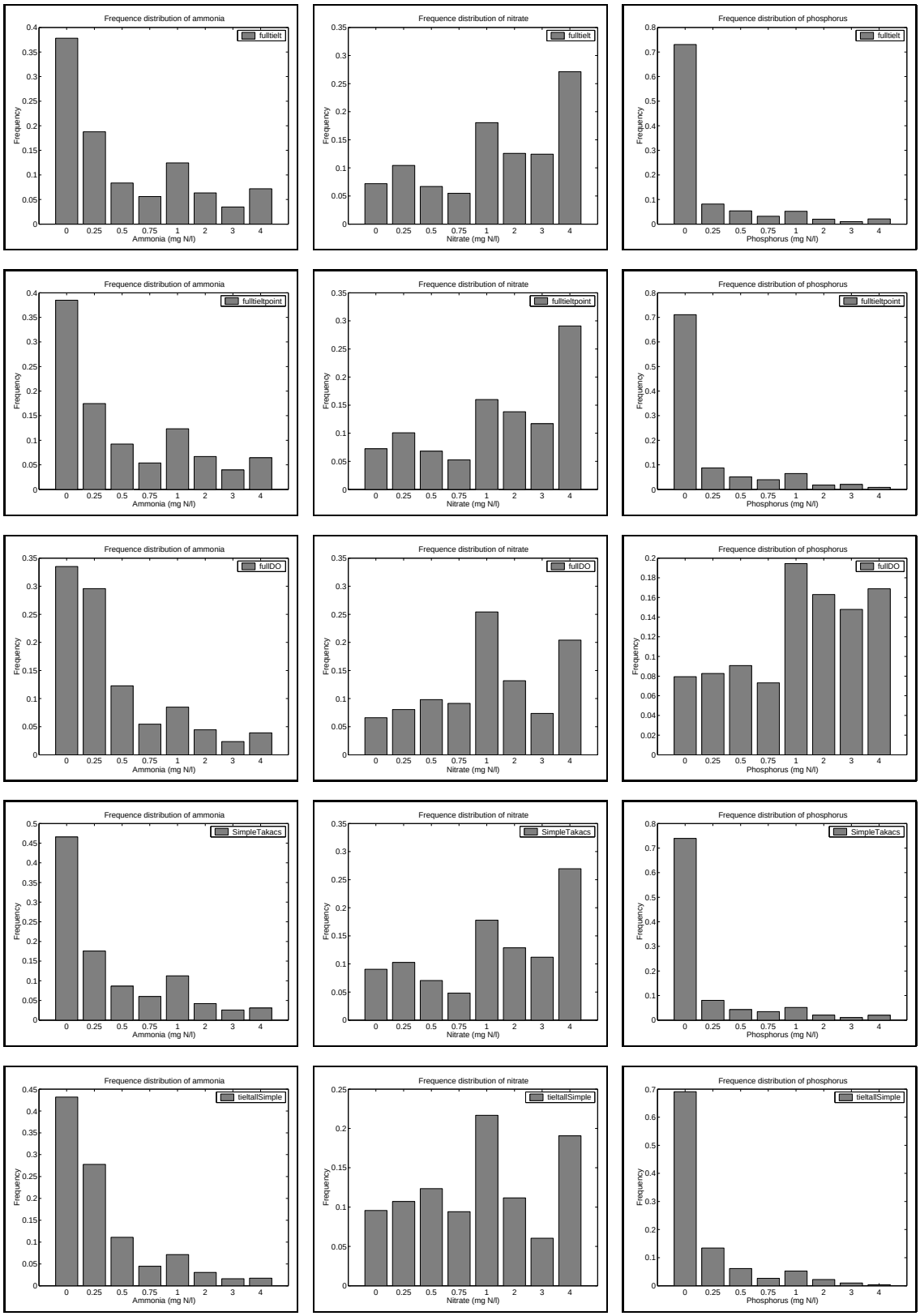


Figure 5.19: Histograms for the different model simplifications for ammonia (left), nitrate (middle) and phosphate(right)

and unacceptable reductions. By using statistical techniques, this discrimination might be possible, but still expert judgement is necessary to interpret the results.

Chapter 6

Modelling river flow and pollutant propagation with CSTRs

6.1 Introduction

In the integrated urban wastewater treatment system, which considers the sewer system, the treatment plant and the river, mathematical models are used to study the impact of combined sewer overflows and of the effluent of the treatment plant on the receiving water. Since the whole system is very complex and shows a lot of interactions, it would be interesting to describe all processes in detail. However, when trying to do so, the resulting model has a huge number of parameters, most of which are not identifiable. In addition the calculation time becomes very large due to the large number of equations involved. Therefore, it is desirable to choose an adequate model complexity in order to be able to describe the processes and pollutants under study and to ignore the other ones.

The equations with probably the largest impact on the calculation time of a model of the IUWS, are the “de Saint-Venant” equations. These equations are based on the conservation of mass and momentum in open channel flow. Since the “de Saint-Venant” equations are partial differential equations, they require sophisticated numerical algorithms to be solved. These models are very useful when focusing on river hydraulics only and can e.g. be used for flood-forecasting. When focusing on river water quality however, the accuracy reached by the “de Saint-Venant” equations is disproportional to the accuracy the river water quality model can attain. Hence, it appears acceptable to replace the hydraulic part of the river model by a simplified model. In this work a tanks-in-series model is proposed as an alternative model to describe the hydraulic behaviour of the river.

Tanks-in-series models are known to be able to reasonably describe the hydraulics of a river (Beck, 1976). The improved CSTRs-in-series model developed by Reda (1996), was already described in section 2.3.5. However one of the main disadvantages of the tanks-in-series modelling approach is the fact that no backwater effects can be modelled directly. The model proposed in this work is able to describe the backwater effect at a weir by calibrating the tank parameters on a sufficiently large amount of information rich data. Also, the propagation of flood waves that travel faster along the channel than the

corresponding pollution wave, is known to be a problematic point when using CSTRs-in-series models (Reda, 1996), and will be discussed in this chapter.

A procedure to calibrate a CSTRs-in-series model (i.e. a surrogate model) on the basis of data generated by a complex mechanistic model is outlined and tested on the river Zwalm. The different steps can be outlined as follows and refer to the general procedure outlined in section 4.2.

- set up a complex mechanistic model (section 6.3)
- generate data with the complex mechanistic model (section 6.3)
- define a model structure of the surrogate model (CSTRs) (section 6.4.1)
- calibrate the geometry parameters of the surrogate model (section 6.4.2)
- calibrate the flow parameters of the surrogate model using the data generated with the complex model (section 6.4.3)
- validate the model for flow and pollutants propagation in rivers (section 6.5)

Only the hydraulic data will be used for the calibration of the surrogate model. The pollutant data are only used to validate the capacity of the model to describe the flood-wave propagation properties of the model.

6.2 Catchment description

The river Zwalm is a small, meandering river in Flanders. Its sources are located near the town of Brakel (South of Gent). The river Zwalm starts at the confluence of two smaller creeks, the Dorenbosbeek and the Molenbeek. The river is part of the Schelde catchment and has a total surface of about 114 km^2. The total length of the Zwalm is 21.75 km and the average flow is 1.14 m^3/s. The river has an unsteady flow, with dry weather flows in summer below 0.3 m^3/s, while much higher values (up to 4.7 m^3/s) are encountered in wet weather periods. This strongly varying flow has important consequences for the river's diluting capacity and, hence, its pollutant concentrations. Four weirs were built to prevent the previously regular floodings (Carchon and De Pauw, 1997; Ponnet, 1994).

In total 10 subcatchments drain into the part of the Zwalm under study, while the WWTP of Brakel (7000 PE) also discharges into the river. The section under study is about 5km long and ends at the flood control weir in Rozebeke. Since this catchment has been part of another study dealing with the impact of the CSOs on the quality of the Zwalm (Fronteau and Bauwens, 1999), extensive data sets were available.

Field data were collected at different locations along the river. For every location, the distance to the beginning of the stretch, the level and the cross-sectional profile were available. A typical cross-section is shown in Fig. 6.1.

6.3 The complex mechanistic model

Fronteau *et al.* (1999) constructed, calibrated and validated a model of the Zwalm using ISIS software (Wallingford, UK). The data used to construct this model were available,

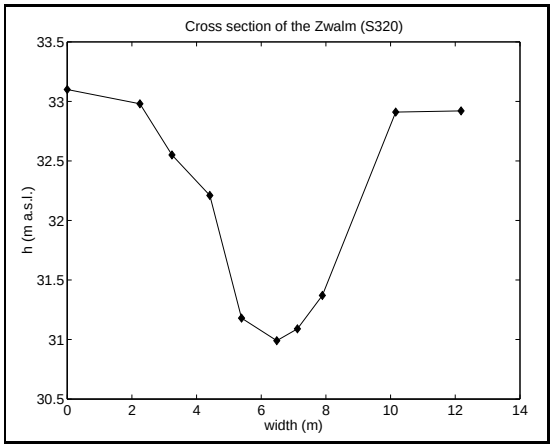


Figure 6.1: Typical cross-sectional profile in the Zwalm

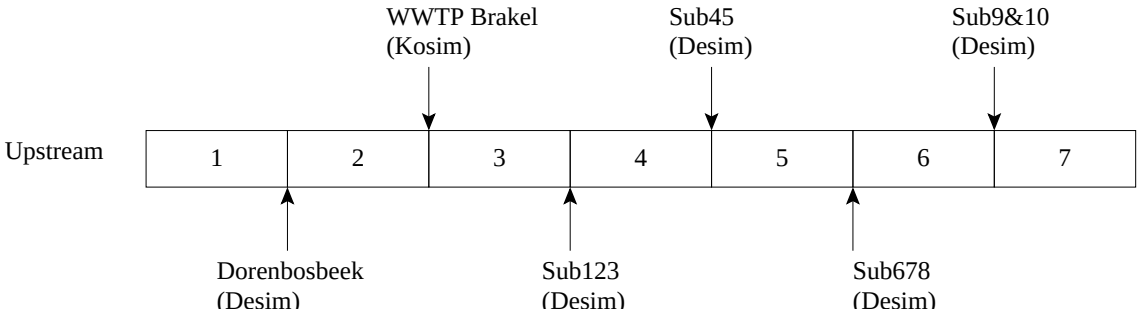


Figure 6.2: Schematic representation of the Zwalm model

but no software license however was available for use in this research, so it was decided to rebuild this model into Aquasim (Reichert, 1998). The river section compartment of Aquasim was used to model the hydraulic behaviour of the Zwalm.

As mentioned before, several tributaries join the Zwalm along the stretch under study. A schematic overview of the stretch is given in Fig. 6.2. The effluent flow rate of the treatment plant was calculated using a Kosim model (itwh, 1995) of the treatment plant of Brakel (Fronteau *et al.*, 1999). The tributary flows were calculated with Desim, which is a mathematical model derived from Kosim. Changes of Desim compared to the Kosim model are the inclusion of a delayed runoff from infiltration water from unpaved areas and the possibility to simulate larger catchments with an important natural flow (Fronteau, 1999).

The available data had to be transformed in order to implement the model in Aquasim. For every section, the data as shown in Fig. 6.1 are transformed into look-up tables with the following format

$$P = f(h) \tag{6.1}$$

$$w = g(h) \tag{6.2}$$

$$A_{cross} = y(h) \tag{6.3}$$

where

P wetted perimeter (m)

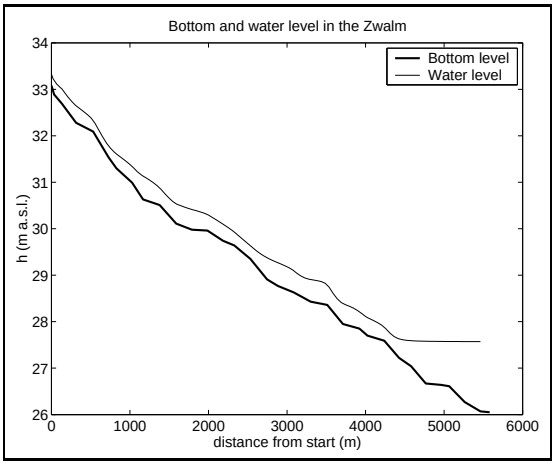


Figure 6.3: Water level during dry weather flow

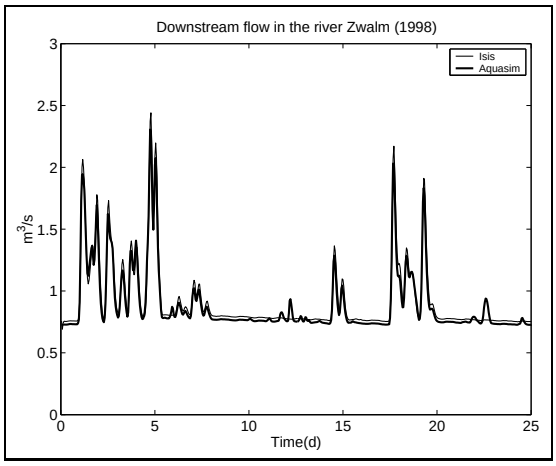


Figure 6.4: Comparison of flows simulated by Isis and Aquasim

w width of the water surface (m)
A_{cross} cross-sectional area of the water body (m^2)
h water height (m)

It has been assumed that the river bed could be approximated by a straight line between two data points. In this way, the perimeter, surface width and cross-sectional area could be calculated as a function of the water height.

These data are entered into the Aquasim model, together with the elevations of every section, and used in the “de Saint-Venant” equations. Seven river compartments were used and the beginning and end of every compartment was located at places where a tributary flows into the river. The diffusive wave approximation of the “de Saint-Venant” equations was used to solve the model. This approximation allows for the modelling of flood wave propagation and backwater effects. The bottom level elevation, together with the water level during dry weather flow are shown in Fig. 6.3. Near the end of the stretch under study, the effect of the downstream weir can clearly be noted. A comparison between the simulation results obtained with Aquasim and the results obtained earlier with ISIS is shown in Fig. 6.4. It can be concluded that the Aquasim model has the same behaviour as the Isis flow model. Therefore, the Aquasim model can be used to generate data which are necessary to calibrate the CSTRs model.

Three types of data were collected during the data-generating simulations: flow rate, water depth and tracer concentration. The flow rate is measured at the end of each tank. The water depth is averaged over each river compartment since in the CSTR model, the water level is always horizontal and, as a consequence, only one depth can be used to calibrate the CSTR model. As with the depth of the water, only one value for the concentration can be used in a CSTR. For the concentration of the pollutants, different options may be chosen. The first option is to fit the outflux of each tank in order to have a correct flux of pollutants out of each stretch. The second option is to fit the average concentration of the pollutant. This would allow the conversion rates of the pollutants to be approximated better. Depending on the situation, one or the other might be chosen. If the pollutants have a high conversion rate, and will not be transported over long distances, the average

concentration may be used. On the other hand, if inert pollutants or pollutants with a low conversion rate are important, the outflux should be used as a calibration function.

In this study, the outflux of pollutants was considered more important in order to have the correct flux of pollutant from one tank to the next. If this is not the case, an accumulation of errors along the different tanks occurs.

Summarising, for each tank in the river model, flow series at the beginning and at the end were collected. Also, average water depths in the compartment were calculated. For the tracer, the concentrations at the end of the tank were collected. These data were used for the calibration and validation of the CSTR model.

6.4 A modified tanks-in-series model

6.4.1 Non-rectangular tanks

In traditional water quality modelling use of Continuous Stirred Tank Reactors (CSTRs), the implicit assumption is that the river stretch can be approximated by a rectangular box. This means that the relationship between the volume and the height in the tank can be written as

$$\frac{dV}{dt} = Q_{In} - Q_{Out} \tag{6.4}$$

$$h = \frac{V}{w * l} \tag{6.5}$$

$$A_{cross} = w * h \tag{6.6}$$

$$v = \frac{Q_{Out}}{A_{cross}} \tag{6.7}$$

$$Q_{Out} = f(h, Q_{In}) \tag{6.8}$$

where

h	The height of the water (m)
l	The length of the tank (m)
Q_{In}	The incoming flow rate ($m^3 s^{-1}$)
Q_{Out}	The outgoing flow rate ($m^3 s^{-1}$)
v	The average water velocity (ms^{-1})
V	The volume of water in the tank (m^3)
w	The width of the water surface (m)

The assumption of a rectangular box is a good approximation for large rivers, where the variation of the width is small over the total depth of the stretch under study. However, in small rivers, this assumption may not be valid. A typical cross-section for the river Zwalm (Belgium), was already shown in Fig. 6.1. It can be seen from this figure that the assumption of a linear increase of the cross-sectional area with the height (which assumes a constant width) is not valid for the Zwalm river. Therefore, an alternative model had to be used in order to describe the flow propagation in the river.

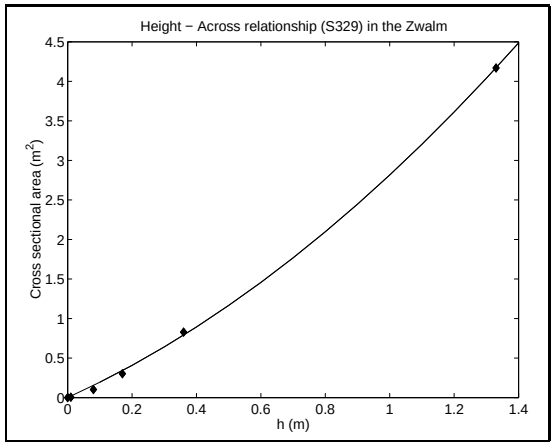


Figure 6.5: Calculated h-A_{cross} relationship for section 329

The model used in this study, exists of a series of CSTRs with variable volume. The outflow rate is related to the height in the water tank in a non-linear way, which is a general rating curve in case the flow is not zero when the water height = 0 (Shaw, 1996).

$$Q_{Out} = \alpha(h-\beta)^{\gamma} \tag{6.9}$$

$$A_{cross} = \frac{V}{l} \tag{6.10}$$

However, the relationship between the height and the volume of the tank, could not be written as in equation 6.5. By plotting the calculated relationship between the height and the cross-sectional area, a second order relationship was found to fit the calculated points. The following relationship was used in the model:

$$A_{cross} = ah^2 + bh \tag{6.11}$$

which can be rewritten as

$$h = \sqrt{\frac{A_{cross}}{a} + \frac{b^2}{4a^2}} - \frac{b}{2a} \tag{6.12}$$

An example of the calculated and fitted cross-sectional area can be found in Fig. 6.5. Since the cross-section is zero when there is no water in the tank, the zero-order term of the second order relationship was set to zero by default. The other two parameters, *a* and *b* were estimated to minimise the sum of squared errors. Equation 6.12 forms, together with the mass balance 6.4 and equations 6.9 and 6.10, a set of equations which can be solved by numerical algorithms. The hydraulic model has five parameters: *a*, *b*, α, β and γ. The parameters *a* and *b* could, as explained before, be estimated on the basis of field measurement data of the profiles of the river bed. The parameters α, β and γ need to be estimated by comparison of the flow predicted by the tanks-in-series model with the real flow. The data generated by the Aquasim model will be used for this purpose (see section 6.4.3).

Table 6.1: Overview of the geometry parameters for the different tanks in the CSTR model

	a	**b**	**L**
Tank1	0.304	1.830	134
Tank2	1.241	1.589	693
Tank3	1.581	0.979	340
Tank4	1.392	1.258	1161
Tank5	1.290	1.161	1697
Tank6	1.207	1.536	1040
Tank7	1.338	1.531	398

6.4.2 Calibration of the geometry parameters

Every location for which data about the cross-sectional profile were available has a different shape. This yields different h-A_{cross} pairs and different estimated values for the parameters a and b are obtained for different sections. Only one value for each parameter can be used in the CSTR model. Therefore, lumping of the different parameter values was necessary in order to estimate unique values for a and b in every tank.

For every section i within a tank, the parameters a_i and b_i were estimated. The parameters used in the CSTR model are then calculated as

$$a_{T_j} = \frac{1}{n_j} \sum_{i=1}^{n_j} a_i \tag{6.13}$$

$$b_{T_j} = \frac{1}{n_j} \sum_{i=1}^{n_j} b_i \tag{6.14}$$

where

a_{T_j} average value for parameter a in tank j
b_{T_j} average value for parameter b in tank j
n_j the number of sections with data points in tank j

An overview of the parameter values obtained is given in Table 6.1. The resulting relationships are also plotted in Fig. 6.6. It can be seen that the relationships are similar for tank 2-tank 7, while tank 1 has a different shape. This could be expected since a part of the river in the first tank is a concrete tunnel with a rectangular shape.

6.4.3 Calibration of the flow parameters

The hydraulic parameters (α, β and γ) were calculated for each of the seven tanks separately. In this way, a deviating behaviour of the upstream tank could not influence the parameter estimation in the next tank. For every tank, a "correct" input flow series was generated by Aquasim simulations. Also, a data series for Q_{Out} and h was generated. As mentioned before, the tracer concentrations were not used for calibration of the hydraulic

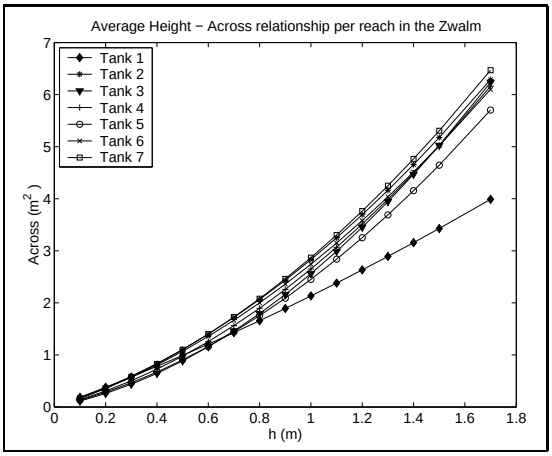


Figure 6.6: Average h-A_{cross} relationship for all tanks

parameters, but will be used to check the behaviour of the model once the hydraulic calibration is finished.

Several problems occurred during the calibration phase of the separate tanks. The first problem was the choice of a suitable data series from the Aquasim simulations. Two degrees of freedom had to be fixed: the length of the calibration period and the frequency of data sampling.

The length of the calibration period needs to be sufficient to cover a reasonable range of different conditions in the river such as dry weather and storms of different magnitudes. To a large extent, the time needed for the parameter estimation is determined by the length of the calibration period. Indeed, during the parameter estimation, several hundreds of runs need to be performed and a doubling of the simulation period, leads (approximately) to a doubling of the time needed to estimate the best values of the parameters.

The frequency of data sampling was determined by a trial and error approach. In the first try, an hourly interval was chosen. This seemed reasonable since the flow in the river changes only gradually. However, with this interval, no unique parameter values could be obtained. Therefore, the interval was reduced to 15 minutes, which gives more data points and hence, more information. Also with this interval, the optimisation algorithms used (simplex and Praxis, see chapter 3) had problems in finding unique parameter values for most of the tanks.

These problems may, in future research, be solved by optimal experimental design. In this way, an automated procedure can be used to determine the length and frequency of the data collection.

Two main steps were used in the calibration of the hydraulic parameters. In a first step, the stage-discharge relationship at the end of the tank was estimated from the data generated by the Aquasim simulations. In a second step, the values obtained in the first step were used as initial values for parameter estimation by dynamic simulation. This is necessary since the stage-discharge relationship determined in the first step only accounts for one location in the river, while the tank takes into account the geometry of its complete length. Therefore, different values can be expected from these two methods.

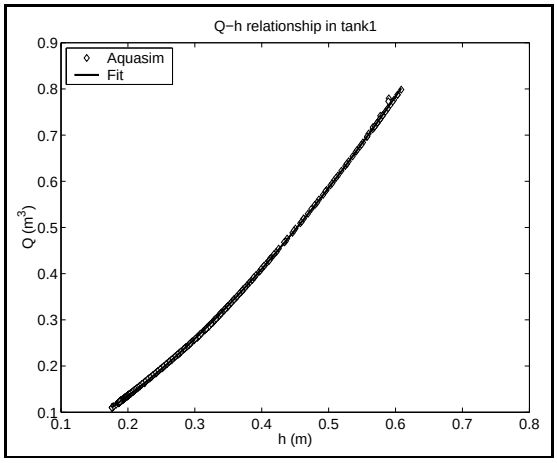


Figure 6.7: Q-h relationship for tank 1 with three parameters

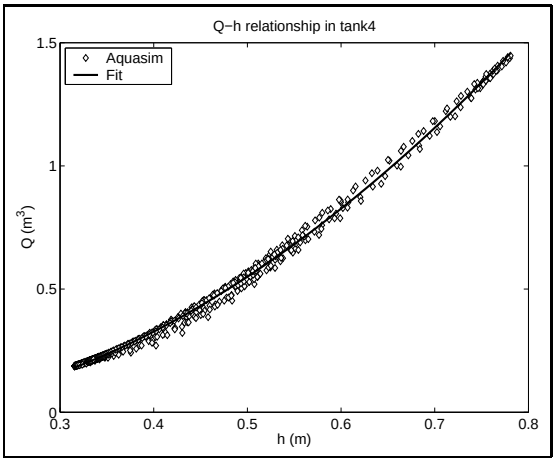


Figure 6.8: Q-h relationship for tank 4 with three parameters

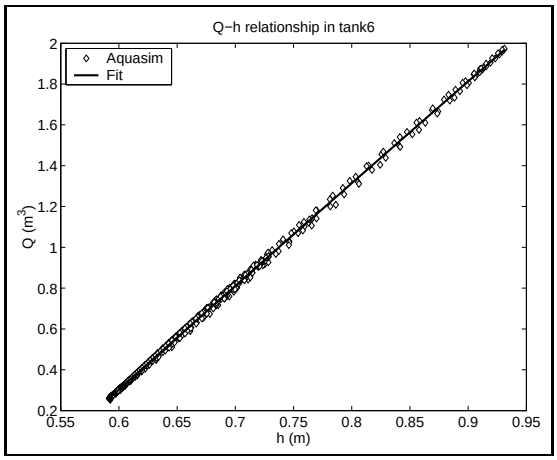


Figure 6.9: Q-h relationship for tank 6 with three parameters

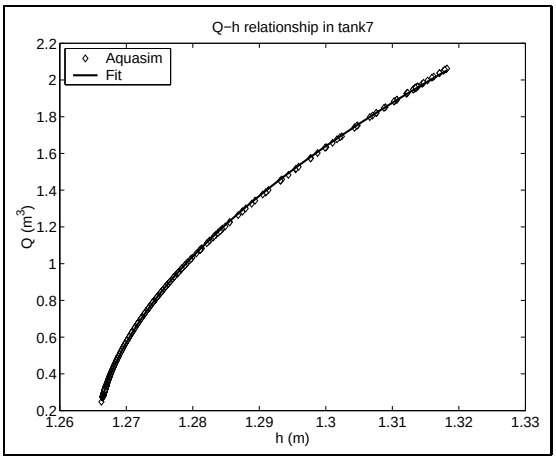


Figure 6.10: Q-h relationship for tank 7 with three parameters

Estimating Q-h relationships

The flow measurement of rivers is often done using measurements of the water depth in combination with a formula relating the measured depth to the flow rate. These formulae can generally be written as (Shaw, 1996) (see also eq. 6.9):

$$Q = \alpha(h - \beta)^{\gamma} \tag{6.15}$$

where α, β and γ are parameters of the gauging station. As the outflow formula chosen in the CSTRs-in-series model uses the same formula, the relationship between Q and h at the end of every tank can be used to get a first estimate of the parameters α, β and γ. This was done using a Matlab routine to minimise the sum of squared errors (SSE) between the curve and the Q-h data from the Aquasim simulations.

When analysing the Q-h data, 4 different cases could be distinguished. The first three tanks could be described by a single curve as shown in Fig. 6.7. It can be seen from this figure that the data generated by Aquasim and the curve match very well. In Fig. 6.8 the

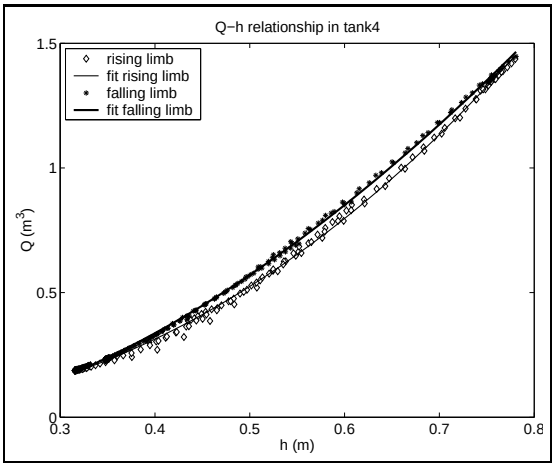


Figure 6.11: Q-h relationship for tank 4 with falling and rising limb

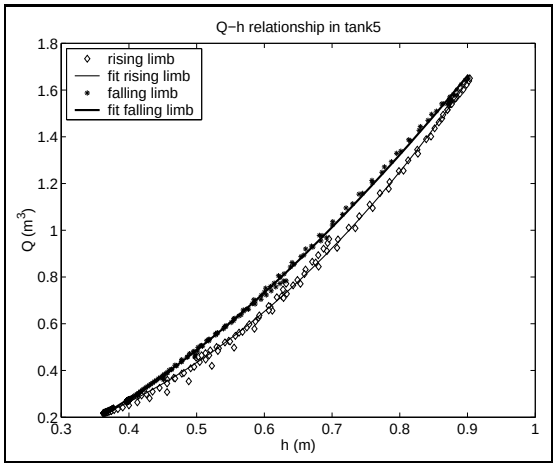


Figure 6.12: Q-h relationship for tank 5 with falling and rising limb

data are more scattered around the average curve. This is the case with tank 4 and 5 where there is a difference between the Q-h relationship in the rising and the falling limb of a flood wave. Tank 6 (Fig. 6.9) shows a linear relationship between the flow rate and the water depth, while tank 7 shows a saturating relationship (Fig. 6.10).

The observed data points in tank 4 and 5 (with the scattered data) can be better approximated if an extra equation can be added to the model. As known from river hydraulics (Shaw, 1996) there might be differences in the Q-h relationship at a certain point depending on the part of the storm considered. The rising limb (i.e. with an increase in flow rate) has a different Q-h relationship compared to the falling limb (with a decrease in flow rate). Therefore, the data were split in two series: one where dQ/dt is positive and one where dQ/dt is negative. Two curves were fitted to these two series as illustrated in Fig. 6.11 and Fig. 6.12. It is clear that the use of these two curves increases the accuracy of the model, but at the cost of more parameters. This model was not used during the dynamic simulations, as the fit found without the extra equation was considered to be sufficiently accurate.

The behaviour of the first three tanks can be better understood by applying the Darcy-Weisbach formula under uniform flow conditions. In uniform flow conditions, the "de Saint-Venant" equations simplify to:

$$S_f = S_0 \tag{6.16}$$

while the Darcy-Weisbach equation can be written as:

$$S_f = \frac{f}{8g} \cdot \frac{Q^2 P}{A^3} \tag{6.17}$$

where

Q Flow rate (m^3/s)
S_f The friction slope (-)

S_0 The bottom slope (-)
f The friction factor (-)
g The gravity constant (m^2/s)
P The perimeter of the cross-section (m)
A The cross-sectional area (m^2)

which can be combined to

$$Q = \sqrt{\frac{8gS_0}{f}} \cdot A\sqrt{R} \tag{6.18}$$

where

R The hydraulic radius (A/P) (m)

In this formula A and R are function of the water depth. Assuming a rectangular tank $A = B * h$ and $R = Bh/(B+2h)$ where B is the width of the tank. Assuming a wide tank ($B >> 2h$), this yields:

$$Q = \sqrt{\frac{8gS_0}{f}} \cdot Bh^{1.5} \tag{6.19}$$

Hence, $Q \sim h^{1.5}$ for rectangular tanks. For triangular shape cross-sections, the same reasoning may be made and yields $Q \sim h^{2.5}$. Looking at the results from the parameter estimation in Matlab™ (Table 6.2), it can be concluded that the behaviour of the Zwalm system modelled with Aquasim is something in between the behaviour of a wide rectangular and a triangular tank.

From the theory described above it becomes clear that two parameters (i.e. α & γ) might be sufficient to describe the Q-h curve. The results obtained from the parameter estimation with three parameters (Table 6.2) indicate that the parameter β is close to zero for tank 1-5.

The results of the parameter estimations with two parameters are also given in Table 6.2. It can be noted that for tank 1 to 5, the fits are still very good, with low SSE, but, as could be expected, the SSE for the fit with three parameters is always lower. Some examples of fitting with the estimation of two parameters are shown in Fig. 6.13 and Fig. 6.14. For tank 6, however, no good results were obtained with this 2 parameter model (α and γ). Looking at Fig. 6.9, it can be noted that the relationship is more or less linear for tank 6. Consequently, γ was put to 1, while β was estimated, with good results. For tank 7 no good results could be obtained by estimating only 2 parameters.

It can be concluded that the general model (eq. 6.9) is applicable to the Q-h data generated by the solution of the diffusive wave approximation of the "de Saint-Venant" equations. The parameters estimated for these curves will be used in the parameter estimation for the dynamic simulation of the flow propagation in the river. The values obtained in Table 6.2 will be used as initial values for the parameter estimation.

Table 6.2: Best estimated values for the parameters of the Q-h relationship

	2 parameters				3 parameters			
	α	β	γ	SSE	α	β	γ	SSE
Tank 1	1.7722	0	1.5971	0.00096	1.7722	0.0002	1.5961	0.00096
Tank 2	3.4033	0	1.9709	0.0345	3.2274	-0.0708	2.3491	0.01769
Tank 3	1.9274	0	1.927	0.04494	1.5291	-0.1256	2.4053	0.01138
Tank 4	2.579	0	2.2578	0.1637	2.8886	0.0853	1.884	0.1302
Tank 5	2.0984	0	2.1974	0.3529	2.479	0.1022	1.8168	0.3041
Tank 6	5.0411	0.5398	1	0.05	4.9746	0.5422	0.9822	0.04762
Tank 7	36.7242	1.2567	1	4.6547	9.81	1.2652	0.53259	0.0058

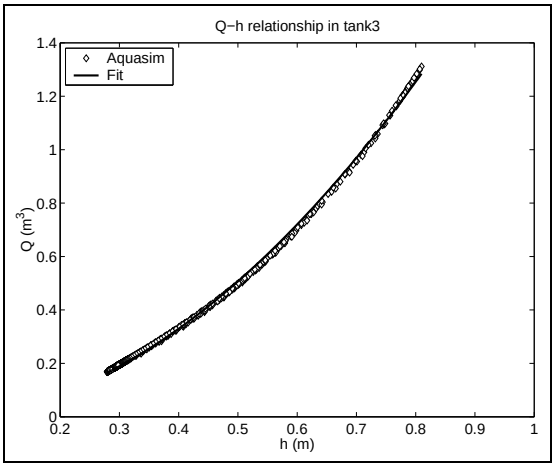


Figure 6.13: Q-h relationship for tank 3 with two parameters

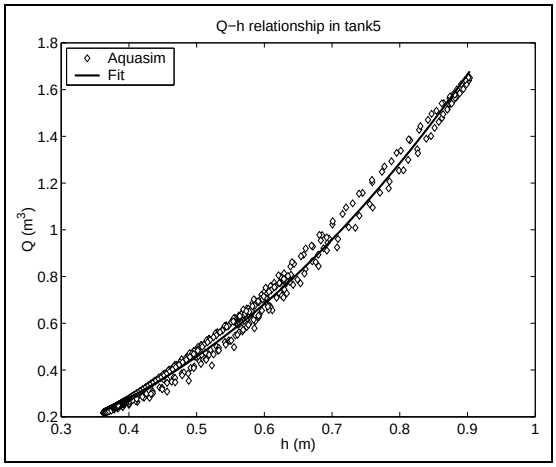


Figure 6.14: Q-h relationship for tank 5 with two parameters

Estimation by dynamic simulation

The model described by equations 6.4, 6.9, 6.10 and 6.12 was implemented in WEST. The data generated by Aquasim were used to estimate the parameters α, β, and γ. The objective function was defined as the sum of squared errors between the generated and predicted data for flow at the end of the tank and for the averaged height data. Since both variables have the same order of magnitude, they were given the same weight in the objective function.

As mentioned above, the number of parameters may be reduced for almost all tanks. Since the search algorithms were not able to find a unique minimum with three parameters it was concluded that the model was not practically identifiable. Therefore, an extra optimisation was performed in which β was put to 0 (tanks 1 to 5), or γ was put to 1 (tanks 6 and 7). An iterative approach was used with different initial values given to both the Praxis and the Simplex algorithm. After several iterations, a minimum was found which gave good results for both the predicted height and flow rate at the end of the tank.

Selected examples of the fits obtained by the CSTR model with three parameters to the Aquasim model are shown in Fig. 6.15. In Fig. 6.16 the same results are shown for the

Table 6.3: Best estimated values for the parameters of the Q-h relationship in dynamic simulation

	2params				3params			
	α	β	γ	SSE	α	β	γ	SSE
Tank 1	1.7841	0	1.6046	0.0766	1.7740	0.0091	1.5544	0.0768
Tank 2	3.3933	0	1.9610	0.0477	3.3834	0.02277	1.8353	0.0515
Tank 3	1.9088	0	1.9038	0.1081	1.9633	0.0173	1.8425	0.1114
Tank 4	2.6796	0	2.3150	0.0412	2.8893	0.06057	2.0229	0.0403
Tank 5	2.1610	0	2.2558	0.0722	2.4220	0.06435	2.0025	0.0704
Tank 6	5.2111	0.5439	1	0.0930	5.0238	0.54519	0.9737	0.0955
Tank 7	48.1561	1.2618	1	0.2416	48.4382	1.2561	1.1059	0.2541

CSTR model with two parameters.

It can be noted that, in general, both parameter sets give good fits for both the flow rate and the water height in the river, and this for all tanks. A summary of the fitting results is given in Table 6.3. When comparing the SSE for the optimisation with two and three parameters, it can be noted that the optimisation algorithms were not able to detect that the parameter β was best set to zero in certain cases (e.g. tank 2). The numerical problems are caused by local minima in the objective function. This is illustrated in Fig. 6.17, which shows the variation of the objective function for varying α, while β and γ are kept constant.

The results for the water height in tank 7 look less good than the others (Fig. 6.15 and Fig. 6.16). This can also be concluded from the SSE in Table 6.3, which is the highest for tank 7. The difficulty is that a strong backwater effect is present in tank 7. Therefore, water level changes more along this tank than in the other tanks. As a consequence, the behaviour of this tank is more complex than for the other tanks, and the fits are less good. To compensate for this, tank 7 was split in two tanks, but the performance of the model did not change considerably and was therefore not used any further. It should however be noted that the absolute differences in water height are small (a few cm). Therefore, it was concluded that the fit was still acceptable for simulation within the framework of water quality modelling where other uncertainties and errors are much larger.

A second remark can be made about the differences in the estimated parameters by the direct estimation of Q-h relationships and by dynamic simulation. When comparing Table 6.2 with Table 6.3, it can be seen that most parameters are in the same order of magnitude. This dynamic simulation based parameter estimation adjusts the parameters of the Q-h relationship so that the dynamic behaviour is improved. This behaviour is different from the behaviour in the complex model since in the tanks-in-series approach only one set of geometry parameters can be used in a tank and, hence, deviations from the behaviour of the complex model occur. These deviations are corrected by adjusting the hydraulic parameters. The important corrections made for tank 7, can again be explained by the non-uniform geometry along this tank. If the simulation results obtained for this tank were considered not satisfactory, the tank could have been split in more tanks to have a better approximation of the geometry.

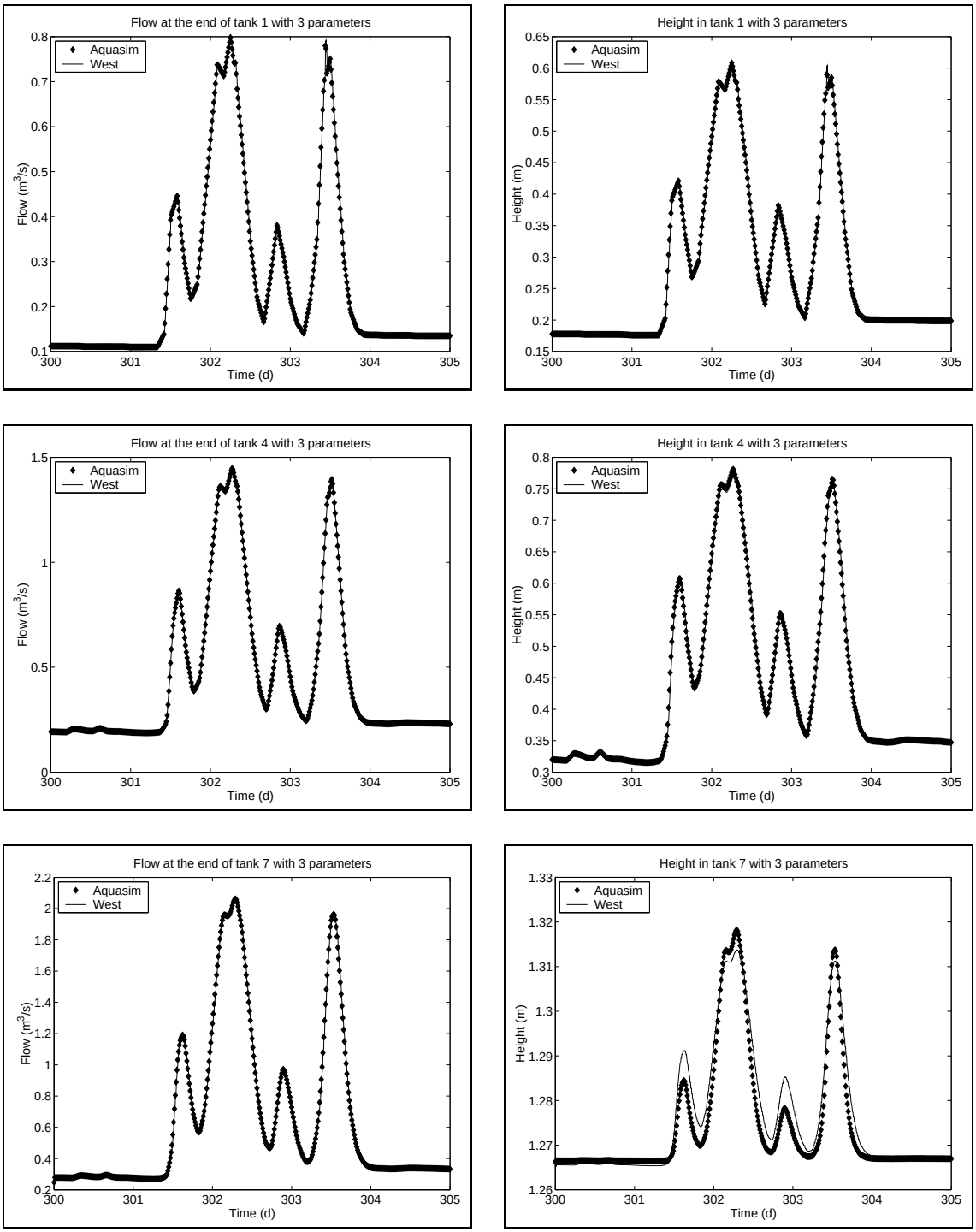


Figure 6.15: Comparison of the flow rates (left) and the water height (right) for the CSTR model with 3 parameters

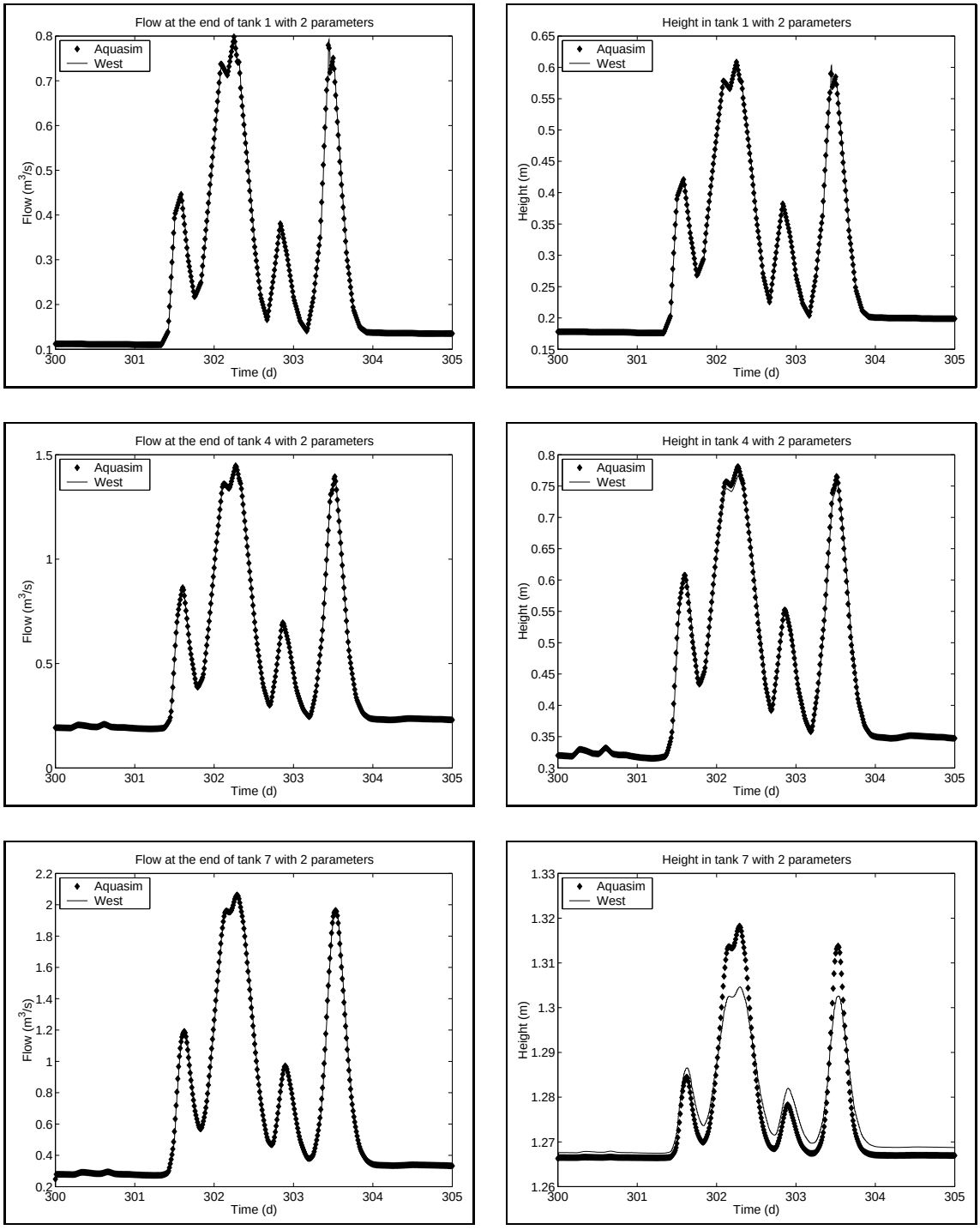


Figure 6.16: Comparison of the flow rates (left) and the water height (right) for the CSTR model with 2 parameters

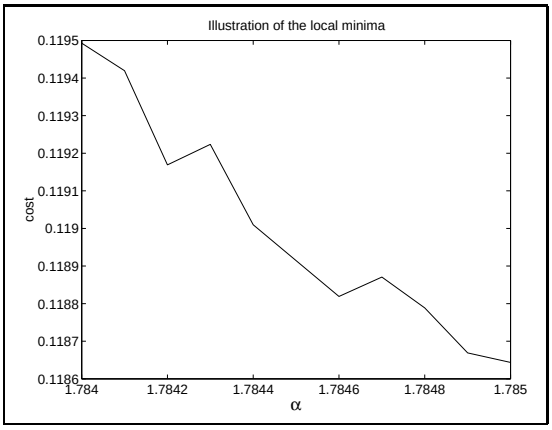


Figure 6.17: Objective function for tank 1 with $\beta = 0$ and $\gamma = 1.6046$

All parameters from the tanks were also checked with a flow series that was not used for calibration. The results obtained show similar fits to both the flow rate and the water height in all tanks. It could thus be concluded that the model was able to describe the dynamic behaviour of a river stretch along the tank sufficiently well.

6.4.4 Summary of the calibration procedure

A summary of the procedure to calibrate the CSTR model is given in Fig. 6.18. The first step is to set up a complex mechanistic model using the "de Saint-Venant" equations. This model is then used to generate information rich data.

In a second step, the surrogate model is constructed. A first phase is to calibrate the geometry parameters of the selected surrogate model. For this, the data collected during field measurement campaigns are used. In a second phase, the hydraulics are calibrated using the data generated with the complex mechanistic model. The separate tanks are calibrated by using an estimated Q-h relationship and parameter estimation using dynamic simulation.

As a final step, the model needs to be validated. The model is checked for both the flood wave and pollution wave propagation. For this, the separate tanks are connected. In this way, the complete river is modelled and it can be checked if the model is accurate enough for the selected use. The validation results are described in the next sections.

6.5 Simulating the flood and pollution wave propagation

So far, only individual tanks were calibrated, and the propagation of the flood wave by the CSTR model was not checked. In this section, the behaviour of the CSTR-in-series model will be checked against the predictions made by the Aquasim model. Two types of simulations will be performed: in the first one, only an upstream flow that is generated, without any inflow from the tributaries, and in the second simulation, tributaries do discharge into the stream. This is an important difference, since the water level downstream

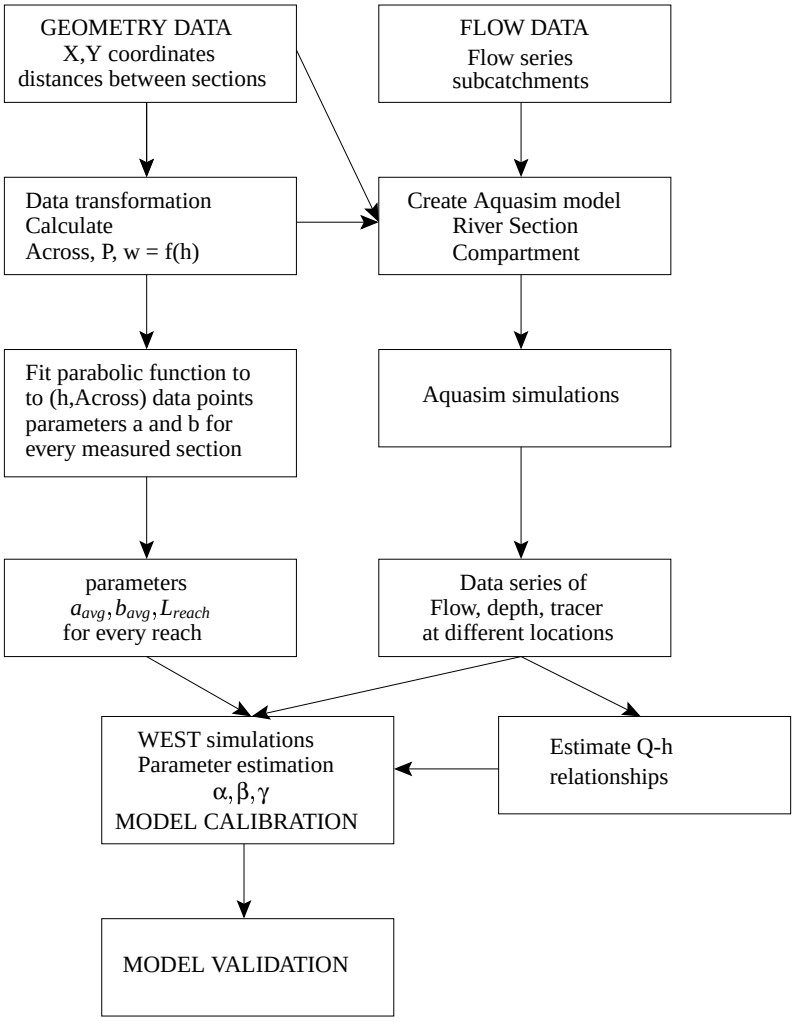


Figure 6.18: Procedure to calibrate a CSTR model

may create a backwater effect if the inflow from the tributary is large. For both types of upstream inputs, the propagation of a pollution wave along the river will be checked as well.

6.5.1 Simulating the flood and pollution wave – no side inflows

The data generated in this section are obtained by simulating the river Zwalm with the model built above. However, the tributaries were disconnected so that only the upstream conditions determine the behaviour of the river. Additionally, a tracer was added to this inflow with a concentration proportional to the flow rate. This allowed to judge the time difference of the flood wave and the pollution wave at the end of the river. This difference could be expected since it is known that a flood wave travels in a channel at a velocity that is higher than the water velocity as was clearly observed before (Huisman *et al.*, 2000; Krebs *et al.*, 1999b).

The CSTRs-in-series model was constructed by connecting the seven tanks, as calibrated above to each other in such a way that the outflow of the upstream tank was the inflow to

the downstream tank. The simulations were performed with the same influent data as the Aquasim simulations, i.e. a tracer was also added to the upstream flow.

The general wave propagation showed a similar behaviour as with the separate tanks. However, when looking into some more detail (Fig. 6.19) some small differences can be noted. For the tracer concentration of a model with seven tanks in Fig. 6.20 (solid line), more important differences can be noted. The tracer concentration starts to rise too early compared to the Aquasim model, while the peak concentration is reached too early. Also, the amplitude of the peak is lower, which can be explained by the higher dispersion of the pollution wave with the CSTR model.

Since the dispersion of a CSTR model can be decreased by increasing the number of tanks (Levenspiel, 1972), the original 7 tanks were each split in two and three tanks to check the model behaviour with more tanks. This resulted in a model with 14 tanks and a model with 21 tanks. The original lengths of the tanks were divided by 2 or by 3 in order to keep the same total length. All other parameters (i.e. a and b for the geometry and α, β and γ for the hydraulics) were kept to the original values. The simulation results are shown in Fig. 6.19 and Fig. 6.20.

It can be noted that the flow rate dynamics are hardly changed by the increased number of tanks, while the effect on the tracer concentrations is more pronounced. Both the peak time and the peak height are closer to the Aquasim predictions if the number of tanks increases. The desired accuracy of the model with respect to this aspect of modelling the river water quality will determine how many tanks are necessary to approximate the “de Saint-Venant” equations sufficiently close, but still have a simulation time that is shorter than the simulation time of the complex model. Care should also be taken not to use too many tanks, since this would decrease the dispersion too much. An infinite number of tanks reduces the dispersion to zero (Levenspiel, 1972).Hence, there is an optimum number of tanks with respect to fitting the dispersion observed in the Aquasim model. A compromise between model accuracy and calculation time needs to be found. It should also be noted that the CSTR-in-series model has a time delay of the pollution wave compared to the flood wave, which is correct and also noticed in the hydrodynamic simulation. This can be seen by comparing the maxima of the flow rate and the tracer concentration.

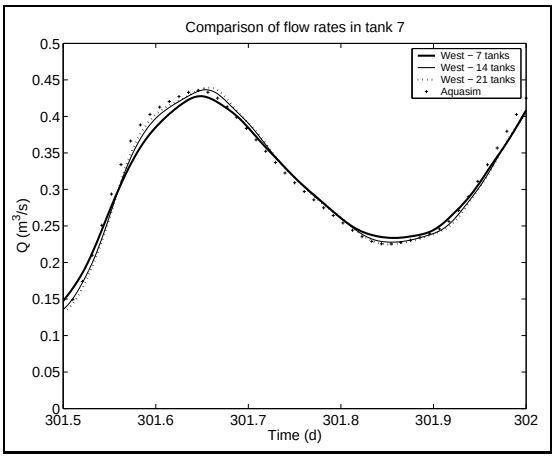


Figure 6.19: Comparison of flow with different number of tanks

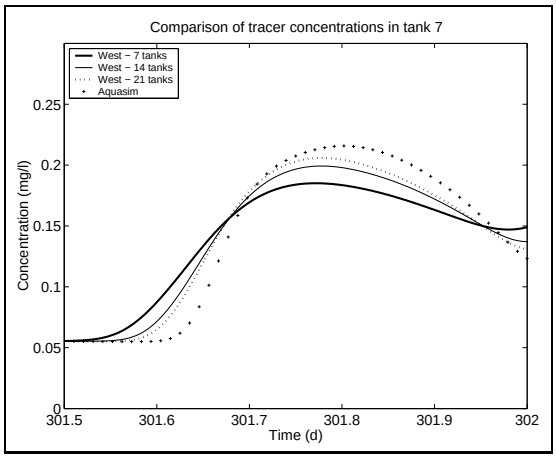


Figure 6.20: Comparison of tracer concentration with different number of tanks

These maxima are imposed at the same time in the input file of the simulation, but are, as Fig. 6.19 and Fig. 6.20 show, clearly shifted at the end of the river.

6.5.2 Simulating the flood and pollution wave – with tributary inflows

The flow of a tributary might influence the water level at a certain location and could therefore create a backwater effect towards upstream parts of the river. It is therefore important to consider the behaviour of the CSTR-in-series model while the tributaries are discharging into the main stream. The same data were generated as in the above model and used to check whether the estimated parameters were able to describe the flood and pollution wave propagation through the river.

In Fig. 6.21, the water height and flow rate for some tanks are shown for the same period that was used to calibrate the parameters of these tanks. It can be seen that the fits are very good for all tanks, except for tank 7 where deviations of a few cm in water height can be noted.

In Fig. 6.22 similar plots are shown for a period that was not used for calibration of the model parameters. Again, the flow and the water depth are simulated very close to the data. When looking into some more detail (the middle plots in Fig. 6.22), small differences in phase (i.e. time between the maxima) can be noted.

The predicted tracer concentrations are shown in Fig. 6.23. The presence of the tributaries does not have an influence on the prediction capacities of the CSTR-in-series model. This is due to the fact that these sidestreams were present when the data for the calibration of the separate tanks were generated. This means that in the training data, the flow limitations generated by the tributaries are present and can hence be incorporated in the parameters of the CSTR model. The flow data for the tributaries are generated by the Desim software package, which generates similar data series for the same type of events. This means that if the flow in the main stream reaches a certain point, also the tributaries will have a similar behaviour which can be modelled by the simple equations used in the CSTR models. If non-uniform rainfall is present in the catchment, and hence a non-uniform behaviour of the different subcatchments would occur, the CSTR-in-series model could have more problems incorporating this type of behaviour. So far, the results of the CSTR model are satisfactory for the research goals set: modelling river water quality.

6.6 Conclusions

In this chapter, a procedure to calibrate a CSTR-in-series model on the basis of data generated by a complex mechanistic model was outlined and tested on the river Zwalm. The first step was to set up a model for a non-rectangular tank, since the river under study could not be modelled with the assumption of a rectangular cross-section. A quadratic relationship ($A_{cross} = ah^2 + bh$)was found to be a good function to describe the field measurement data. In this way the geometric data could be estimated for every tank.

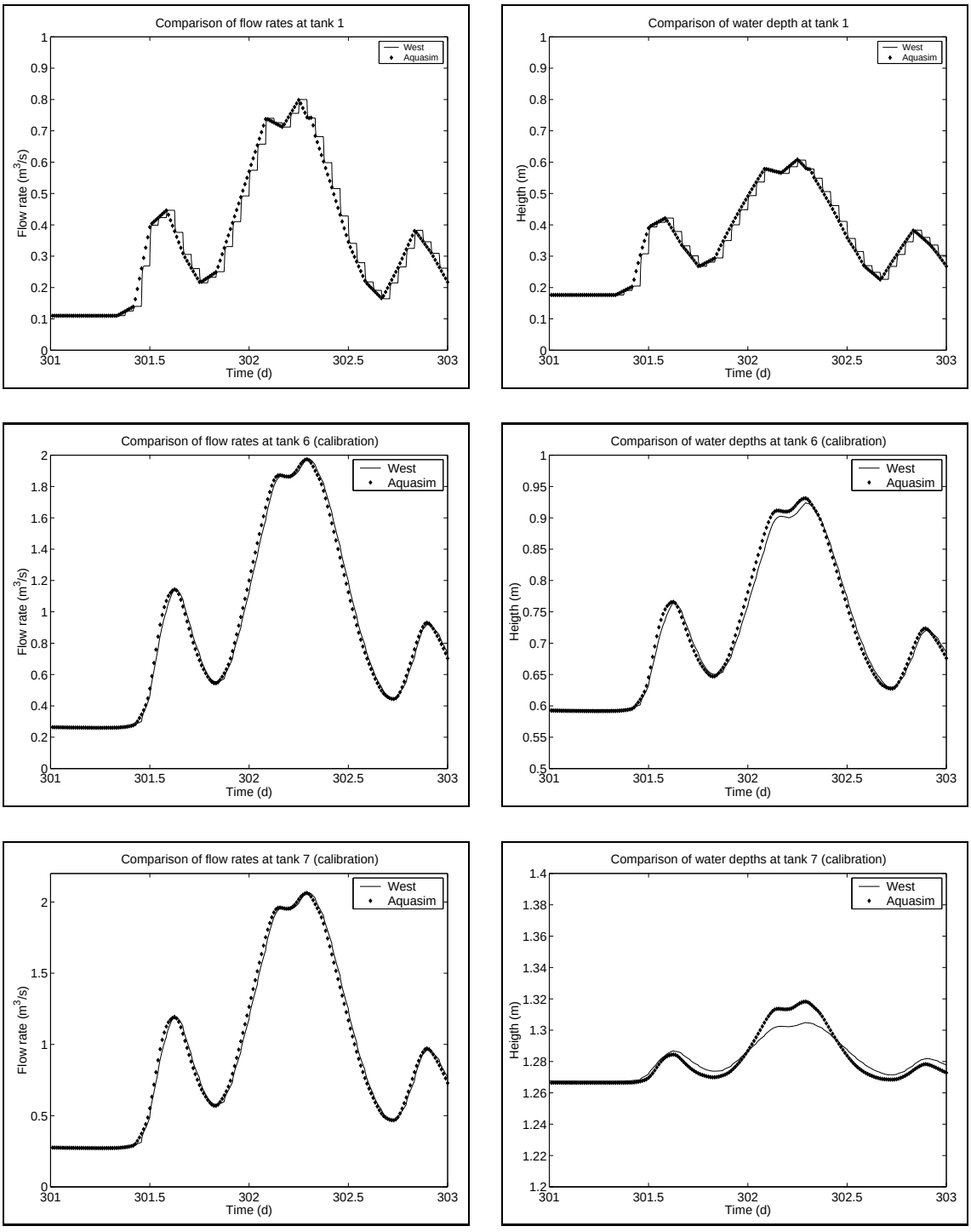


Figure 6.21: Comparison of the flow rates (left) and water height for the complete river model for different tanks for the calibration period

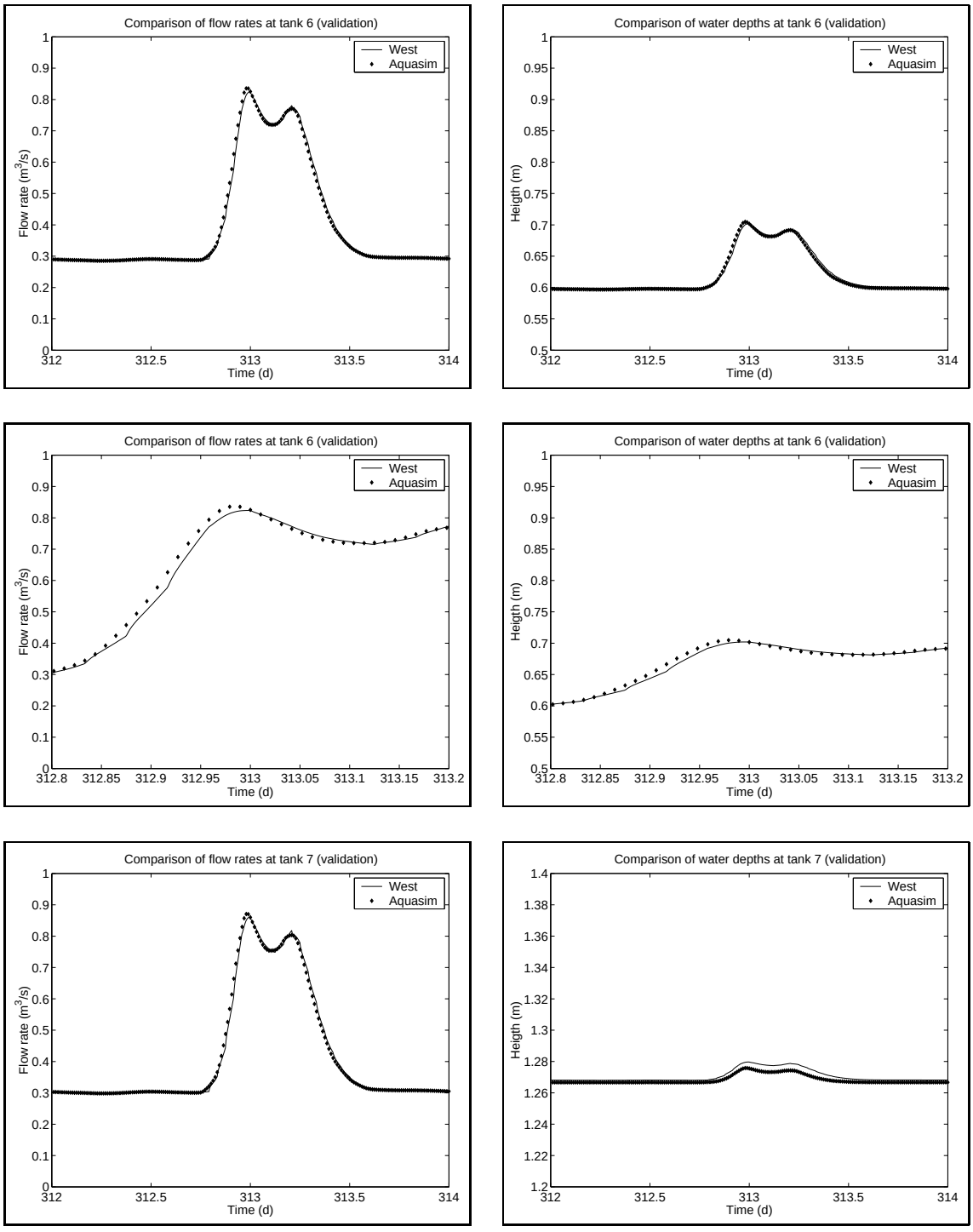


Figure 6.22: Comparison of the flow rates (left) and water height for the complete river model for different tanks for a validation period

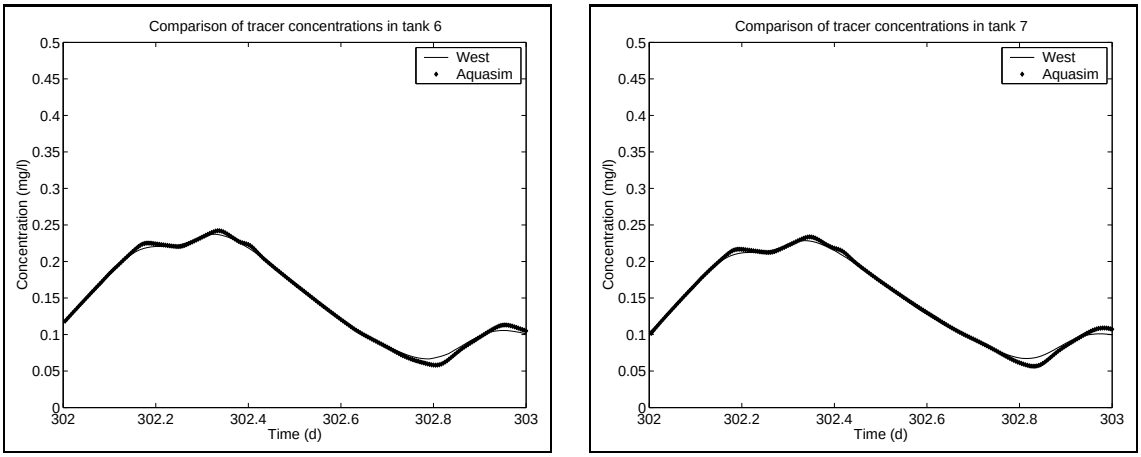


Figure 6.23: Tracer concentration at the end of tank 6 (left) and tank 7 (right)

The data generated with the complex model (implemented in Aquasim) were used to calibrate the hydraulic parameters of the model. Two sequential approaches were followed to estimate the parameters of each tank separately. In the first approach, the Q-h data pairs were plotted and an exponential curve ($Q = \alpha(h-\beta)^{\gamma}$) was fitted to these data. In some cases, the number of parameters could be reduced to only two. Depending on the type of tank, α and β or α and γ are needed. In the second approach, dynamic simulation was used to estimate the same parameters. In this optimisation the values obtained by the first approach can be used as initial values, since, in most cases, only small changes need to be made to the parameters in order to find the optimal parameter set.

In the last part, the propagation of the flood wave along the river channel was checked, together with the propagation of a pollution wave. It could be concluded that the CSTR model was able to describe the behaviour of the complex model sufficiently close. An increasing number of tanks used to describe the river hydraulics, allows to reduce the difference with the diffusive wave approximation of the “de Saint-Venant” equations. A compromise between accuracy and calculation time needs to be made in order to find the most suited model for the problem.

Chapter 7

Integrated modelling: the river Lambro case study

7.1 Introduction

In this chapter, the possibilities of integrated modelling with WEST® are demonstrated in a case study on the river Lambro (Italy). The interesting aspect of this system is that the WWTP plant in Merone has a hydraulic capacity that is insufficient to treat even the maximum dry weather flow. As a consequence, a daily overflow of untreated wastewater occurs, resulting in a daily peak of pollution in the river. A monitoring campaign has been set up in order to better understand the behaviour of the river (Gandolfi and Facchi, 1998a,b). In an initial study, a simple plug flow model has been used to describe the propagation of the pollution plug in the river (Whelan *et al.*, 1999).

One of the main problems when developing an integrated model is the incompatibility between state variables, processes and parameters used in the different submodels (see also chapter 4). An example of the difference between state variables is given by the treatment plant model and the river model, the former being typically based on COD and the latter on BOD. Maryns and Bauwens (1997) tried to avoid the problem by using the ASM model in riverine conditions but this approach did not give satisfactory results. To tackle this problem more fundamentally, the IWA task group on river water quality has developed a new COD based model, RWQM1 (Reichert *et al.*, 2001b). The connector between the ASM1 and the RWQM1 has been described in section 4.4. The states of this model are more like the ASM states, but some differences still remain. This is due to the fact that the full RWQM1 model is very detailed and describes more components than the ASM1 model.

For the calibration of both the treatment plant and the river model only a limited amount of data was available. The results of this study should therefore be considered only indicative. The main goal of this chapter is to illustrate the possibilities of the CSTRs-in-series river model to describe dispersion and water quality processes. A second goal is to illustrate the connection of the treatment plant model with the river model. Boron coming from the household wastewater has been used as a tracer to determine the number of tanks

in series to describe the mixing and dispersion behaviour of the Lambro. The concentration of Linear Alkylbenzene Sulfonate (LAS), was used as an indicator of pollution. Also some other water quality parameters have been taken into account in the paper, in order to check the capability of RWQM1 to predict the river water quality.

7.2 The Lambro catchment

7.2.1 Site description

The river Lambro lies North of Milano, Italy. The headwaters of the river Lambro lie in the Pre-Alps at approximately 1450m above sea level (a.s.l.), between the southern arms of Lake Como in northern Italy. The river flows southwards for approximately 130 km to its confluence with the River Po at approximately 50m a.s.l. The total catchment area of the Lambro is approximately 1950 km^2. The average annual rainfall for the catchment varies between 900 mm and 1500 mm (Holmes *et al.*, 1999).

The reach under study starts at Mulino del Baggero and ends at Biassono, with a length of 26 km, a decrease in bottom elevation of about 70 m, and a total drained area of approximately 300 km^2. The Lake Pusiano, which lies just upstream of Mulino del Baggero, feeds this part of the river, giving it a steady flow regime. The undulating land between Lake Pusiano and Milan contains large areas of intensive industrial and residential land-use such as the city of Monza and the Brianza area, as well as large tracts of arable land. An overview of the catchment and the location of the monitoring stations is shown in Fig. 7.1.

The whole reach can be divided in two stretches with two different bottom slopes. These stretches are characterised by a light average bottom slope increasing downstream, respectively 0.0015 and 0.0041 (m/m). The river profile in Fig. 7.2 shows the relative distance between sections along the reach. The river Lambro between Mulino del Baggero and Biassono S.Giorgio has a rather constant cross-section, which has been approximated by a trapezium with a bottom 11m wide and with side slope of 45°.

The most important pollution source in this stretch is the treatment plant of Merone, located 0.6 km downstream of Mulino del Baggero. This treatment plant receives the wastewater of approximately 120.000 inhabitant equivalents (IE). Prior to July 1998 the Merone WWTP was constantly working at its maximum hydraulic capacity (25400 m^3/d), but this did not avoid the daily overflow of dry weather wastewater (approximately 40% was regularly discharged untreated directly into the river). The daily bypass of raw wastewater imposed a marked diurnal cycle in pollutant concentrations in the river for a considerable distance downstream of the plant.

7.2.2 Monitoring activity

Six automatic water quality samplers were placed along the study reach between November 1997 and May 1998, in order to collect 24 hours composite samples (which allowed

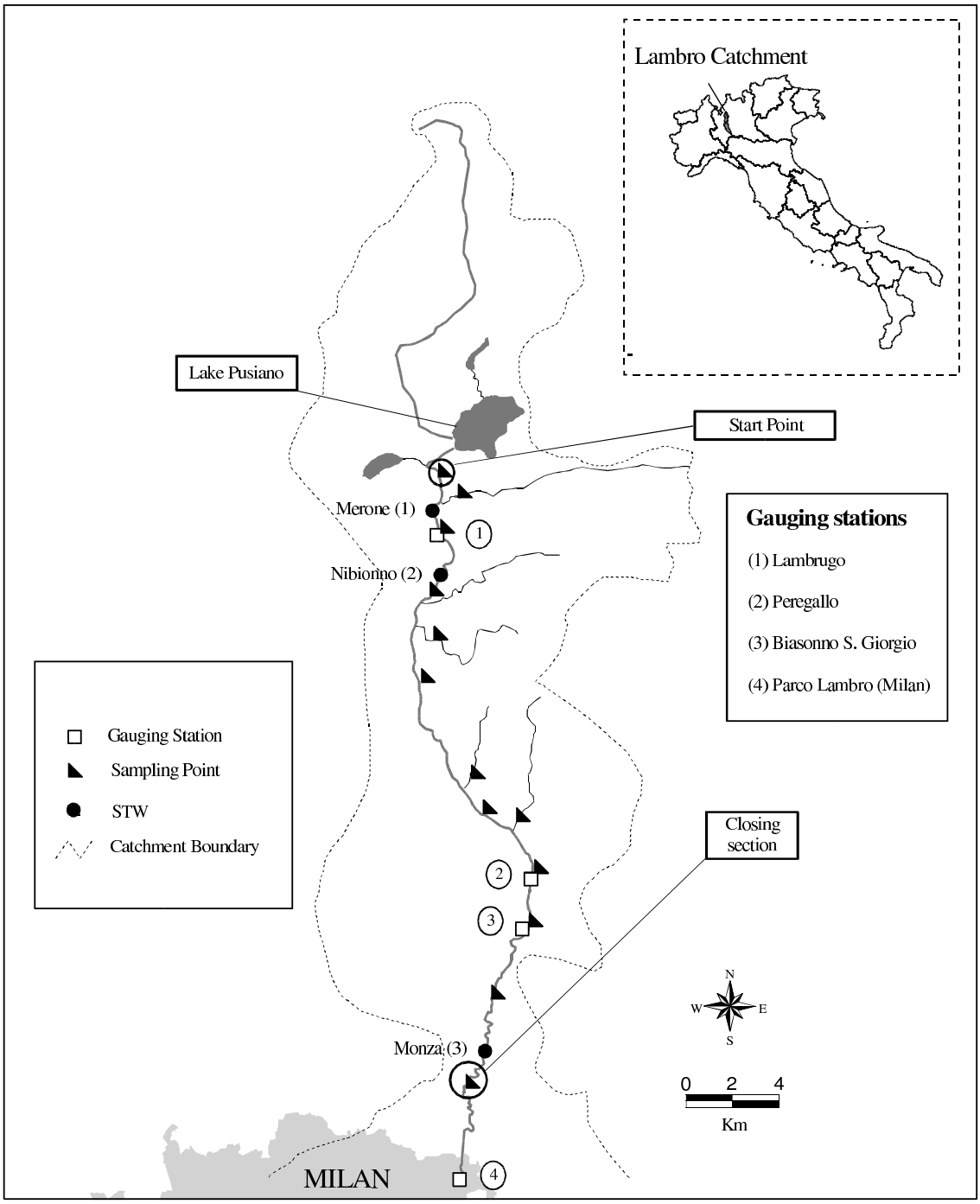


Figure 7.1: The Lambro catchment

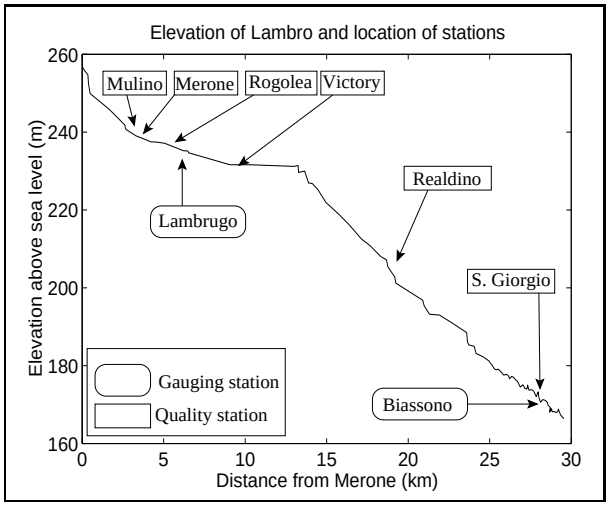


Figure 7.2: Altimetric profile of the river Lambro

Table 7.1: Distances between quality/gauging stations and bottom elevations.

Site at the end reach	Distance from Merone (m)	Bottom elevation (m)	Type of station
Mulino del Baggero	-600	239.0	quality
Merone	0	239.0	quality at WWTP
Rogolea	900	237.4	quality
Lambrugo	1100	237.4	gauging
Victory	5776	231.6	quality
Realdino	15032	208.0	quality
Biassono	25299	169.8	quality
Biassono	25500	168.6	gauging

the diurnal variability imposed by the Merone WWTP to be accounted for). One sampler was placed upstream of the Merone treatment plant, one to sample the untreated outflow of the treatment plant itself (i.e. also the inflow), while the other four were placed along the river downstream of the plant (Table 7.1).

A nine-day study was performed between the 7^{th} and the 15^{th} of July 1997 at the Merone WWTP with the aim of evaluating plant efficiency. The study was executed using automatic water samplers at the inflow and the treated outflow of the plant. Twelve two-hourly composite samples were collected over 24 hours on one day, while one 24 hour composite sample was collected on each of the remaining days. Water samples were analysed for LAS, boron, total phosphorus, total nitrogen and suspended solids.

Two measurement campaigns (February 1998 and May 1998) were performed to follow the diurnal wave of pollutants as it moved along the river stretch. Two hourly samples were taken at the different stations and analysed for LAS, boron and a series of standard water quality variables. Boron and LAS data were collected during one of the two measurement campaigns together with some other significant water quality parameters, have been used for this study. During both campaigns the flow was considered to be

steady (Gandolfi and Facchi, 1998a). Two gauging stations are present within the studied river stretch (Table 7.1). For these sites good quality rating curves (Q-h relationships) are available. The data for the May campaign were incomplete due to a malfunctioning of the samplers in the downstream part of the river. Therefore, these data cannot be used for the calibration of the river model.

7.3 The Merone treatment plant modelling and calibration

The WWTP in Merone consists of a coarse and fine grid, sand removal, oil removal, a mixing and flocculation tank (700m^3), a primary settler (area: 908 m^2; working height: 2.5 m, double weir), two circular biological oxidation tanks with surface aeration (total volume of 6300 m^3), two secondary settlers (area: 1018 m^2; working height: 3.3 m; double weir) and a disinfection unit.

In the oxidation tank a control system for dissolved oxygen is present, consisting of the raising or lowering of the weirs in order to change the water level, so that the immersion of the rotors of the surface aerators increases or decreases. The set point of the controller is 2.5 mg O_2/l.

The sludge concentration in the aeration tanks was about 4 g TSS/l, of which 70% is organic. Settling was modelled by assuming a constant non-settable fraction of the inlet solids going into the effluent. For the primary settler this fraction was set to 30%, while for the secondary settler it was set to 0.6%. These values were adjusted to match measured average effluent suspended solids concentrations. The reactions in the activated sludge units are described by the ASM1 (Henze *et al.*, 2000), with the parameters suggested in the report as a starting point. An extra component was added to the model in order to describe the behaviour of LAS in the plant. LAS is known to degrade almost completely in activated sludge treatment plants (Boeije *et al.*, 1998), but only in aerobic conditions. A first order removal mechanism was assumed, combined with a switching function for oxygen which turned off degradation in anoxic conditions. Corresponding oxygen uptake and growth of heterotrophic biomass was also included, while the yield was taken the same as the yield during degradation of readily biodegradable COD, S_S.

The available data were scarce and hence only an approximate calibration could be accomplished. Steady state calibration was performed on the average of the nine days, while dynamic calibration was performed on the data of day nine. The suspended solids concentration in the activated sludge tanks was mainly influenced by the amount of inert solids present in the influent to the plant since these inerts accumulate in the system. Good results were obtained with a ratio of 40% X_I and 60% X_S in the inlet particulates (Table 7.2).

Although both activated sludge tanks are aerated, total nitrogen balances indicated simultaneous nitrification and denitrification in the plant. A macro-scale idea on how the water flows in circular tanks with two surface aerators is presented in Fig. 7.3. As both aeration and in- and outflow occur at the top of the tank, some water may find a shortcut without entering the anoxic phase. At the bottom the water has a lower flow velocity and oxy-

Table 7.2: Steady state simulation data and measured data

Variable	Measured	Simulated
SS in aeration tank (g/l)	4	3
SS in outflow (mg/l)	18	17.8
SS in underflow (g/l)	8	7.4
TN (mg N/l)	15	15
LAS (mg/l)	4.6	4.6

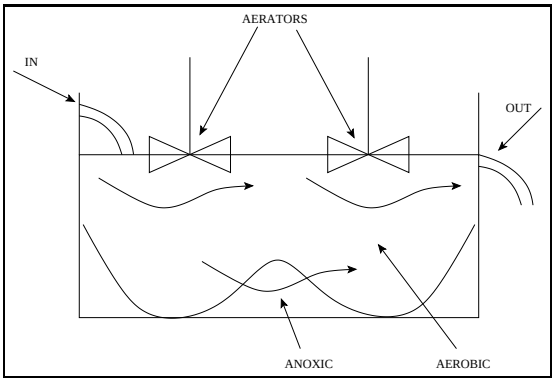


Figure 7.3: Aerated tank and anoxic zone

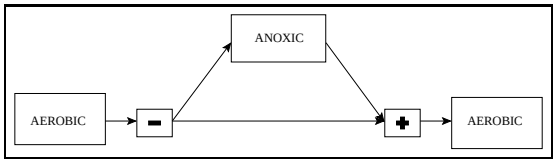


Figure 7.4: Implementation of the aerated tank

gen concentrations. Another explanation for the observed nitrogen removal might be the presence of anoxic zones inside the sludge flocs (Pochana *et al.*, 1998).

This first hypothesis was not confirmed by direct measurements, but it allows to describe dead zones in a reasonable way. Therefore, one anoxic and two aerobic tanks are used in the model, keeping the total volume equal to the existing volume (Fig. 7.4). Total nitrogen in the effluent was mainly influenced by the anoxic volume and the flow to the anoxic tank. Manual adjustment of these parameters yielded a volume of 10% and a flow of 5% to the anoxic tank (Table 7.2). A simple sensitivity analysis showed that the volume of the anoxic tank did not have a large influence on the LAS concentration in the effluent, which is the main focus of this work. For example, if the volume of the anoxic tank changed with 10%, the effluent LAS concentration would change only by 2.2%. This could be explained by the fact that no degradation occurs under anoxic conditions, and the aerobic residence time was still sufficiently large to degrade most of the LAS.

The first order degradation constant of LAS was calibrated on the basis of the average value of the nine days. The Praxis algorithm (Brent, 1973) was used to estimate the value of the degradation constant K_{LAS}. For the steady state simulation, a value of 176 d^{-1} was found to be the best value. With this value, the steady state effluent concentration for LAS was the same as the average of the data collected during the measurement campaign.

After this steady state calibration, a dynamic simulation was performed with the influent data of day 9. The results for the suspended solids and the total nitrogen concentrations are shown in Fig. 7.5 and Fig. 7.6. As expected, the model does not reproduce the dynamic behaviour of SS concentration, and this is due to the characteristics of the Pointsettler model. As for TN, the simulation follows the data set, even if not too closely. A pos-

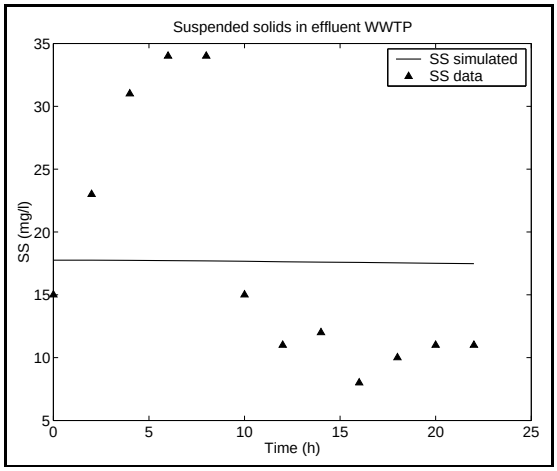


Figure 7.5: Dynamic simulation of the suspended solids in the effluent

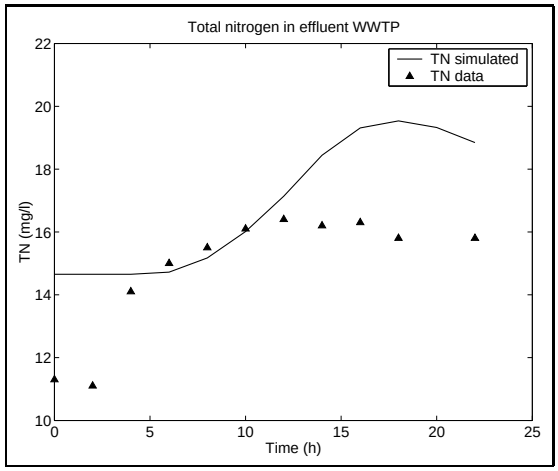


Figure 7.6: Dynamic simulation of the total nitrogen in the effluent

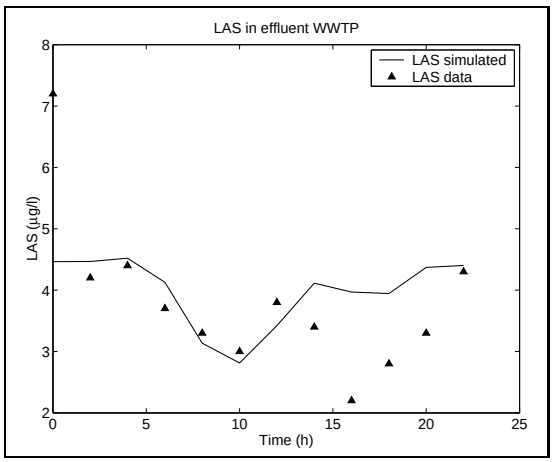


Figure 7.7: Dynamic simulation of the LAS in the effluent

sible explanation is the delay between the measured influent and corresponding effluent concentrations. The hydraulic residence time in the aeration basins is about 12 hours, while the total hydraulic residence time is about 20 h (primary and secondary settlers included). Hence, the measured effluent on the day during which the two hourly samples were taken is still largely influenced by the influent on the previous day for which only average information is available.

An automatic parameter estimation of K_{LAS} has been performed by means of a trajectory optimisation. The optimisation algorithm used was Praxis (see section 3.6). The value for K_{LAS} that minimises the difference between the simulation output and the data set is equal to 194 d^{-1}. This value is higher than the one found for the steady-state conditions, since from the data a faster degradation is supposed, considering that the average LAS concentration in that day is lower than the average for the nine days. In Fig. 7.7 the output of the model with the optimised K_{LAS} is compared to the actual data set for that day. Taking into account a measurement error of 15%, one could state that the modelled effluent concentration corresponds to the observed data.

The value of K_{LAS} = 176 d^{-1} or 194 d^{-1} found by steady state or dynamic estimation

Table 7.3: Comparison between literature and actual conditions

WWTP Characteristic	**Boeije *et al.* (1998)**	**Merone WWTP**
loading [gLAS / (gSS·d)]	$3.43 \cdot 10^{-4}$	$2.67 \cdot 10^{-4}$
O_2 [mg/l]	3.5	2.5
T [°C]	18-23	> 25
% removal	98.6	99.5
K_{LAS} [d^{-1}]	96	176.74

respectively, is almost the double of what has been found in literature (Boeije *et al.*, 1998). In Table 7.3 the conditions in the ASU of the WWTP in Merone are compared with the conditions of the experiments conducted by Boeije (batch experiments on a small-scale pilot plant). This difference for the value of K_{LAS} is explained by a higher temperature and by a longer exposure of the bacteria in the plant to LAS, so that the biomass present in the WWTP is more adapted to consume that compound. Also absorption to the activated sludge was not taken into account in this model, and may add to the observed removal rate (Boeije, 1999).

7.4 The river Lambro modelling and calibration

7.4.1 Calibration of the hydraulics

The hydraulics of the river Lambro have been modelled by using CSTRs with variable volume in series. This modelling approach requires the river to be divided into stretches, in which the end of a stretch usually coincides with river discontinuities or sites where information is available as input data or required as model output (Reda, 1996). The number of CSTRs-in-series has been used as a calibration parameter.

The rating curves at Lambrugo and Biassono are very similar, probably due to the fact that the hydraulic geometry (i.e. section shape) of the river is more or less uniform along the study reach. Consequently, the assumption has been made that the rating curve varies linearly along the river. The number of tanks has been increased step wise and the rating curves were linearly interpolated between the two known rating curves. To allow an interpolation of the rating curves, both equations have been transformed to second order polynomials with similar parameters (see Table 7.4). A comparison of the two curves is shown in Fig. 7.8.

The river reach under study was initially divided into five stretches, with the end of each stretch coinciding with sites at which water quality data were available. This first division immediately proved its inadequacy to model the hydraulic behaviour of the Lambro. Therefore, these five stretches had to be split up into smaller tanks.

The pollution wave of boron coming from the bypass household wastewater has been used as a tracer to optimise the number of tanks necessary to model the hydraulic behaviour of the river Lambro. Boron is chemically inert and is a well-established conservative tracer

Table 7.4: The original and transformed rating curves of the gauging stations in the catchment - h is expressed in meters and Q in m^3/s

Gauging Station	**Rating curve relationship**	**Limits of applicability**
Lambrugo	$Q = 13.05h^2 - 3.886h - 1.396$	0.51 <h< 2.32m
Biassono	$Q = 19.05(h - 0.35)^{1.926}$	Not specified
Lambrugo (transformed)	$Q = 15.925h^2 - 8.667h + 0.5$	$0.51 < h < 1.20m$
Biassono (transformed)	$Q = 16.108h^2 - 8.1939h + 0.4$	$0.3 < Q < 12m^3/s$

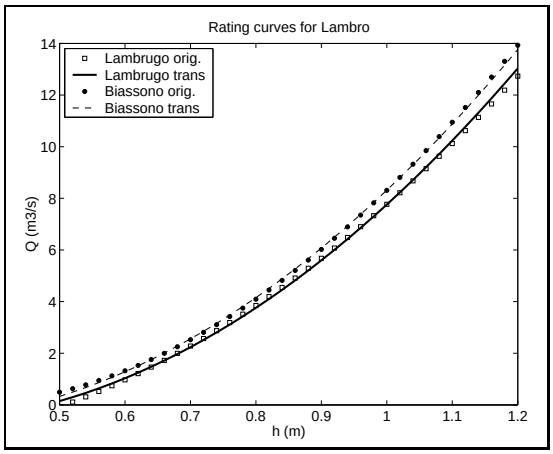


Figure 7.8: Comparison of the original and transformed rating curves at Lambrugo and Biassono

for use in environmental monitoring studies since it is not removed significantly in sewer systems, treatment plants or rivers (Matthijs *et al.*, 1997).

Fig. 7.9 shows the simulation results of the boron concentration in the last section at Biassono, 26 km downstream the Merone WWTP. Measured data are compared to the simulated data with 10, 24 and 47 tanks. Increasing the number of tanks raises the peak delay, in agreement with the behaviour of a pollution wave in a cascade of tanks described earlier (see section 6.5). For the 10-tanks simulation, the simulated boron peak arrives early to the measurement data in the last section of Biassono. For the 24- and 47-tanks simulations the peak arrives too late (Table 7.5 and Fig. 7.9). The simulated pollution travel time with 47 tanks is slightly longer than observed in the measured data: the delay is 1.6h, which is 2.4% more than the whole travel time from the plant to that section. This may be caused by some imprecision, i.e. underestimates of the velocity field along the river, measured discharge slightly lower than the real flow discharge during the campaign, strong simplification of the river geometry, etc. However, a more accurate analysis is not feasible, since all available hydraulic and morphologic data are already used.

With increasing number of tanks, dispersion decreases, but the maximum amplitude of the simulated boron peak concentration is still lower than indicated by the measurement data for each studied case. Again, the low number of data, and the missing beginning and end of the peak, do not allow for further improvement of the simulation.

The average length of each tank was found to be about 500 m. The fitting between simulated and measured data was judged on the basis of (1) a visual comparison (Fig. 7.9) and (2) a comparison of the sums of squared errors (SSE) (Table 7.6). In both cases the

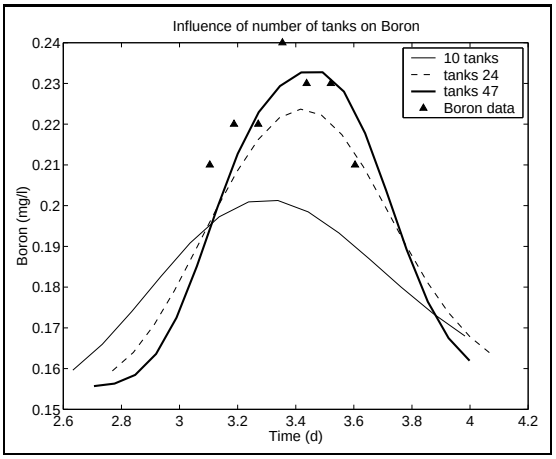


Figure 7.9: The effect of the number of tanks on the boron concentration in the last stretch of the Lambro

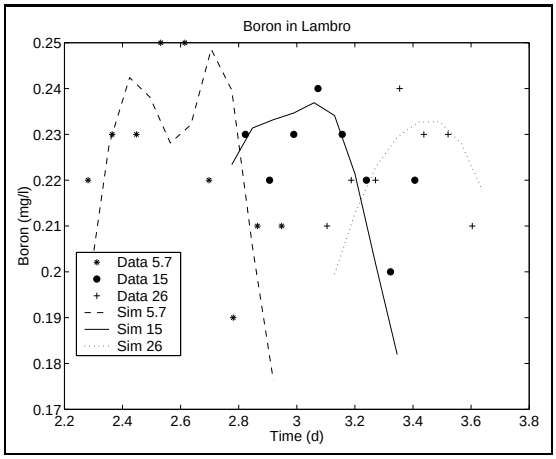


Figure 7.10: The boron concentration along the river at different stretches

Table 7.5: Peak Delay and differences in amplitude for boron

No. of tanks	Delay [h]	Difference in amplitude
10	-1.6	-19%
24	+1.4	-7%
47	+1.6	-3%

Table 7.6: SSE for boron and LAS for the model with 47 tanks and $K_{LAS} = 2.04$

Quality station	SSE boron	n	SSE LAS	n
Rogolea (km 1)	0.0100	8	0.0019	8
Victory (km 5.7)	0.0038	8	0.0050	8
Realdino (km 15)	0.0004	8	0.0013	8
Biassono (km 26)	0.0004	7	0.0002	7

model with 47 tanks turned out to be the best model (i.e. the model looked the best and had the lowest SSE). For a statistical comparison of the different models, F-tests were performed on the SSE (Dochain and Vanrolleghem, 2001). This analysis showed that the model with 47 tanks was significantly better than the models with 5 and 10 tanks, but was not significantly different from the model with 24 tanks (at a significance level of 95%). Nevertheless, the model with 47 tanks was kept, since it had a lower SSE for the same number of parameters.

The large number of tanks needed to approximate the dispersion in the river Lambro, makes the model fairly complicated, in spite of the basically very simple model. This has as a consequence that the model is more difficult to handle as a whole. However, the hierarchical model structure in WEST® aids in structuring the complex model. It is practically impossible and not necessary to monitor at 47 places along the river in order to have data for every tank. Since no intermediate sources of the pollutants are expected and pollutant concentrations change gradually, the location of the monitors was found to be appropriate, but a longer time series of samples would have helped with the calibration of the model.

Once the total number of tanks was determined by fitting the boron profile at the end of the river reach, the model was validated by comparing the predicted and the measured data at the intermediate sampling points along the whole reach (Fig. 7.10). At Victory station (km 5.7), the observed data indicate an increase in average and peak concentrations of boron,

Table 7.7: LAS in-stream removal rates in the literature (Boeije *et al.*, 2000)

Authors	**Rate coefficient (d^{-1})**	**River**	**Notes**
Waters	3.12 - 21.6	Avon, Tean	-
Schröder	1.92 - 11	mesocosm	-
Steber	3.6 - 7.44	mesocosm	LAS conc. 0.1-5 mg/l
Hennes	0.48 - 2.88	Rapid Creek	5 °C
Amano	1.68	Oohori	25 °C, large river+lake
Amano	0.14 - 0.216	Teganuma	5 °C, large river+lake
Schöber	26.2	Isar	Below WWTP outfall
Takada	10.3 - 41.5	Nogawa	7 - 27 °C, small river
Schröder	5.04 - 15.12	Anger, Rur	small river
Grob	0.72 - 18.5	Itter	river source to mouth
Fox	6.24 - 7.44	Red Beck	9 °C, small river

in comparison to the first station downstream of the treatment plant (Rogolea station). Since there were no relevant input discharges entering the river between the two points, this could only be explained by the absence of complete lateral mixing of river water and the outflow of the treatment plant, by the time the river reaches Rogolea less than 1 km downstream of the treatment plant. The sampler was located on the opposite side of the river in comparison to the effluent discharge point. This issue can also be noticed in the mass balance of the model, which predicted higher concentrations of boron than the measured ones for the first station. After 15 and 26 km (Realdino and Biassono stations) the model gives an acceptable fitting of the boron observed data.

Taking into account the previous remarks, the simulation results shown in Fig. 7.10 were considered sufficiently close to the measured data points. In fact, both the travel time and the amplitude of the pollution wave were approximated reasonably well. Therefore the tanks-in-series model was considered to be able to reproduce the hydraulic behaviour of the river Lambro in the given conditions.

7.4.2 Calibration of the in-stream LAS degradation constant

The most important parameter influencing the concentration of LAS in the river is the first order degradation constant K_{LAS}. The best value of k was found to be 2.04 d^{-1}, based on the manual minimisation (trial and error) of the SSE value at the different sites. The SSE values for the LAS concentrations for all measuring station sites can be found in Table 7.6. This value is close to other values previously used for the Lambro (1.25 d^{-1} in (Gandolfi and Facchi, 1998a, steady state model), and 1.92 d^{-1} in Whelan *et al.* (1999, plug flow model). In literature this parameter is found to vary between 0.14 to 41.5 d^{-1} (Boeije *et al.*, 2000). Water temperature and microbial population density are the most important factors explaining this large variability. The water temperature during the measurement campaign was found to be 18°C.

In order to find out more about the hydraulic behaviour of the river, two theoretical formula can be compared. The theoretical delay (i.e. the time between the maxima at the

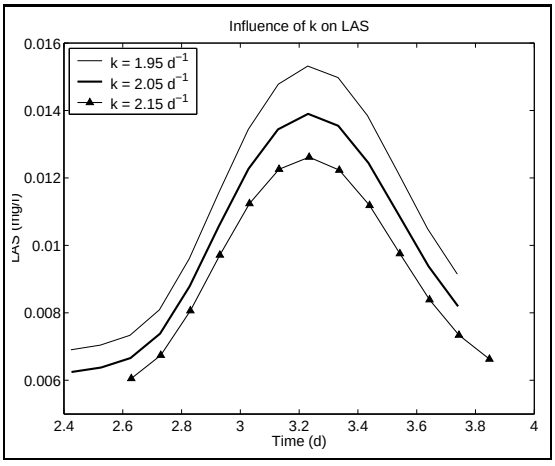


Figure 7.11: The influence of K_{LAS} on the peak height and travel time

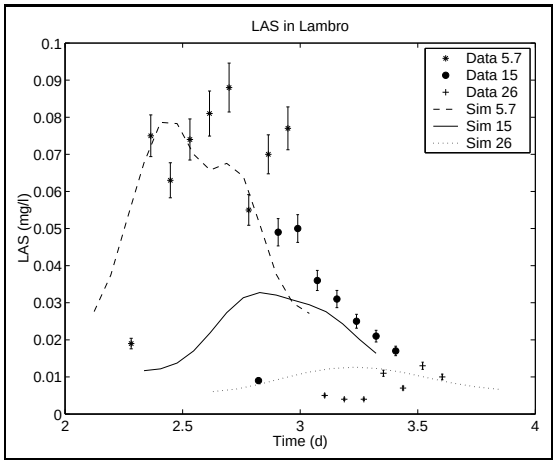


Figure 7.12: The LAS concentration along the river at different stretches

beginning and the end) for an impulse response with first order degradation kinetics, in case of a cascade of n-reservoirs with equal volume, is (Levenspiel, 1972):

$$t_m(d) = \frac{n-1}{k}(1-\beta^{\frac{1}{n}}) = 1.043 \tag{7.1}$$

where

n the number of tanks
k the first order degradation constant
β the ratio between the final and the initial concentration

It is possible to use the above formula to evaluate the travel time with the 47-tanks model, because this model has tank lengths that are very similar for each reservoir. Note that the delay time is not dependent on *k* for a plug flow:

$$t_m(d) = \frac{L}{u} = 1.067 \tag{7.2}$$

where

L the length of the plug flow
u the average flow velocity

Hence, the peak travel time in a cascade of 47 tanks turned out to be very similar to the peak travel time in a plug flow. For this reason, the effect of *k* on the peak travel time can be neglected here. On the other hand, *k* has a clear influence on the amplitude of the peak at the end of the river reach (Fig. 7.11). A good estimation of the first order decay value of LAS is important to get a good approximation of the peak height, but has only little influence on the time-delay of the peak.

Some simulation results are shown in Fig. 7.12. It can be observed that despite the large measurement error (15% coefficient of variance), the simulation results do not match the

observed concentrations very closely. For the Victory station (5.7 km) the data are still reasonably close, but further downstream only the mean values are approximated well. The dynamic behaviour at both the Realdino (km 15) and Biassono (km 26) sampling site show that the modelled dispersion for LAS is too large, while the simulated peak anticipates the measured one. It turned out that 47 tanks are not sufficient to describe all phenomena contributing to the propagation of this degraded compound. These results are somewhat contradictory with the results obtained for the boron simulations, and need to be investigated further.

7.4.3 Submodel selection

In addition to the LAS simulation, a submodel of the RWQM1 was used in the river to model the other processes occurring in the water. Therefore, the model could also be used to judge the effect of an upgrade of the plant on the other water quality components such as ammonia and oxygen. Since some processes used in the RWQM1 were considered unimportant in the present case study, and since insufficient data were available to calibrate the full RWQM1, it was decided to eliminate some states and reactions from the model.

Since instream river oxygen data indicated the oxygen concentrations to be always higher than 7 mg O_2/l (Gandolfi and Facchi, 1998a), processes taking place in anoxic conditions were considered not to be of any importance in the Lambro and hence eliminated from the model. Nitrifying bacteria and oxidised nitrogen were grouped together in one group of organisms X_A and one species of S_{NO}, since no data on nitrite were present in the data set. No data were available for algae and consumers, so they were not taken into account in the model. The carbonate equilibrium was also considered irrelevant for this case study and adsorption and desorption of the phosphates could not be judged since no data were available. More info about submodel selection of the RWQM1 can be found in Reichert *et al.* (2001b).

The full connector as described in 4.4, had to be reduced as well, but the concept still proved to be useful in connecting the two models. Both the treatment plant model ASM1 and the submodel of the RWQM1 are available in the model base of WEST® The integrated model could be created easily, since WEST® allows the reuse of models.

7.5 Integrated simulations

The two calibrated models as described above were used to study the impact of the daily dry weather overflow on the river Lambro. The following situations were considered: the situation before June 1998 with the treatment plant as described above and the situation after June 1998 with an increased plant capacity. Indeed, from June 1998, another primary settler identical to the first, an oxidation tank (volume: 3150 m^3) and a third secondary settler with the same characteristics as the existing ones have been operational at the plant. This increased the hydraulic capacity of the plant to 38000 m^3/d. However, all available data were collected in the period before this extension of the plant.

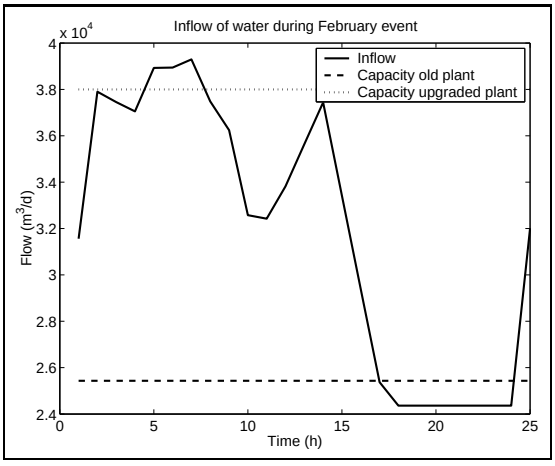


Figure 7.13: The water flow at the Merone WWTP during the February campaign

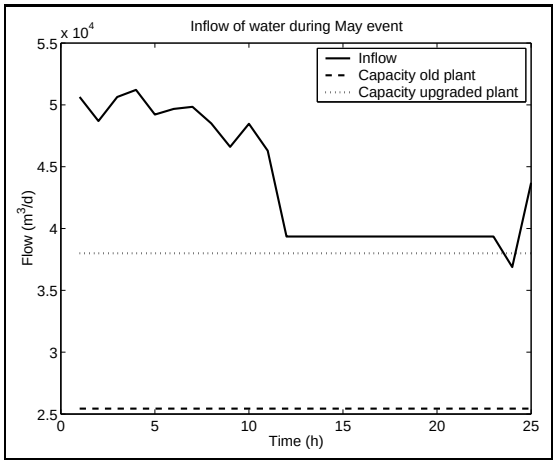


Figure 7.14: The water flow at the Merone WWTP during the May campaign

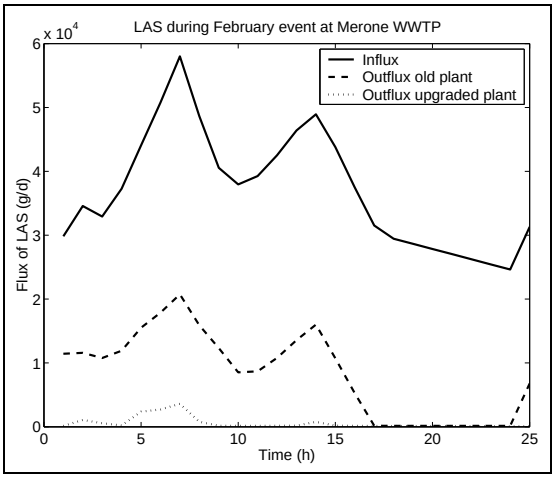


Figure 7.15: The flux of LAS coming from the WWTP and the CSO during the February campaign

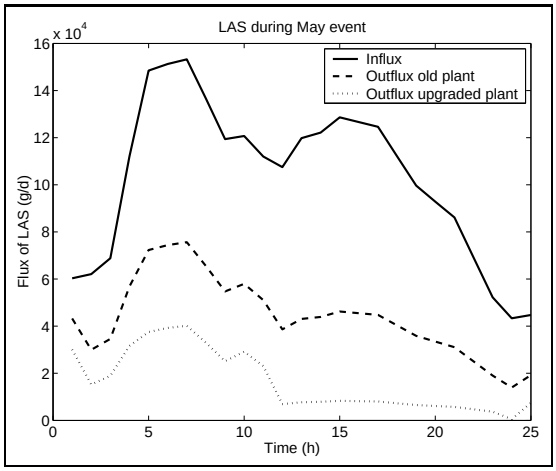


Figure 7.16: The flux of LAS coming from the WWTP and the CSO during the May campaign

The effect of the upgrade can be clearly seen when looking at the water flow at the WWTP compared to the capacity of the plant (Fig. 7.13 and Fig. 7.14). With the old plant capacity, a large bypass will occur in both cases. With the new plant capacity, more water can be treated and the bypass will be smaller in any case, and shorter during the May 1998 event studied here. As mentioned before, the data for LAS at the end of the river were missed during the May campaign, but the upstream data could still be used to evaluate the effect of the WWTP on the river.

The volume of untreated water during each event determines the amount of LAS that is discharged into the river. It is clear that this will be less with the upgraded plant, as can be seen in Fig. 7.15 and Fig. 7.16. The reduced emission of LAS from the effluent and the bypass together can be noted. This is due to the fact that the LAS concentration in the effluent of the plant is very low, due to the biodegradable character of LAS.

The integrated model also allows the evaluation of the effect of the upgrade of the plant on the LAS concentration in the river. The results of the simulation with the old and the

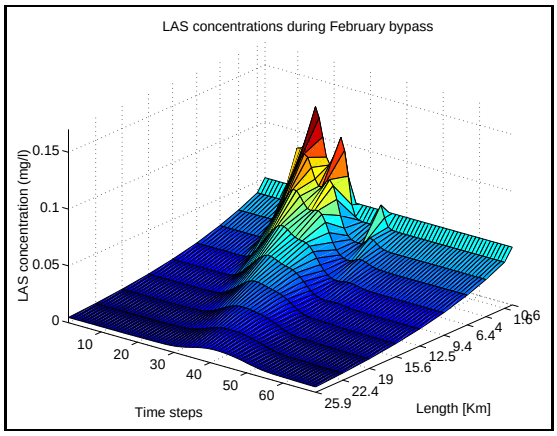


Figure 7.17: The LAS concentrations during the February campaign with the old WWTP

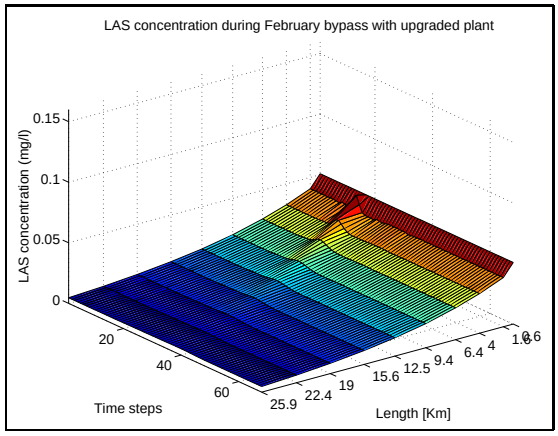


Figure 7.18: The LAS concentrations during the February campaign with the upgraded WWTP

new plant configuration respectively, are shown in Fig. 7.17 and Fig. 7.18. It is clear that the upgrade of the plant has a positive effect on the river water quality of the Lambro during the daily high dry weather flow conditions. These predictions should, however, be confirmed with field data. The obvious decrease in concentration of LAS at the end of the river is a combination of the dispersion and degradation phenomena.

In conclusion, this integrated model allows to judge the water quality of the river Lambro in the given conditions. It can be used to predict the evolution of the LAS concentration in the river. However, both field data measurements and model predictions are uncertain, and the results should thus be looked at with care, certainly when applying the model in other conditions than the one the data were collected in.

Since also a submodel of the RWQM1 was implemented, the effect of the upgrading of the treatment plant can also be qualitatively judged for other water quality variables (Fig. 7.19 to Fig. 7.24). It should be stressed that these result from an uncalibrated model, and should be carefully interpreted. In general, one can say that the beneficial effect of the upgrading of the plant cannot only be noted in LAS, but also in ammonium and oxygen concentrations. For nitrate, an adverse effect was noted. This is due to the fact that more ammonia is converted to nitrate in the WWTP, while almost no denitrification occurs. Hence, the nitrate concentrations in the river are higher after the upgrade than before. Since ammonium concentrations are lower, toxic effects from unionised ammonia are less likely. Also oxygen depletions were less deep with the upgraded plant.

7.6 Discussion: data requirements

This case study illustrates the fact that a lot of data are needed to create an integrated model. For both the WWTP and the river model, measurement campaigns have been designed and performed. The goal of these campaigns was to gain insight in the behaviour of LAS in the Merone WWTP and the river Lambro.

For the calibration of the Merone WWTP, data about nitrogen, phosphorus, boron, LAS and suspended solids have been analysed. While this allows to make a mass balance for

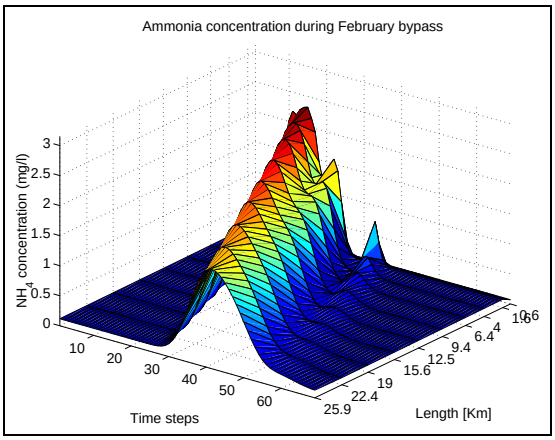


Figure 7.19: The ammonium concentration during the February campaign with the old WWTP

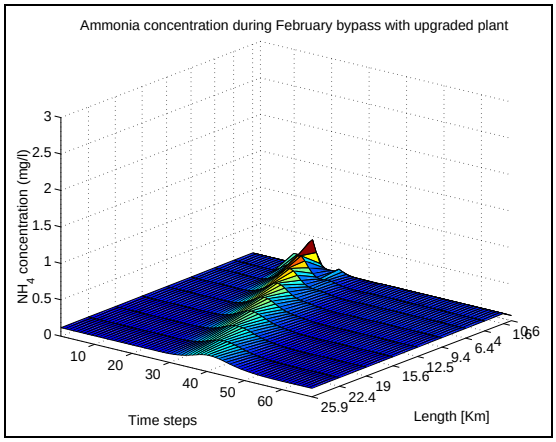


Figure 7.20: The ammonium concentrations during the February campaign with the upgraded WWTP

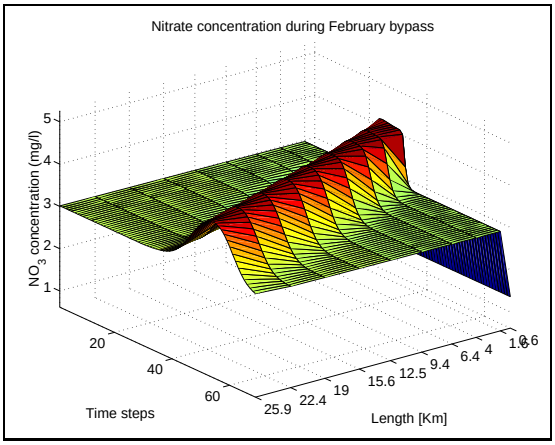


Figure 7.21: The nitrate concentration during the February campaign with the old WWTP

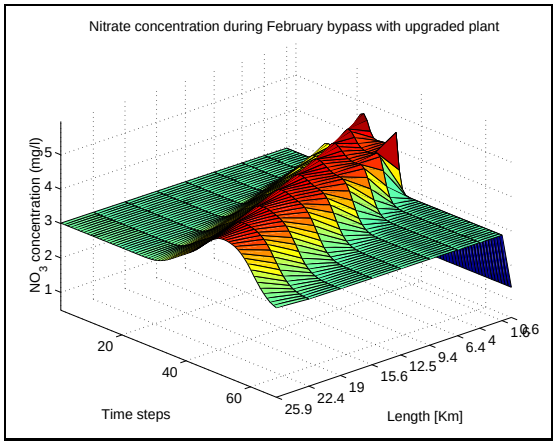


Figure 7.22: The nitrate concentrations during the February campaign with the upgraded WWTP

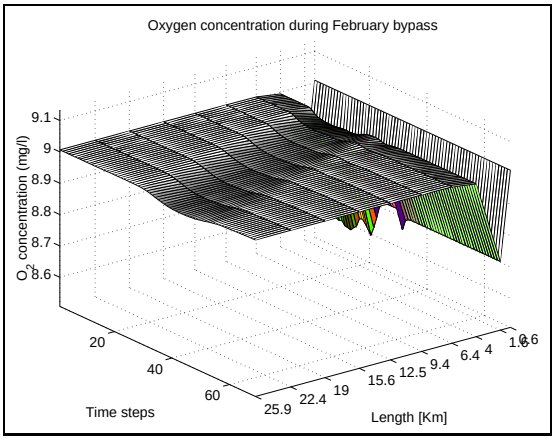


Figure 7.23: The oxygen concentration during the February campaign with the old WWTP

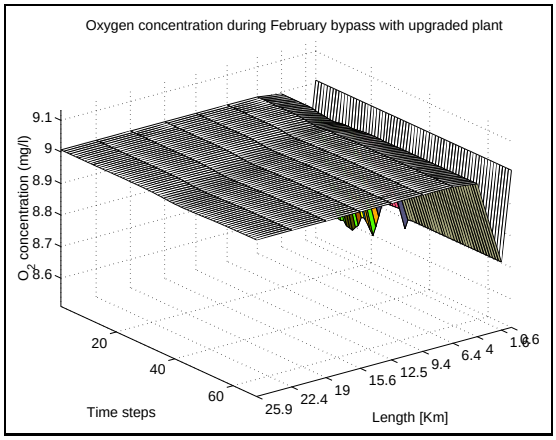


Figure 7.24: The oxygen concentrations during the February campaign with the upgraded WWTP

the nutrients and estimate a removal efficiency or a degradation constant for LAS, this is insufficient for the calibration of the parameters of a model like ASM1. The use of a calibrated deterministic model would allow for a scenario analysis of different upgrading possibilities. However, the sampling (8 24h samples and one day with 2h samples), was too short since the hydraulic residence time in the plant causes a delay in the influent-effluent response (Petersen *et al.*, 2001b).

For the calibration of the river model, six water quality samplers were installed and the samples analysed for boron and LAS. From the measurement data it was clear that no background concentration could be determined and that parts of the plug were missed by the samplers. This made it difficult to make mass balances for the inert tracer. Moreover, the behaviour of boron and LAS was found to be contradictory. The dispersion behaviour was different for these two soluble compounds. The cause of this could not be found, but may be due to insufficient mixing at the first measurement station downstream of the treatment plant. Another possibility is a small, but concentrated inflow somewhere along the river. Errors in flow measurement or the assumptions that the flow is steady during the campaign are other possible sources of errors and model uncertainty.

Despite the large uncertainties related to the scarce data, the integrated model shows that both the dispersion phenomena and the degradation of LAS can be predicted in a CSTRs-in-series model. If more (or more accurate) data had been collected, a better and less uncertain model calibration could have been performed. This is always a difficult choice the model builder has to make: more data are available only at the expense of a serious financial and manpower effort (Vanrolleghem *et al.*, 1999).

7.7 Conclusions

An integrated model of the treatment plant of Merone and the river Lambro has been created with the aid of a connector between the ASM1 and RWQM1 models. Inherent features of this connector are its closed mass and elemental balances. The COD fractions of the ASM1 have been split over the COD fractions of the RWQM1, while balance terms were used to close elemental balances. Also the different environmental conditions in the activated sludge system and the river system have been taken into account. The treatment plant model was only calibrated on steady state data, and a simple tanks-in-series model was able to adequately describe the dispersion in the river Lambro using boron as a tracer. Also, LAS data could be modelled sufficiently well and the first order degradation constant found for LAS is within the range of degradation constants found in literature and close to the value found in other studies on the same river. As an example of application, the integrated model was used to simulate the effects of an upgrade of the undersized Merone plant. Simulation results show a clear improvement in river water quality with the upgraded plant, both for LAS and traditional pollutants. In a last section, it was concluded that, in order to create a calibrated model of an IUWS, a large measurement campaign has to be set up, which requires a large investment of money, equipment and time.

Chapter 8

Immission based real-time control: the Tielt case study[1]

8.1 Introduction

As outlined in chapter 4, immission based real-time control can improve the water quality of the receiving waters in urban catchments. In order to design and tune such immission based strategy, a fast simultaneously simulating model of the (part of the) catchment under study is necessary. In this chapter a simultaneously simulating model of the Tielt case study is described. The developed immission based control strategy focuses on the maximum ammonia concentration in the river.

After a description of the catchment, the complex deterministic models that have been built previously are outlined. In the next section, the model simplifications and model reductions applied in this case study are explained. This results in a control model which can be used for controller evaluation and optimisation.

Once the controller is tuned, the secondary objectives of the controller must be checked, in case the effect of the controller on the dissolved oxygen concentrations. As a final step, the robustness of the control strategies against system changes is tested and discussed.

8.2 Catchment description

The catchment under study is part of the catchment of the town of Tielt (Belgium, 20 km West of Gent). This catchment has been described in previous studies as part of European

[1]Parts of this chapter were published as:
Meirlaen J., Van Assel J. and Vanrolleghem P.A. (2002). Real-time control of the integrated urban wastewater system using simultaneously simulating surrogate models. *Wat. Sci. Tech.*, 45(3), 109–116.

Meirlaen J. and Vanrolleghem P.A. (2002). Model reduction through boundary relocation to facilitate real-time control optimisation in the integrated urban wastewater system. *Wat. Sci. Tech.*, 45(4-5), 373-381.

Other parts were submitted as: Meirlaen J. and Vanrolleghem P.A. (submitted). Modelling and real-time control of the integrated urban wastewater system. *submitted to Urban Water*.

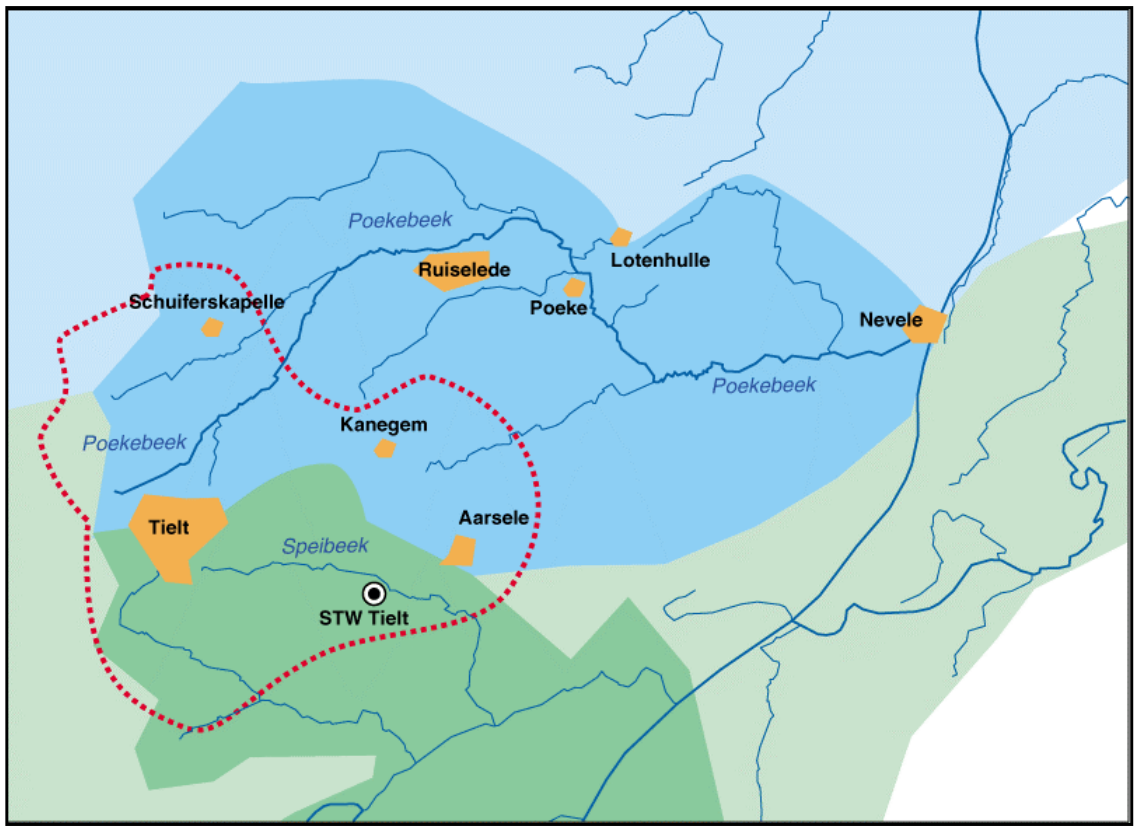


Figure 8.1: An overview of the catchment of Tielt

TTP projects (Van Assel, 2000b). Two watercourses drain the catchment, the Poekebeek and the Speibeek. An overview of the catchment is given in Fig. 8.1. The total area is about 11000 ha, about 250 ha of which are impervious.

The main sewer system is a fully combined system and serves the area of the town of Tielt and some surrounding villages. The total population is about 20000 connected people, while also some industries are connected (5000 IE on flow basis). It has a branched structure, with the different branches ending in a large collector which transports the water towards the treatment plant. Combined sewer overflows are present on both watercourses, while the effluent of the treatment plant is discharged towards the Speibeek.

The treatment plant of Tielt is an extended aeration plant with biological phosphorus removal. The plant has an anaerobic tank (1000 m^3), two aeration basins (total volume of 5938 m^3), two secondary clarifiers (2152 m^3 each, diameter = 28m) and a storm tank (also 2152 m^3).

To judge the effect of the interaction between the sewer system, treatment plant and river, the Speibeek was chosen as the river to be optimised in terms of river water quality, without altering the water quality of the Poekebeek. The river water quality has been judged according to a simple, though very important criterion, the maximum ammonia concentration in the river along the reach under study, while the minimum oxygen concentration was considered as a secondary objective.

Four important overflows are present on the Speibeek, which is of a bad quality in both dry and wet weather (e.g. 90% of the time oxygen concentrations are below 50% saturation).

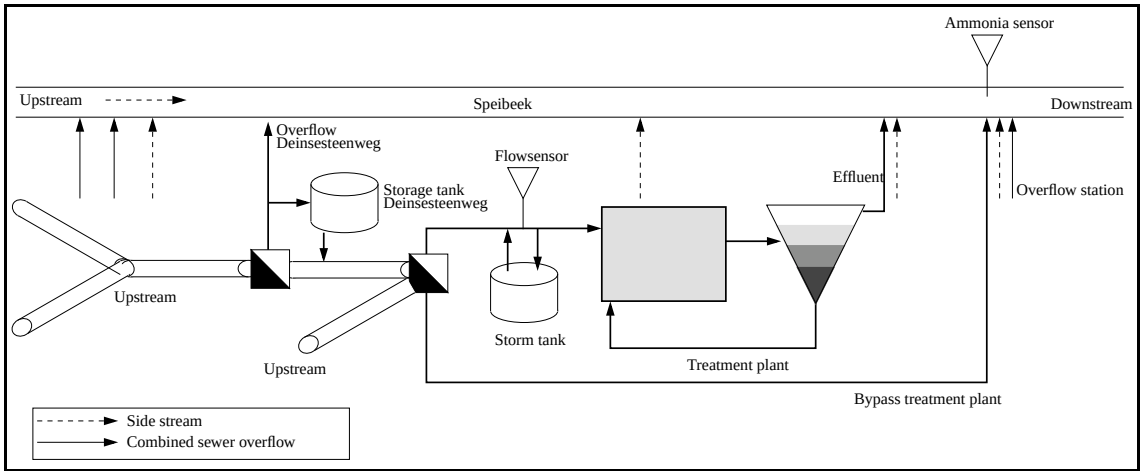


Figure 8.2: Overview of the catchment under study at the Speibeek

The base flow of the Speibeek is very low, and has been assumed to be 10 l/s during the period under study (i.e. summer period). This causes a very low dilution capacity which is typical for Flemish rivers. During this period, the impact of CSOs will probably be the most critical. In fact, the overflow Deinsesteenweg acts as the main source of flow during rain events. A schematic overview of the modelled part of the catchment is given in Fig. 8.2.

8.3 Mechanistic model description

8.3.1 Sewer model

The sewer system has been modelled using Hydroworks (Wallingford Software, UK) and has been calibrated on the basis of several measurement campaigns. The model contains 1379 nodes, 22 outfalls, 1381 conduits and 51 control links (Heip *et al.*, 1997; Van Assel, 2000a). The model building has been performed in four consecutive steps: DWF and WWF hydraulic calibration and DWF and WWF water quality calibration. It was concluded that the model was calibrated correctly for the hydraulic part and reasonably well for dry weather quality. The wet weather quality could not be checked in detail due to the too short sampling periods (Heip *et al.*, 1997).

8.3.2 Treatment plant model

The treatment plant has been modelled using the ASM2d model (Henze *et al.*, 2000) for the activated sludge conversion part, while the settling model of Takács *et al.* (1991) was used to describe the behaviour of the clarifier. Intensive measurement campaigns have been carried out to allow the calibration of the most important parameters (Carrette *et al.*, 2001a). The influent fractionation (i.e. the division of the incoming COD in the COD fractions used in the ASM2d model) was the factor most influencing the predicted

effluents. The original model consisted of 11 different submodels and is described in chapter 5.

8.3.3 River model

A complex mechanistic model was built for the Poekebeek system (Van Assel, 2000a). Both a hydrologic and hydraulic model were built and calibrated using ISIS (Wallingford Software). Also, a river water quality model has been constructed using ISIS-Qual (Wallingford Software). It was concluded that the flow could be modelled reasonably well, but that, due to software and data problems, the water quality dynamics could not be described. No complex mechanistic model of the river Speibeek was built, due to a lack of data.

8.4 Control strategy description

In this case study, the existing sewer system and treatment plant (designed to comply with the Flemish emission standards) are, with the current static operation, not able to ensure a good water quality in the Speibeek. This can be concluded from the measurements which show that oxygen is lower than 50% of the saturation concentration about half of the time (Van Assel, 2000a). To tackle this, immission based control strategies are developed to evaluate whether the problem can be solved without rebuilding the sewer system, change the treatment plant or add large storage tanks. Two control strategies are compared to the current static control strategy. The first control strategy uses measurements in the river to act on the WWTP. The second strategy extends the first one, by also acting on the sewer system.

An efficient control strategy acting on both the sewer system and the treatment plant might improve the quality of the Speibeek, since the impact of the CSOs is very serious due to the very low dilution capacity. Although this is a typical Flemish situation, the ideas presented below might be (in a modified format) applicable in other situations as well.

8.4.1 Reference control strategy

The reference (existing) control strategy is acting on the storm tank at the treatment plant. If the incoming flow at the plant is higher than the design capacity for biological treatment (3Q14 = 23000 m^3/d), the flow exceeding this capacity is redirected to the stormtank. Once this tank is filled, the water that cannot be treated is bypassed and spills 2 km downstream of the plant at the overflow Station. The aeration of the biological tanks is controlled by local time based controllers, which implement a predefined time schedule. No dynamic control is currently implemented in the sewer system.

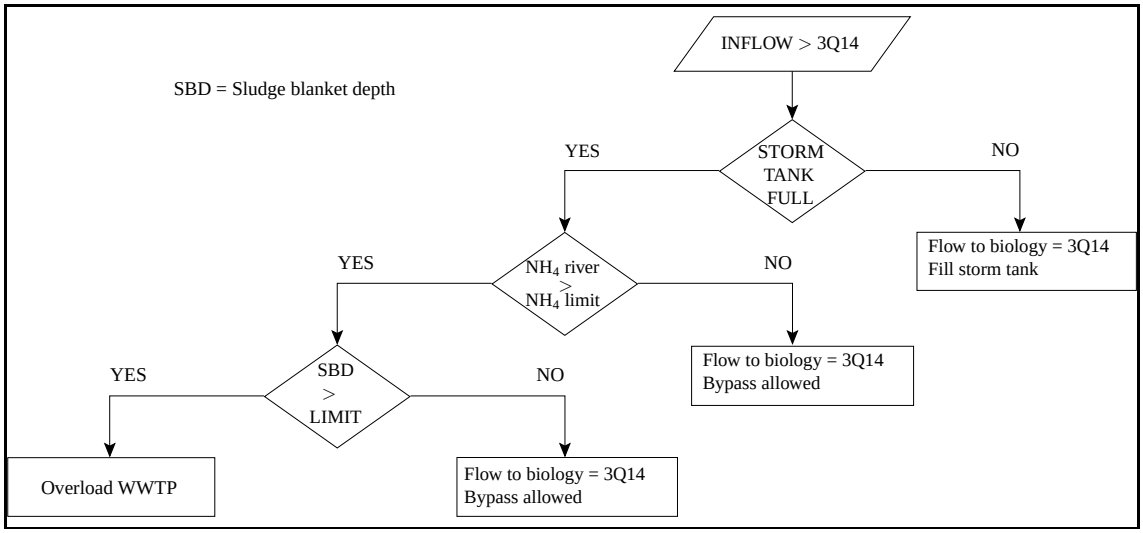


Figure 8.3: Overview of strategy 1

8.4.2 Control strategy 1

This first immission based control strategy focuses on the elimination of peak ammonia concentrations in the river downstream of the treatment plant. For this, an ammonia sensor is located into the river at the point where the highest concentrations of ammonia occur, this is at the overflow Station. The ammonia sensor used has no delay, which in reality will not be the case. The idea of the controller is to avoid the overloading of the treatment plant as long as the river is not in a critical situation with respect to ammonia or, in other words, bypassing is allowed in those situations. Once the ammonia in the river gets too high, the bypass is reduced by putting more water through the biological treatment.

The overloading of the treatment plant is controlled on the basis of the ammonia measurement in the river with a proportional controller with a maximum value. This means that the inflow to the treatment plant is proportional to the difference between the ammonia concentration in the river and a given set point. The set point concentration of 1.5 mg/l for (unionised plus ionised) ammonia was chosen based on the Fundamental Intermittent standards (FIS) of UPM (FWR, 1998). These criteria take the concentration of unionised ammonia (NH_3) in the water into consideration. According to these criteria the concentration of NH_3 should not exceed 0.03-0.05 mg/l for more than 24 hours assuming a return period of 1 month. With a pH of around 7.5, which is the value most frequently encountered in the Speibeek (Van Assel, 2000b), a NH_3 concentration of approximately 0.03 mg/l leads to the limit of 1.5 mg/l for total ammonia.

The proportional constant was chosen in such a way that the maximum overloading of the plant (4 Q14) was reached if this difference was 1 mg NH_4-N/l. Note that the overloading of the treatment plant is only activated when the storm tank is completely filled. In addition, a supervisory controller on the sludge blanket is implemented to prevent massive sludge wash-out: if there is any risk of sludge loss via the settler (defined as the sludge blanket reaching a certain height, i.e. 0.5m from the top of the settler) the flow is restricted again to 3 Q14. A schematic overview of the controller is given in Fig. 8.3.

Table 8.1: Summary of the three control strategies tested

Name	Description
Reference control strategy	Local control of the stormtank, local aeration control
Control strategy 1	Reference control + integrated control on the overloading of the TP based on the ammonia measurement in the river and supervised by the sludge blanket height
Control strategy 2	Strategy 1 + pump in the sewer system, pumping more water downstream when the storage tank at Deinsesteenweg is not completely filled and the WWTP is not overloaded

8.4.3 Control strategy 2

Control strategy 2 extends control strategy 1 in order to optimise the operation of the sewer system. The simulations showed that the hydraulic capacity of the connection between the storage tank at the Deinsesteenweg and the overflow Station, was only completely used when the storage tank was completely filled. This is due to the flow being dependent on the head of water in the tank. It was therefore evaluated whether adding a pump to this system would increase the capacity since the downstream flow would no longer be dependent on the water head in the tank, and the hydraulic capacity of the pipe could be completely used, even before the tank is filled. In this way more water can be sent to the treatment plant in the beginning of an event, while at the end of an event the storage tank can be emptied faster. To protect the plant, the pump is only activated when the plant is not hydraulically overloaded.

A summary of the different control strategies is given in Table 8.1 while the location of the sensors is shown in Fig. 8.2.

8.5 Model simplifications

To tune the control strategies described above, the mechanistic models are simplified (see chapter 4). In this way, the iterative simulations to tune the control strategies have a shorter calculation time, which allows this procedure to be completed faster. In the next section, the simplification of the different mechanistic models is explained.

8.5.1 Sewer model

Starting from the detailed model, a simplified Kosim model was constructed. Determining the different elements in the simplified model is straightforward at the hydraulic breakpoints. In other cases, simulation results of the hydrodynamic model have to be studied in order to construct the most suitable model. The Kosim model of the complete catchment of Tielt consists of 33 subcatchments, 18 storage elements, 16 transport elements and 1 flow splitter and is shown in Fig. 8.4 (Van Assel and Carrette, 2001). It was found that

total overflow volumes and overflow peak discharges were modelled with the same accuracy in both types of models. A comparison between the overflow volumes produced by Hydroworks and the ones produced by Kosim is given in Fig. 8.5. Consequently, it was concluded that the model could be used for control tuning purposes, especially in view of the considerably shorter calculation times.

8.5.2 Treatment plant model

For the treatment plant model simplifications, several options were tried. The first idea was to replace the deterministic model by a neural network. This approach did not work, mainly due to the feedback of errors back into model. Indeed, when using a neural network to predict a long time series of model variables, the states predicted for time step k need to be fed back into the network, since the predicted output at time step k+1 depends on them. If the prediction is slightly wrong, a wrong input is given for the next time step. This leads to accumulated errors and useless simulation results and was described in detail in chapter 5.

In a second approach, it was tried to exclude some phenomena from the model. First, the model described by Takács *et al.* (1991) was replaced by a conceptual model (point settler). In this model, a fixed fraction of the incoming solids is directed towards the effluent, while the remaining part is concentrated in the return/waste sludge. Second, the oxygen dynamics were taken out of the activated sludge tanks, assuming either the complete absence of oxygen in the non-aerated case and no limitation of the biomass by oxygen in the aerated case. In this way a fast process was eliminated from the model, which would in principle allow faster numerical integration.

In chapter 5, a comparison was made between the simulation results of the different simplifications. The results for the effluent concentration of ammonia, nitrate and phosphorus did not correspond well to the complete model. Moreover, since the control strategy allows hydraulic overloading of the plant, both the oxygen dynamics and the behaviour of the sludge blanket are important phenomena during storm events. Therefore, the proposed model reductions of the treatment plant model could not be used in order to be able to realistically describe the behaviour of the treatment plant during storm conditions.

8.5.3 River model

The river model is built as a series of completely stirred tank reactors (CSTRs) to approximate the hydraulic routing of the river (see chapter 6). Since only the complex mechanistic model of the Poekebeek was available, a pragmatic approach had to be followed to build a simplified model of the Speibeek. The tanks were chosen in such a way that all important inflows (like side streams or CSOs) could be taken into account. The length of the stretches was estimated on the basis of a detailed map (scale 1:1000). Parameters were taken according to earlier experience in calibrating this type of models for small rivers in Flanders (see chapter 6 for details).

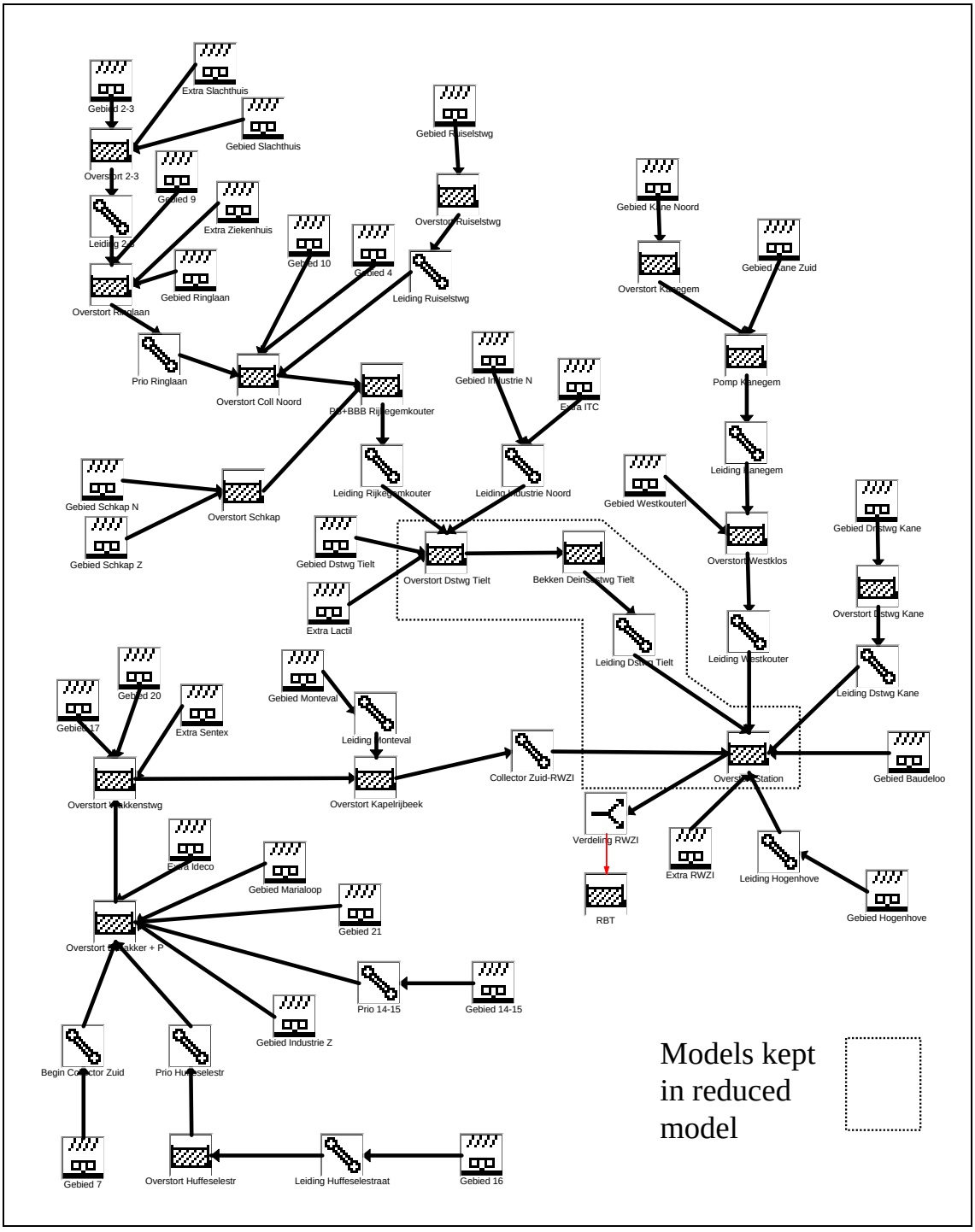


Figure 8.4: Overview of the Kosim model of the Tielt sewer system

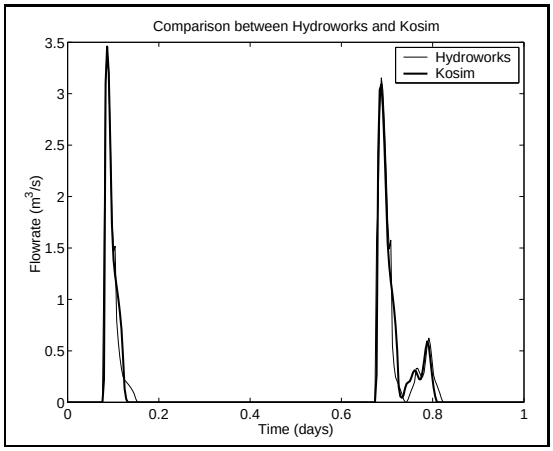


Figure 8.5: The overflow volumes predicted by Hydroworks and by Kosim (Van Assel, 2000a)

Two different models were used to describe the water quality of the river. The first model was part of the fast calculating control model whereas the second, more complex model was only used for the evaluation of the secondary objectives.

The sensitivity of the control model towards the elimination of the conversion model was checked. In the studied example, the nitrogen discharged from a sewer system is already ammonified to a large extent (Holzer and Krebs, 1998) and, therefore, the ammonia concentrations in the wastewater make up most of the total nitrogen content. When focusing on controlling the peak ammonia concentration, it was found that not taking into account the conversions (like ammonification or nitrification), did not lead to significant differences compared to the model with conversion included. This means that the peak ammonia concentration can be modelled by only taking hydraulics and mixing into account. In this way, by eliminating the river conversion model from the mass balances, only retaining the transport term, considerable simulation time, and hence optimisation time is saved.

In the complete model used for the evaluation of the secondary objectives, a submodel of the RWQM1 (Reichert *et al.*, 2001b) has been used to describe the biological conversions. The most important differences with the full RWQM1 are the lumping of the two step nitrification into a one-step nitrification process with one type of nitrifying biomass. Moreover, no pH variations, algae or consumers were taken into account.

An overview of the resulting state vector is given in Table 8.2. Since very few data were available about the water quality of this small river and calibration was therefore very limited, this model should be considered a hypothetical model, which can however be used to evaluate the impact of the different control strategies. It is important to note that no hydrological model was used and that the upstream flow of the river did not increase during storms. This results in a worst case scenario of the impact of the CSOs and the effluent on the river water quality. Moreover, no sedimentation or resuspension processes were taken into account.

Table 8.2: List of state variables in the sub-model of the RWQM1

State variables	
S_I	Inert soluble COD
S_S	Readily Biodegradable soluble COD
S_S	Biodegradable soluble COD
S_O	Oxygen
S_{NH}	Ammonium nitrogen
S_{NO_3}	Oxidised nitrogen
S_{HPO_4}	Ortho-phosphate
X_I	Inert particulate COD
X_S	Slowly biodegradable COD
X_H	Heterotrophic biomass
X_N	Nitrifying biomass

Table 8.3: The biological reactions in the sub-model of the RWQM1

Biological reactions
Hydrolysis of particulate material
Aerobic growth of heterotrophic biomass with NH_4
Aerobic growth of heterotrophic biomass with NO_3
Anoxic growth of heterotrophic biomass with NO_3
Aerobic respiration of heterotrophs
Anoxic respiration of heterotrophs
Growth of nitrifying biomass
Aerobic respiration of nitrifying biomass

8.6 Model reductions

8.6.1 Sewer model

Since the most important overflows are located close to the treatment plant (both the overflow at Deinsesteenweg and at Station), only four out of the 68 elements of the full Kosim model had to be retained in the control model (Fig. 8.4). These were the CSO structure at Deinsesteenweg, the storage tank at Deinsesteenweg, the pipe connecting this CSO with the Station and the overflow structure at Station itself. This resulted in a substantial model simplification and only this part of the sewer model has been implemented into WEST® The upstream parts of the sewer model were calculated once and used as an input file for the simulation. This is a clear example of system boundary relocation.

Since the Kosim model uses discrete time steps, it cannot be implemented efficiently as such in the WEST® simulator (Hemmis NV, Kortrijk, Belgium) because this package is very effective in solving differential equations, but less so in solving discrete time equations. Consequently, the differential equations corresponding to the Kosim difference equations have been worked out and implemented in the WEST® simulator. More details about the implementation of the Kosim model into WEST were given in section 3.7.4.

8.6.2 Treatment plant model

Since the complete treatment plant is important for the river water quality, no upstream or downstream parts could be left out in this case. However, if the sludge treatment processes would also have been taken into account in the full model (e.g. to model sludge treatment cost), this part could clearly have been left out for the control model.

8.6.3 River model

The complete river model of the Speibeek used to evaluate the effect on the oxygen dynamics is composed of 18 tanks in series. Leaving out the part of the model upstream of the first controlled overflow (at Deinsesteenweg) and the part of the model describing the part downstream of the overflow at Station where the ammonia measurement was made, resulted in a control model of only six tanks.

8.6.4 Time boundary

The first important rain event only occurs during the 7th day of the studied period (see also Fig. 8.8 on page 189). Since the controllers do not act in either of the cases before the end of the sixth day, the behaviour of the system is independent of the control system under study. Therefore, a relocation of the time boundaries can be performed: one simulation was performed to determine the state of the system at the beginning of the seventh day, and all other simulations were run starting from that time and with the initial conditions being determined by this single simulation.

8.6.5 Secondary objectives

In the example used in the study, it was tried to maximise the model reduction via system boundary relocation and submodel selection, leading to a so-called control model. The control system only focused on the ammonia concentration and in this way the section of the river downstream of the ammonia sensor could be eliminated. The secondary objectives looked at in this study are the minimum oxygen concentration, the time the oxygen is below a given limit (4 $mg\ O_2/l$) and the time the river concentration at the critical section is above a given ammonia limit. For these secondary objectives, the complete river model with conversions taken into account, is used. Finally, as a last part of the procedure described in chapter 4, the robustness of the different control strategies is calculated, as another means of evaluating the performance of the strategy.

8.7 The resulting control model

The WEST® simulator was originally used mainly for simulation of wastewater treatment plants and an extensive WWTP model base is available. Both the simplification of the runoff/sewer model and the tanks in series river model are now implemented in this package as well. Hence, the three parts of the integrated urban wastewater system (IUWS) are now available in a single software tool and, thanks to this, linking of the submodels is straightforward. Moreover, problems with file or data transfer between different simulators are avoided and, most importantly, simultaneous simulation is possible. A schematic overview of the resulting control model in WEST® is given in Fig. 8.6.

For the evaluation of the secondary objectives, a separate river model was used, which included the river processes and the complete downstream river part. In this way, the

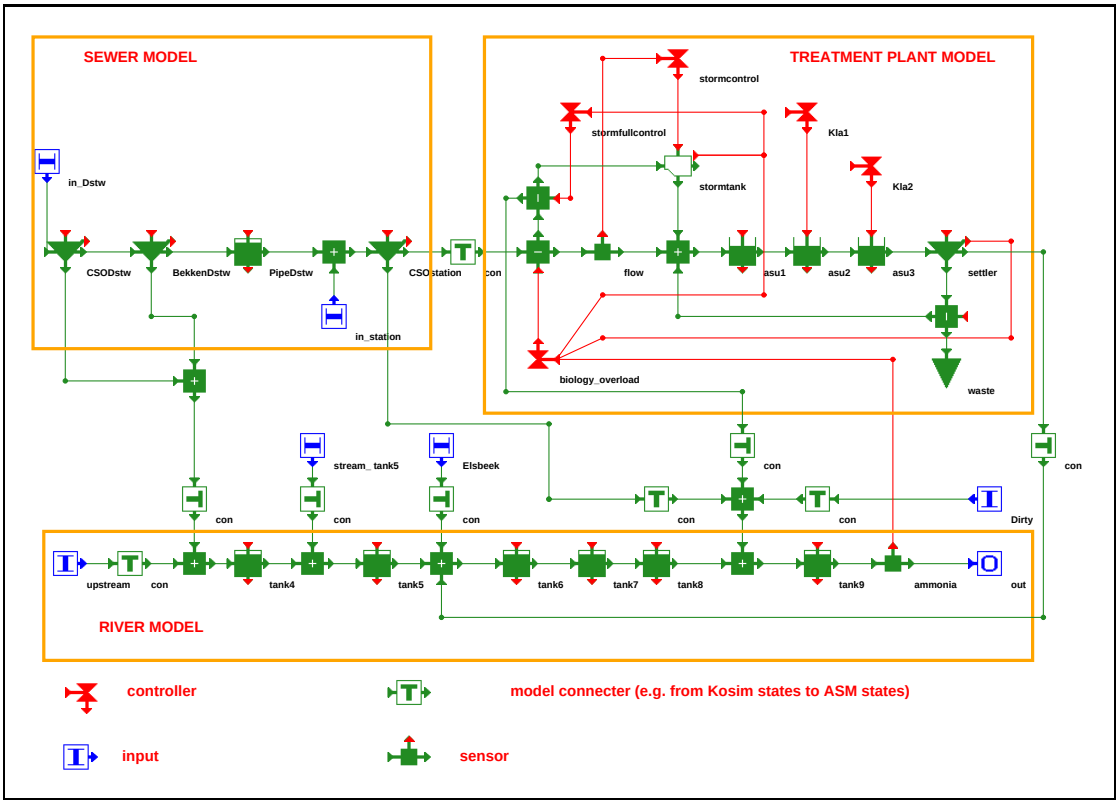


Figure 8.6: The control model as implemented in WEST

overall oxygen dynamics of the river could be judged. Since in this case, only the river subsystem is considered, all inputs to the river are specified as input files calculated at particular locations with the control model.

Particular attention has to be paid when creating these influent files. As CSOs are very dynamic, the time interval used in the input files must be rather small, e.g. one minute. In order to avoid huge files, this time interval might then be relaxed to, for instance, 15' in other situations (e.g. dry weather). This is illustrated in Fig. 8.7 which shows the simulation results of a CSO event with a file communication interval of 0.01 d ($\approx$ 15min) and with an interval of 0.001 d ($\approx$ 1.5 min). It is clear that the 15 minutes interval is a very rough approximation of the simulated behaviour during storm periods.

It should be noted that both the control model and the secondary objective evaluation model are still rather slow in the current implementation. The control model needs 2 hours for a simulation of 8 days on a Pentium III, 800MHz PC, while the secondary objective evaluation model needs 8 hours for the same simulation period[2]. For the control model, this is due to the fact that the Kosim model is currently implemented as a continuous rather than a discrete model as is the case in the original software (itwh, 1995). The river model is slow due to the large number of equations used, in combination with a very low time interval used in the input file. In the current implementation of the model and the numerical algorithms, the simulations become very slow when such a small time step is

[2]During the last week of this work, an input routine was optimised reducing the simulation time to 2h 40 min

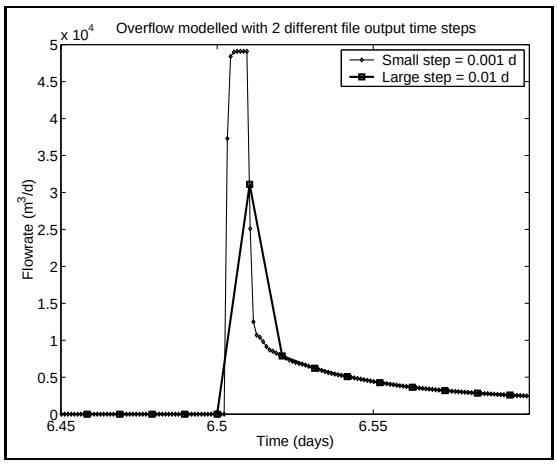


Figure 8.7: Difference in results in the output file for different file communication intervals

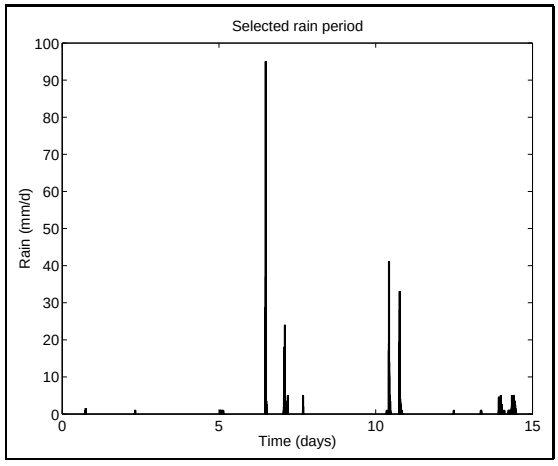


Figure 8.8: Rain intensity during the selected rain period

encountered.

8.8 Simulation results

8.8.1 Performance of the controllers

A two week period was selected from the available data (6 months) to test the control strategies. In these two weeks, two major storms with each two rain peaks are present (Fig. 8.8).

The different control strategies are evaluated at different levels. First, the treatment plant effluent concentrations are compared. In a second paragraph, the resulting ammonia concentrations in the river are shown and discussed. Next, the effect of the control strategies on the resulting in-stream oxygen concentrations is evaluated. Finally, the robustness of the controllers towards system changes will be calculated and discussed.

The effluent concentrations of the treatment plant for the reference control and strategy 2 are shown in Fig. 8.9. The strategy 1 effluent is very close to the strategy 2 effluent and not shown in the graph. It can be seen that the effluent concentrations are not depending a lot on the control strategy applied, even though the plant is overloaded during certain periods. In the reference control case, the inflow goes up to 3 Q14 (design capacity), while in control strategy 2 the maximum overload factor is 4 Q14. Apparently, since the treatment plant is an extended aeration system, sufficient nitrification capacity is available. Also, no major increase of the effluent suspended solids concentration was noted in the different simulation results. This is probably a good assumption since the sludge of extended aeration systems is known to settle well (Arhan *et al.*, 1996).

In Fig. 8.10 however, the effect of the control strategies can clearly be seen, since the river ammonium concentration with the controllers active is always lower than or equal to the concentration in the reference case. However, the effect is not always caused by the same mechanism. In the first part of each storm (from day 6.5 to 6.7 and 7.1-7.3), the

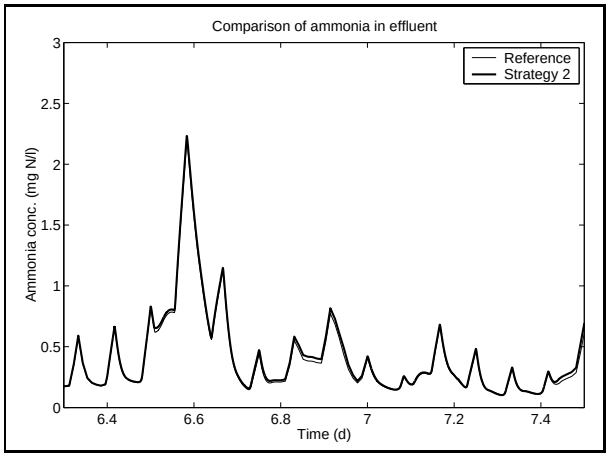


Figure 8.9: The resulting effluent ammonia concentration in both the reference control case and control strategy 2

storage tank at Deinsesteenweg is not completely filled and, hence, the flow rate of water to the treatment plant is not maximised in the reference case and in strategy 1. By adding a pump in the sewer system at the storage tank (strategy 2, Fig. 8.10right), more water can be sent downstream, even without the tank being completely filled. The additional water which is sent downstream, saves some space in this storage tank, which can be used later on to store polluted water. Due to the limited capacity of the pipe downstream of the storage tank at the Deinsesteenweg, not all of the combined sewer overflow can be avoided, leading to peak ammonia concentrations in the river in the early stages of the events. If the hydraulic capacity could be increased, a more substantial reduction in river ammonia concentration in these early phases of the storm events can be expected.

In the second part of the evaluated storms (days 6.7-6.8 and 7.3-7.5), the storm tank is filled in all cases, so the addition of the pump no longer has a beneficial effect. However, in these conditions the overloading of the treatment plant by the first and the second control strategy starts to act. This overloading is only activated if the ammonia concentration in the river at the discharge point is above a given set point, which was chosen 1.5 mg NH_4-N/l in this study. It can be seen that in the second part of the selected rain events, the ammonia concentration can be controlled to this set point. The effect of the control strategies on the ammonia concentrations in the river can clearly be noticed from the difference in the simulation results between control strategy 1 and 2. In the first strategy, an improvement in river water quality is only noticed in the second part of the storm (Fig. 8.10left), while in the second case, both parts of the storm period benefit the control actions (Fig. 8.10right). However, it can be concluded that there is insufficient control authority to completely control the first peak.

Fig. 8.11 shows the minimum oxygen concentration along the whole downstream river stretch in the reference case compared to strategy 1. For this an additional sensor was added to the model, which uses the measurement of oxygen in every tank and determines the minimum. It can be seen that the oxygen is more or less the same in the two cases. The secondary objectives of the control strategy are not worse, so the control strategy may be implemented from the point of view of the secondary objectives. This limited effect of

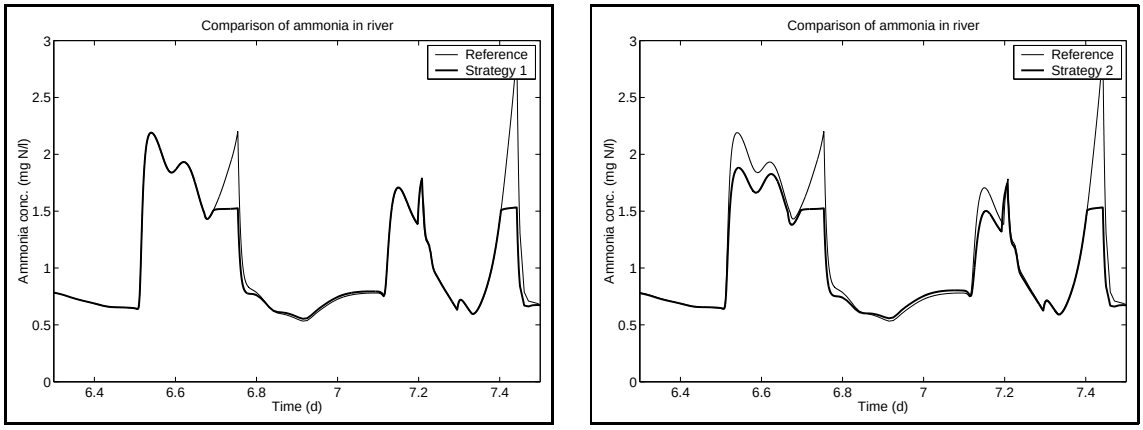


Figure 8.10: The resulting river ammonia concentration at the critical location in both the reference control case compared to strategy 1 (left) and 2 (right)

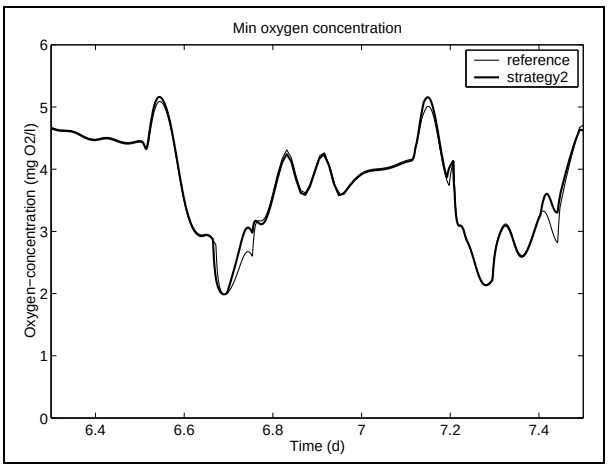


Figure 8.11: The minimum oxygen concentration along the river for the reference strategy compared to strategy 2

the control strategy is mainly due to the limited conversion processes taking place in the river, due to the low biomass concentrations.

8.8.2 Emission analysis

Flow emissions

In the previous section it was shown that the different control strategies do not worsen the effluent quality dramatically and that the ammonia concentration in the river could be decreased at certain time periods. In this section, the behaviour of the different outfalls into the Speibeek is analysed in both a quantitative (volume) and qualitative (pollutants) way.

As can be seen in Fig. 8.2, four outfalls discharge into the Speibeek. These are the effluent and the bypass of the treatment plant, and the CSOs at BekkenDstw and at the Station. The different control strategies influence the behaviour of these outfalls. The first strategy only influences the bypass and effluent flow. The second control strategy influences the

bypass and the effluent flow, but at the same time also the flow at the BekkenDstw by activating a pump, sending more water downstream. This extra water arriving downstream also influences the CSO at Station, since now more water has to be handled at this point. Fig. 8.12 to Fig. 8.19 illustrate these interactions.

In Fig. 8.12, Fig. 8.14 and Fig. 8.16 the different flows from the three CSOs are shown. It can be seen that the CSO at the BekkenDstw spills first and that the CSOstation and the bypass are active more or less at the same time. It can also be seen that strategy 1 and 2 reduce the flow of the bypass at the end of the event, when the ammonia concentration has risen above the limit that was set. It can also be noted that the CSOstation is of less importance, i.e. the total flow spilled by this CSO structure is much lower than the flow spilled by the CSO at BekkenDstw and by the bypass.

When looking in some more detail, some extra conclusions can be drawn. In Fig. 8.13 it can be seen that the activation of a pump in the sewer system with the objective to completely use the hydraulic capacity of the downstream pipe from the start of the event, delays the beginning of the CSO. This is due to the fact that more water is sent downstream in the beginning of the event, hence the storage tank is filled later, so the CSO starts to spill later. However, in this case, the maximum flow is not reduced. When comparing the second event however (Fig. 8.12 and Fig. 8.16) it can be noted that the maximum flow is about 48000 m^3/d in the reference case, while it is about 35000 m^3/d with strategy 2.

Fig. 8.15 shows the differences in the bypass flow rate for the three cases. It can be seen that in strategy 1, the overloading of the treatment plant starts earlier than in strategy 2. This can be explained by the fact that in strategy 2, the ammonia concentration in the river is lower due to the reduced overflow at BekkenDstw and, hence, the critical concentration is reached later. Consequently, the overloading is switched on later as well.

Fig. 8.17 shows the adverse effect of switching on the pump in the upstream section of the sewer system. Since this pump does not know about the flow downstream in the sewer system (only the flow at the treatment plant is important), the overflow at the CSOstation starts to spill earlier in strategy 2 than in the other two cases. So the increased flow downstream causes this CSO to spill more water. However, as noted before, the volume spilled by this CSO is low compared to the other two CSOs and hence the effect on the river water quality is not very important.

The flow at the effluent of the treatment plant is the result of the behaviour of the different CSOs. In Fig. 8.18, the effluent flow rate for the whole simulation period is shown for the reference case. It can be seen that the plant is twice loaded to its design capacity. The dry weather flow is fluctuating periodically. The dry weather flow is obviously the same for the two control strategies, since these are only active during wet weather. The overloading of the treatment plant can be seen in Fig. 8.19. Both control strategy 1 and 2 overload the treatment plant depending on the ammonia concentration in the river. Control strategies 1 and 2 always overload the WWTP at the same time, except at time 10.8, where only strategy 1 is overloading the WWTP. It can hence be concluded that the control strategy 2 overloads the treatment plant less than strategy 1.

As a conclusion it can be said that the two control strategies reduce the amount of untreated wet weather flow that enters the river. However, the second strategy causes a

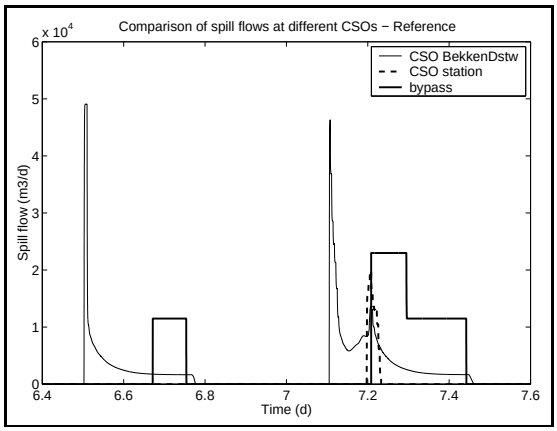


Figure 8.12: Flow data for the reference strategy for the three CSOs

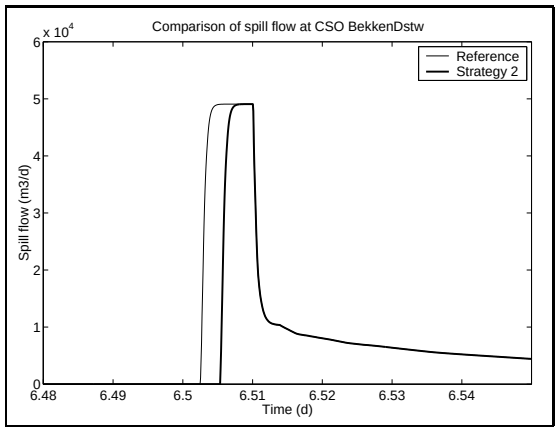


Figure 8.13: Flow data at the BekkenDstw for the reference case and strategy 2

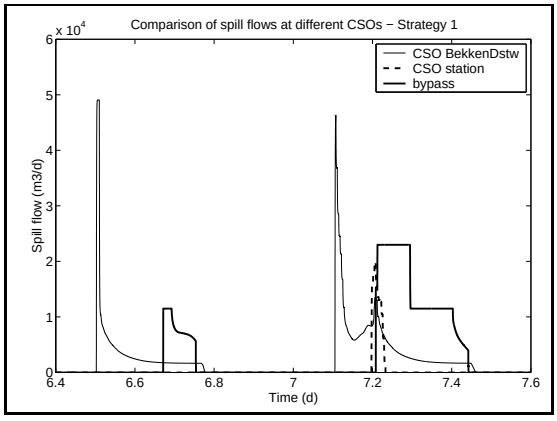


Figure 8.14: Flow data for strategy 1 for the three CSOs

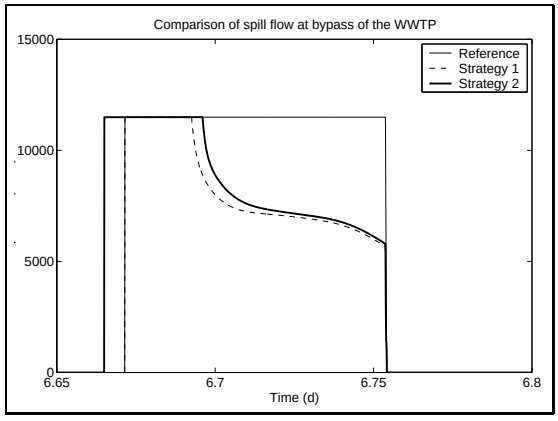


Figure 8.15: Flow data for the bypass for the three cases

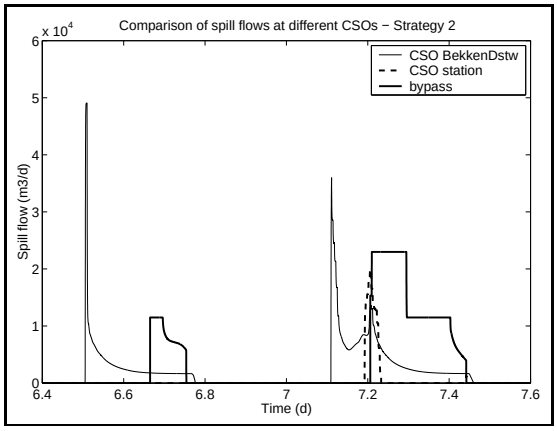


Figure 8.16: Flow data for strategy 2 for the three CSOs

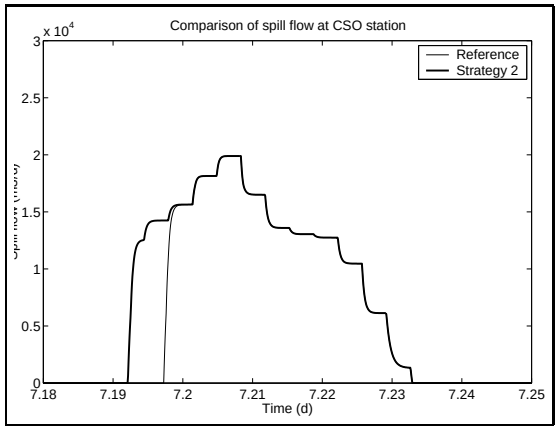


Figure 8.17: Flow data at the CSOstation for the reference case and strategy 2

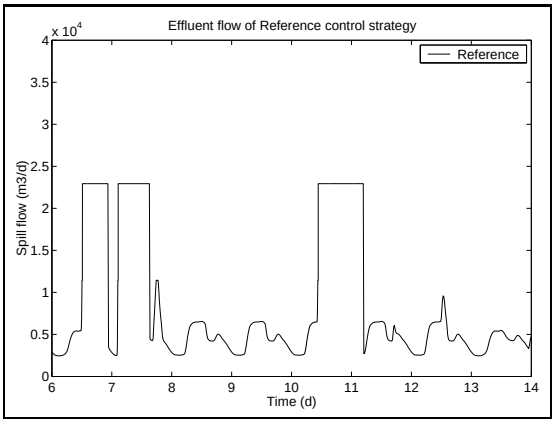


Figure 8.18: Effluent flow data for the reference case

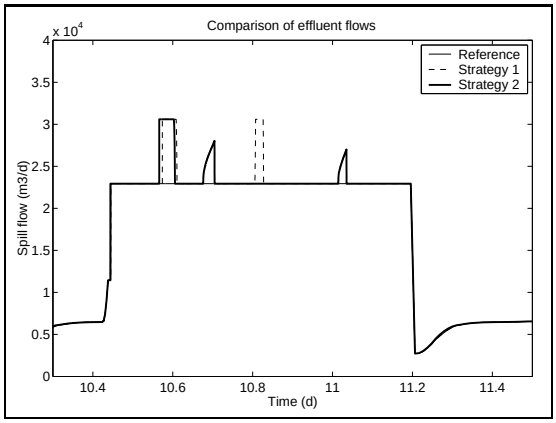


Figure 8.19: Effluent flow data for the three cases (detail)

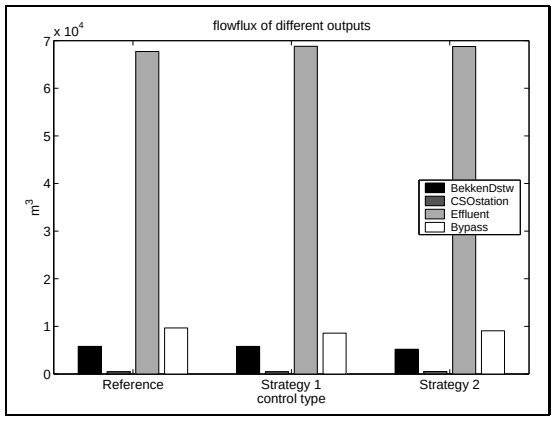


Figure 8.20: Effluent flow data: summary

smaller CSO to spill more due to the increased flow downstream. An overview of the different flows is given in Table 8.4 and in Fig. 8.20.

Pollutant emissions

Since water quality is considered more important than water quantity, the total masses of pollutants discharged in the Speibeek are discussed. Two pollutants have been checked: nitrogen in the form of ammonia and organic nitrogen and COD. It can be seen in Table 8.4 that the total mass of COD discharged into the river is reduced with 3% and 4% for strategy 1 and 2. For strategy 1, the mass discharged via the BekkenDstw CSO and via the CSOstation is equal to the reference case, while the amount in the bypass is reduced with 14%, and the amount discharged via the effluent is increased with only 2%. Strategy 2 has a reduced COD emission of 18% at the CSO BekkenDstw, while the COD emission is increased at the CSOstation. This strategy spills more COD via the bypass than strategy 1, as could also be expected from the higher flows. However, in total less COD is discharged.

For ammonia a similar behaviour can be noted. Strategy 1 remains the same for CSO BekkenDstw and CSOstation, while increasing for the effluent and decreasing for the

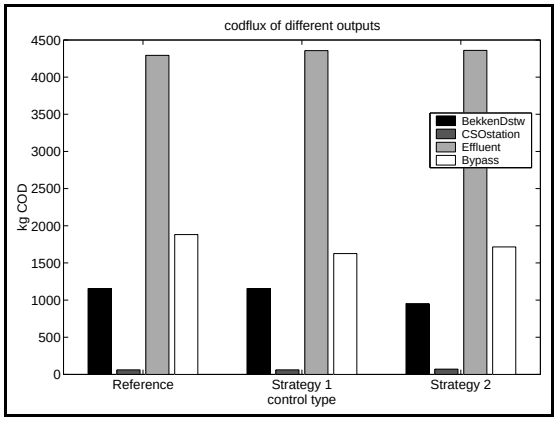


Figure 8.21: COD emissions from the different outfalls

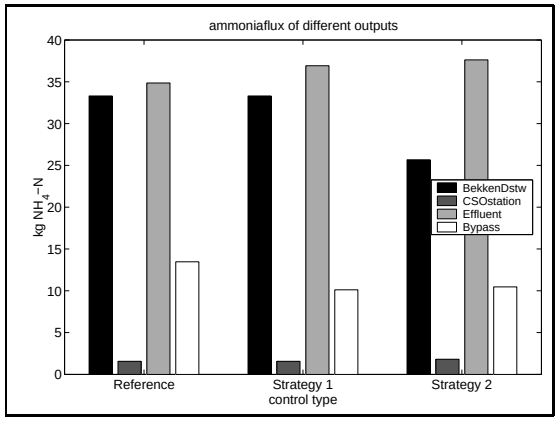


Figure 8.22: Ammonia emissions from the different outfalls

bypass. Strategy 2 decreases at CSO BekkenDstw and increases at CSOstation. The effluent and the bypass spill more ammonia in the river. However, the total amount of ammonia is much lower for strategy 2 than for strategy 1, which is in turn lower than for the reference case. A graphical overview is also given in Fig. 8.21 and Fig. 8.22.

8.8.3 Evaluation of the robustness of the control system

As discussed in chapter 4, a controller is always tuned for a given situation and a given system. As a model never represents reality perfectly, it is important to know how sensitive the controller is towards differences in the system properties to which it is applied. The robustness index as introduced before, is one way to express this and will be discussed for the used control strategies.

The control strategies were tested for robustness against three changes to system properties. In the first case, the growth rate of the nitrifying biomass was temporarily reduced with 10% compared to the reference case. This case mimics for instance a slightly toxic influent entering the treatment plant. In the second case, the aeration capacity was reduced with 10% to mimic mechanical problems with a blower. In the third case, the nitrogen content of the sewage was increased with 10%. All expected ranges ($\Delta\theta$) were chosen to be 20%.

The effect on the performance of the reference control strategy of reducing the Kla with 10% is shown in Fig. 8.23 and Fig. 8.24. For both the ammonia maximum and the oxygen minimum, the system change causes the quality of the effluent and, hence, the quality of the river to worsen. During the first storm (day 6.5-6.8) the reduction in Kla increases the instream ammonia concentration. This can be explained by the fact that during this storm, the WWTP has insufficient nitrification capacity (as can also be noted from Fig. 8.9). An extra reduction in aeration capacity will limit the nitrification further and the effluent ammonia concentration is increased. The in-stream oxygen concentration is decreased as the effluent of the WWTP contains less oxygen.

For some other properties the system changes improved the criterion value. Decreasing μ_A for example, led to a small increase in the minimum oxygen concentration, which is

Table 8.4: Overview of the CSO emissions for the different outfalls for flow, COD and ammonia

Discharge point										
Flow	BekkenDstw		CSOstation		effluent		bypass		Total	
	m^3	%	m^3	%	m^3	%	m^3	%	m^3	%
Reference	5787	100	451	100	67717	100	9664	100	83619	100
Strategy 1	5787	100	451	100	68814	102	8566	89	83619	100
Strategy 2	5187	90	521	115	68767	102	9077	94	83552	100
COD	BekkenDstw		CSOstation		effluent		bypass		Total	
	kg	%	kg	%	kg	%	kg	%	kg	%
Reference	1155	100	61	100	4293	100	1881	100	7390	100
Strategy 1	1155	100	61	100	4357	102	1626	86	7199	97
Strategy 2	952	82	70	116	4360	102	1715	91	7098	96
Ammonia	BekkenDstw		CSOstation		effluent		bypass		Total	
	kg	%	kg	%	kg	%	kg	%	kg	%
Reference	33.3	100	1.6	100	34.9	100	13.5	100	83.2	100
Strategy 1	33.3	100	1.6	100	36.9	106	10.1	75	81.9	98
Strategy 2	25.7	77	1.8	116	37.6	108	10.5	78	75.6	91

quite unexpected. The reason is that the lower μ_A leads to a lower oxygen consumption in the treatment plant and to a higher oxygen concentration in the effluent, and hence also to higher oxygen levels in the river.

The following equations from chapter 4 were used to calculate the individual sensitivities and the robustness:

$$S_i = \frac{\partial CriterionValue}{\partial \theta_i} \cdot \frac{\Delta \theta_i}{CriterionValue} \tag{8.1}$$

$$RI = 1 \Big/ \sqrt{\frac{1}{p} \sum_{i=1}^{p} S_i^2} \tag{8.2}$$

where

S_i The sensitivity of a control strategy
RI The robustness index of the control strategy

The robustness for two criteria was tested: the maximum ammonia concentration, and the time that the ammonia concentration was above 1.5 $mgNH_4 - N/l$. Since the oxygen was not changing when comparing the different control strategies, the robustness of the controller for oxygen was not calculated. The individual sensitivities towards system changes for the two criteria are shown in Table 8.5, while the robustness index is shown in bold in the same table.

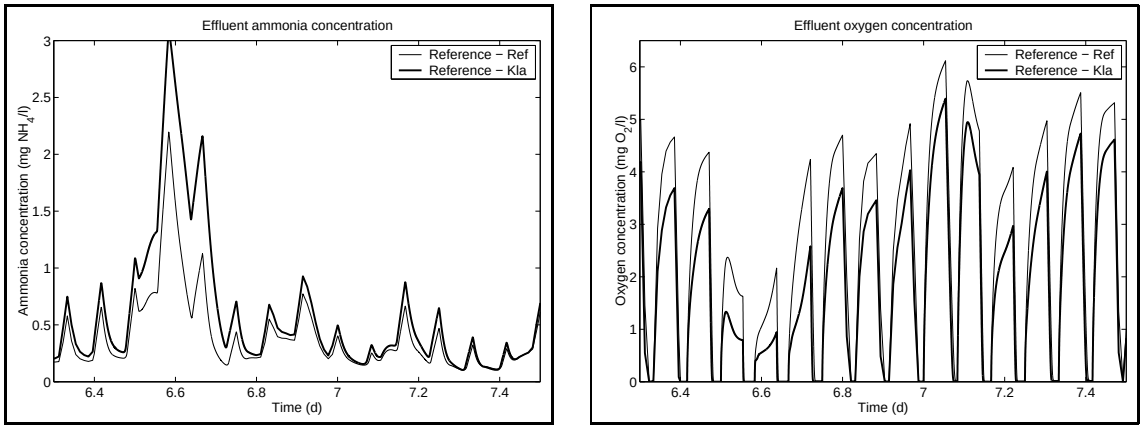


Figure 8.23: The effect of the Kla decrease with 10% on the resulting effluent ammonia (left) and oxygen (right) concentration

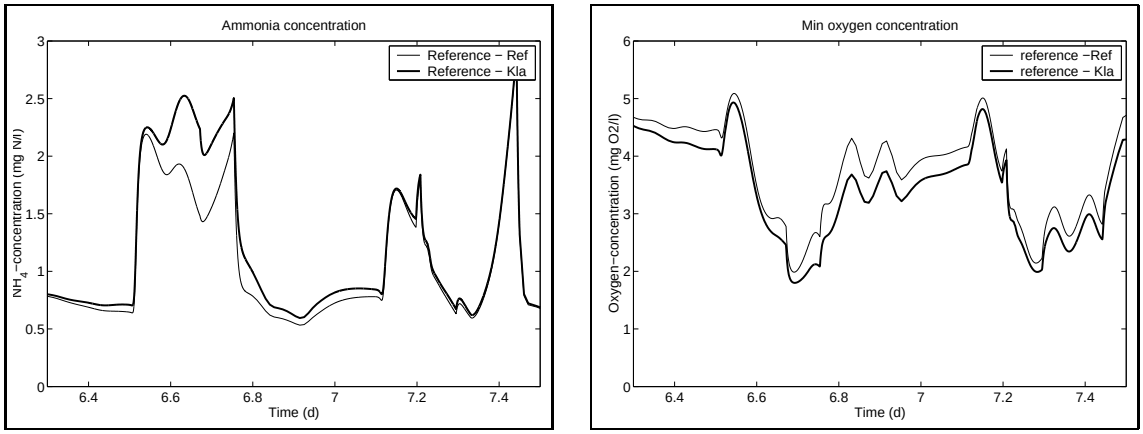


Figure 8.24: The effect of the Kla decrease with 10% on the resulting ammonia concentration (left) and oxygen concentration (right) for the reference control strategy

From Table 8.5 it can be seen that for the two criteria, the robustness of the different control strategies is similar, except for the maximum ammonia concentration where the reference control strategy is more robust. This is somewhat logical, since the controllers have been tuned to perform well in a given situation on the maximum ammonia concentration, and are hence more sensitive towards changes for this criterion. For the other criteria, no substantial change in robustness is noted, but the general performance is better. It can therefore be concluded that it is relatively safe to use the suggested control strategies. As the system is never as it was modelled, the robustness index shows that the controller will also work well in slightly different environments. It should be noted that also different storm and long time series should be evaluated by the model before implementation in practice.

8.9 Conclusions

In this chapter, the different steps of the general procedure for the design and tuning of immission based control strategies in the IUWS (see chapter 4) were applied in a case

Table 8.5: Sensitivities and Robustness (bold) of the different control strategies for different criteria to changes in μ_A, Kla and TKN content (for more details, see text)

		Max, NH_4	Duration NH_4
Ref	μ_A	-0.0087	-5.2313
	Kla	-0.1.7777	-1.5200
	TKN	-0.4038	-1.02
Robustness		**3.2546**	**0.9177**
Strategy 1	μ_A	-0.1523	-0.2921
	Kla	-0.7781	-2.3428
	TKN	-0.3713	-1.1194
Robustness		**1.9799**	**0.6651**
Strategy 2	μ_A	-0.2023	-0.4444
	Kla	-0.9551	-3.2585
	TKN	-0.4401	-1.5835
Robustness		**1.6162**	**0.5328**

study on the catchment of Tielt.

The model simplifications and reductions applied were described and explained. A model including the three subsystems of the IUWS was constructed that could be used for the tuning. For the evaluation of the secondary objectives, a more complex model, only describing the river system, was used.

For the selected rain events, it was shown that a substantial reduction in model complexity could be obtained while still keeping sufficient accuracy for the defined goals. By choosing river ammonia concentration as a primary control variable, the part of the river downstream of the in-stream ammonia measurement could be eliminated from the control model, resulting in a river model consisting of six tanks in series rather than 18. As a first strategy, the measurement of ammonia in the river was used to decide on the overloading of the treatment plant. In a second strategy, a pump was installed in the sewer system, generating an increased flow towards the treatment plant, and hence a reduction in combined sewer overflow volume.

The proposed control strategies, although relatively simple, were able to improve both the emissions and the immission concentration of ammonia at the critical mixing point. However, the improvements were not very large, due to the fact that the CSOs that could not be acted upon by the control strategy, were still polluting the river during storms. For oxygen, no differences could be noted, due to the fact that the biological conversion rates in the river were very low, due to the low bacteria concentrations. Future research could compare the immission based control strategies proposed with a more traditional volume or pollution based approach, in order to decide if the immission based approach is superior to the others.

The robustness of the proposed control strategies was tested by changing three system characteristics, the growth rate of the autotrophic biomass (μ_A), the aeration capacity (Kla)

and the nitrogen content of the wastewater (TKN). The robustness towards two water quality criteria was evaluated: the maximum ammonium concentration and the time the ammonium was above a limit. It was shown that the control strategies had about the same robustness as the reference and could therefore be accepted for implementation.

Chapter 9

Real-time control of the minimum oxygen in rivers

9.1 Introduction

In the previous chapter, an immission based control strategy was designed to minimise the ammonia concentration in the river. This was possible due to an on-line measurement of the ammonia in the river. Oxygen was considered to be a secondary objective. In this chapter, the same integrated model is used as in chapter 8, but now the primary objective is to optimise the oxygen concentration in the river, while the ammonia concentration is the secondary objective. Whereas the maximum ammonia concentration can be measured directly in the river at the critical mixing point, the minimum oxygen concentration can not be measured that easy. This has two reasons which are both related to the oxygen dynamics in the river and are explained below.

The first reason is the fact that the minimum oxygen concentration is usually not due to mixing alone, but is mainly due to consumption of oxygen in the river downstream of the discharge point. This means that there is a time delay between the CSO event, and the time at which the minimum oxygen concentration is reached somewhere in the river. The CSO event may have finished before the minimum oxygen concentration in the river is actually reached. The second reason is the fact that the location of the minimum oxygen concentration in the river varies in time, depending on the BOD concentration, the discharge point and the flow velocity. It is thus not possible to use a hardware sensor on a fixed location.

To overcome these problems, a software sensor is proposed. A software sensor uses field measurements and calculates from these measured data other information which might be more useful (Dochain and Vanrolleghem, 2001; Vanrolleghem and Van Daele, 1994). In this chapter, a software sensor to predict the minimum oxygen concentration in the river is designed. In a second phase, this oxygen predictor will be used in an immission based RTC strategy to optimise the minimum oxygen concentration in the river.

9.2 Minimum oxygen prediction

9.2.1 Principle

The software sensor to predict the minimum oxygen concentration in the river is based on the Streeter-Phelps equation (Streeter and Phelps, 1925). For a constant stream velocity and steady-state discharge of pollution, the following equations can be used to describe the dynamic behaviour of both BOD and oxygen in a river:

$$\frac{dBOD}{dt_T} = -K_1 BOD \tag{9.1}$$

$$\frac{dDO}{dt_T} = -K_1 BOD + K_L a(DO_{sat} - DO) \tag{9.2}$$

where :

BOD	BOD concentration (g/m^3)
DO	Dissolved oxygen concentration (g/m^3)
K_1	First order degradation constant for BOD (d^{-1})
$K_L a$	Reaeration constant (d^{-1})
DO_{sat}	Oxygen saturation concentration (g/m^3)
t_T	Time of travel (d^{-1})

The oxidation of BOD is described as a first order reaction, while the oxygen is consumed during this oxidation. Oxygen is added to the water by reaeration, proportional to the difference between the oxygen saturation concentration and the actual in-stream river concentration.

The solution of these equations in steady-state conditions can be written as (Schnoor, 1996):

$$BOD(t) = BOD_0 e^{-K_1 t} \tag{9.3}$$

$$DO(t) = DO_{sat} - (DO_{sat} - DO_0)e^{-K_L at} - \frac{K_1 BOD_0}{K_L a - K_1}(e^{-K_1 t} - e^{-K_L at}) \tag{9.4}$$

where

DO_0	initial oxygen concentration (g/m^3)
BOD_0	initial BOD concentration (g/m^3)

This is a typical sag curve, shown in Fig. 9.1. The critical time, at which the minimum oxygen concentration is found, can be calculated from equations 9.3 and 9.4 (setting the derivative in eq. 9.2 to 0).

$$t_c = \frac{1}{K_L a - K_1} ln\left(\frac{K_L a}{K_1}\left[1 - \frac{(K_L a - K_1)}{K_1}\frac{(DO_{sat} - DO_0)}{BOD_0}\right]\right) \tag{9.5}$$

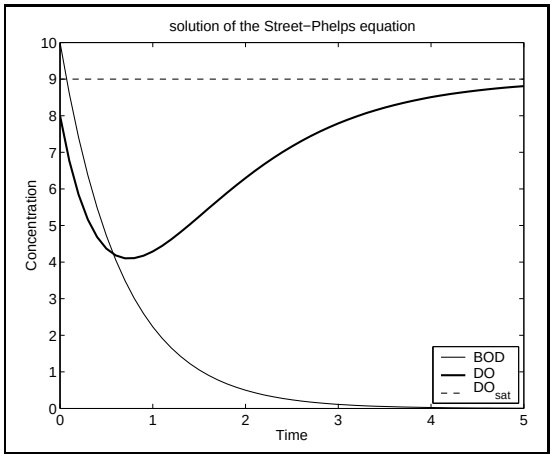


Figure 9.1: Solution of Streeter-Phelps equation, the oxygen-sag curve

By substituting t_c in equation 9.4, the minimum oxygen concentration can be found. If the different parameters (DO_0, K_1 and K_La) and state variables of the model are known, the minimum oxygen concentration in the river can be predicted with these equations.

9.2.2 Estimation of DO_0

In the control model as described in chapter 8, no conversion model is present. Hence, the calculated oxygen concentration at the location of the bypass is the result of mixing alone. This concentration cannot be used as a measure of DO_0. Consequently, the complete model had to be used to estimate an average DO concentration during dry weather conditions.

The average oxygen concentration during dry weather was 4.2 mg O_2/l. This parameter was then used in the model to predict the oxygen concentration at location of the OUR measurement. It is clear that in reality an oxygen sensor could be used to determine the oxygen concentration in the river.

9.2.3 Estimation of K_1

The next parameter to estimate to allow the use of the prediction model, is the first order degradation constant of BOD. As a first approximation the following relationship between measurements of BOD and OUR can be used:

$$OUR = K_1 BOD \tag{9.6}$$

or

$$K_1 = \frac{OUR}{BOD} \tag{9.7}$$

This means that all oxygen consumption is described as if it was caused by the degradation a lumped amount of BOD. From the simulation in the reference case, both the OUR

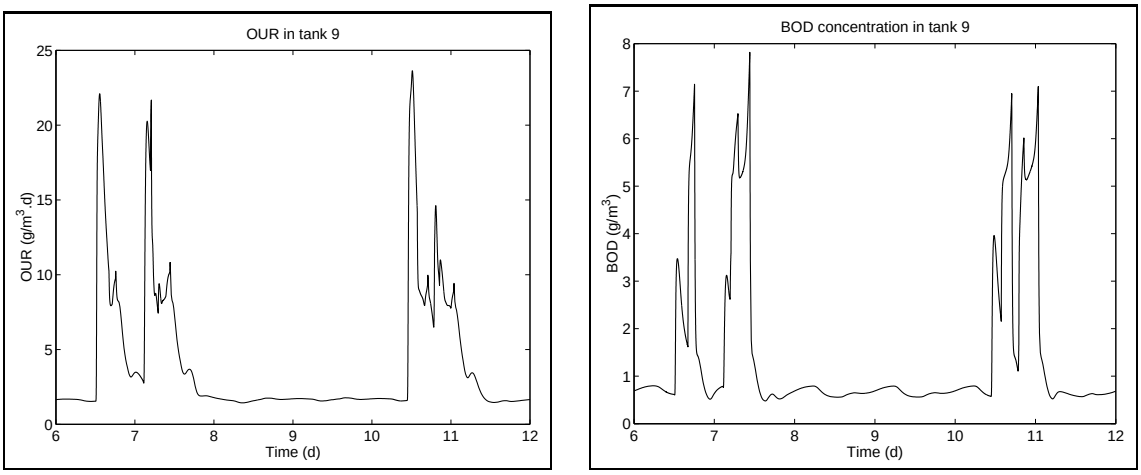


Figure 9.2: The OUR and BOD concentration during the selected simulation period

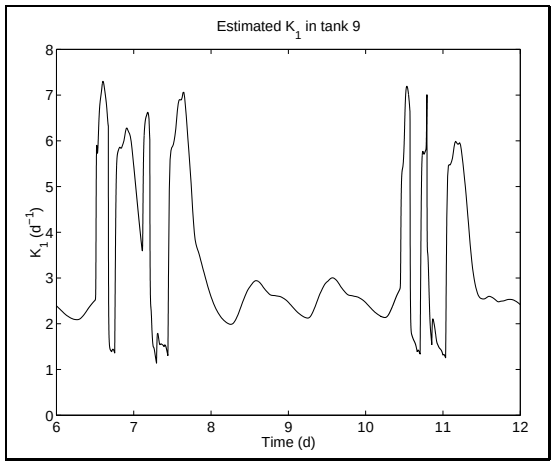


Figure 9.3: The estimated first order degradation constant K_1

time-series and the BOD time-series can be used. Both the OUR and the BOD concentration change during the simulation (Fig. 9.2). In the approach followed, the BOD is approximated by the soluble biodegradable COD fraction, times (1 - Y), where Y is the yield coefficient for soluble COD. The resulting estimation of the K_1 is shown in Fig. 9.3.

It can be seen that the estimated K_1 changes a lot during storm conditions. Since the controller focuses on the negative impact of wet weather conditions, the average of the K_1 estimated during the first two storms will be used in the oxygen prediction model.

9.2.4 Estimation of the $K_L a$

The implemented Streeter-Phelps model uses the OUR as an on-line measurement in the river. Therefore, only one parameter can be adjusted to fit this model to oxygen measurements in the river. This is the parameter $K_L a$. This parameter was changed in order to maximise the correspondence between the predicted and the observed minimum oxygen concentration. The best value was found to be 1.8 d^{-1}.

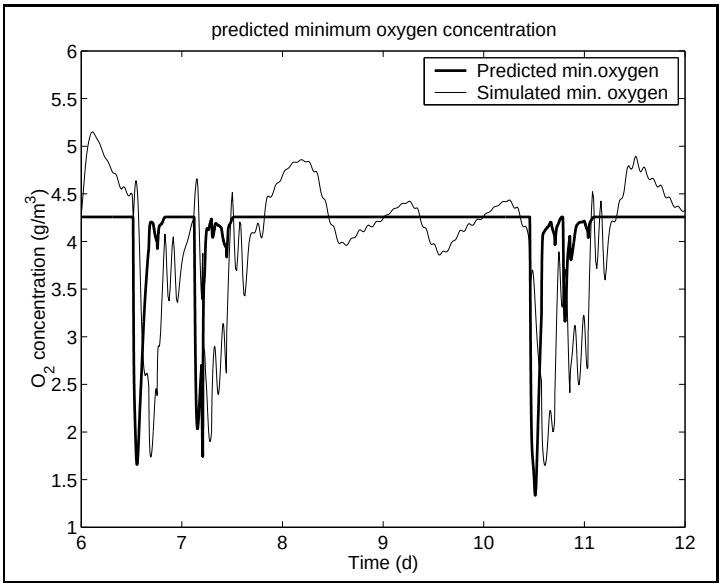


Figure 9.4: Comparison between simulated and predicted oxygen concentrations

Table 9.1: Observed and calculated critical time

Time of storm	Observed t_c	Predicted t_c
6.7	0.15	0.154
7.28	0.13	0.217
10.6	0.1	0.21

9.2.5 The oxygen predictor

Fig. 9.4 shows the results of the oxygen predictions with the simulated data with the river model. It can be seen that the deepest peaks are predicted well, while the smaller peaks are not. The calibration of K_La was done on the storm during days 6-8, while the other storms were used to validate the model predictions.

As an additional check of the model, the critical time as predicted in the Streeter-Phelps model and the observed delay between the predicted and the simulated peak can be compared. It can be seen in Table 9.1 that the predicted and observed critical times match only for the first peak. This is obviously due to the simplifications in the predictor model. It is clear that depending on the flow conditions, the same t_c will result in a different location of the minimum concentration in the river.

9.3 The minimum oxygen control strategy

The control strategy adopted here corresponds to control strategy 1 of chapter 8 which uses an on-line ammonia sensor to determine if the WWTP needs to be overloaded or not. The only differences are the sensor used and the set-point. In this case, the setpoint is set to 4 mg O_2/l and the measurement used is the predicted minimum oxygen concentration

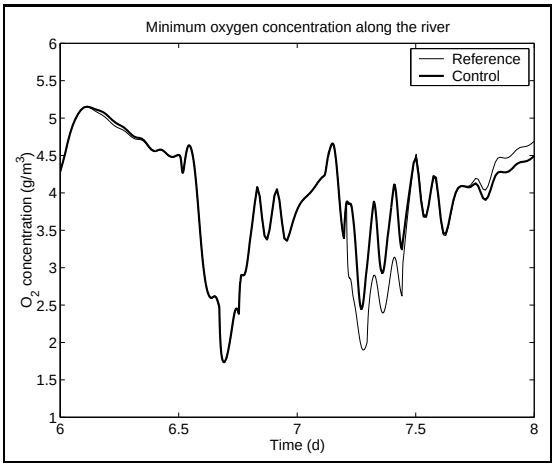


Figure 9.5: Resulting oxygen concentration in the river for the reference and the control case

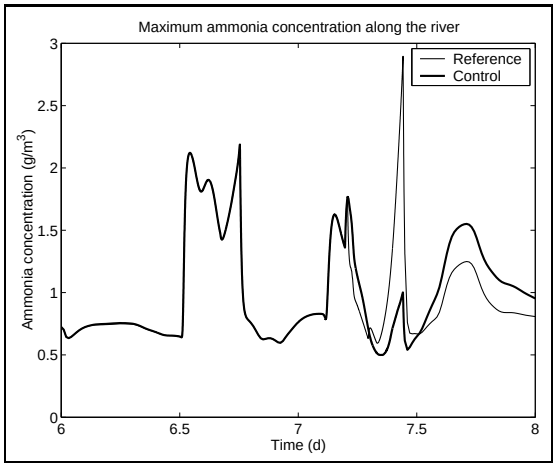


Figure 9.6: The ammonia concentration in tank 9

in the river. If the predicted minimum oxygen concentration in the river is lower than 4 mg O_2/l the WWTP is overloaded. As in control strategy 1, a supervisory controller on the sludge blanket height was also implemented.

The overloading of the WWTP is calculated as follows:

$$e = \begin{cases} DO_{SP} - DO & \text{if } DO < DO_{SP} \\ 0 & \text{otherwise} \end{cases} \tag{9.8}$$

$$Q_{WWTP} = min(3Q_{DWF} + K_P * e, F_{overload} * Q_{DWF}) \tag{9.9}$$

where

DO_{SP}	Setpoint for dissolved oxygen (g/m^3)
K_P	Proportional constant
$F_{overload}$	Maximum overload allowed to the WWTP

$F_{overload}$ determines how much water can go to the WWTP, while K_P determines which deviation from the setpoint is needed before the maximum flow rate is allowed. This overloading is not applied when the storm tank is not completely filled or when there is a risk of sludge loss in the settler.

Different combinations of K_P $(3-5)$ and $F_{overload}$ $(3-6)$ were tried (De Grove, 2002). It turned out that K_P does not have a large influence on the performance of the controller, while $F_{overload}$ = 5 was a good balance between overloading the WWTP and the effect on the receiving water. The resulting oxygen concentrations in the river are shown in Fig. 9.5.

No large effect of overloading the treatment plant on the concentration of oxygen is observed. This is due to the fact that the biological activity in the river is rather low due to the low biomass concentrations. If more biomass is present, the reduced COD load leads to a considerably improved oxygen concentration when overloading the WWTP (results not shown). A large contribution of the decrease in oxygen is due to the fact that bypassed wastewater without oxygen is entering the river (Fig. 9.7). As previously noted

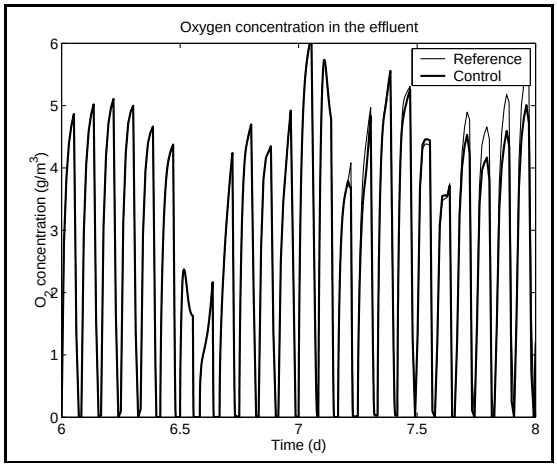


Figure 9.7: The effluent oxygen concentration

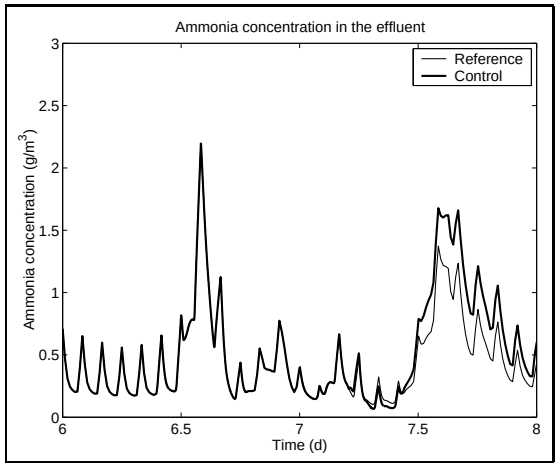


Figure 9.8: The effluent ammonia concentration

(section 8.8), the first storm can not be influenced by this type of control strategy, since the decrease in oxygen is originating from an upstream CSO that is not controlled.

The ammonium concentrations in the river are shown in Fig. 9.6. It can be seen that the control strategy eliminates the ammonium peak at t = 7.4d thanks to the overloading of the treatment plant. However, it can be seen that during the next days, an adverse effect on the ammonium concentration can be noted. This is due to the fact that the overloading of the WWTP disturbs its operation and reduces its nitrification capacity. The overloading of the WWTP in this case has a negative impact on the ammonia concentration (Fig. 9.8).

9.4 OUR measurements

The oxygen predictor assumes that a measurement of the OUR is instantaneously and continuously available. However, this cannot be achieved in practice and the delays caused by this type of measurement will certainly influence the performance of the controller in a negative way. As can be seen in Fig. 9.2, the OUR is about 20 g/m^{3}d in storm conditions. While OUR measurements are well known in activated sludge monitoring and control (Spanjers *et al.*, 1998), the use in river water quality may be limited by the relatively small biomass concentrations present in river water, resulting in low OUR values. Using traditionally respirometric principles, this leads to relatively long measurement times, which in turn have a negative effect on the performance of the controller due to the increased delay. When the OUR is 10 g.m^3/d and the measurement time is set to 15 min, the difference in oxygen to be measured is only about 0.1 g/m^3, when a closed type of respirometer is used. This is close to the accuracy of oxygen electrodes, and hence limits the accuracy of such a measurement.

9.5 Discussion

The problem with the proposed, simple predictor is the fact that it cannot take sediment oxygen demand into account. Depending on the oxygen demand of the sediments down-

stream of the measurement, a different oxygen consumption may noticed on the same location. Indeed, as Harremoës (1982) already noted, two types of oxygen demand can be distinguished: immediate and delayed. While the predictor takes the immediate oxygen into account, it cannot, due to its structure, take the delayed oxygen demand into account. Hence, in a situation where the delayed (sediment) oxygen demand is important, the oxygen predictor will perform poorly. Therefore, it is doubtful whether this controller will allow to keep the oxygen concentration at the desired level.

As an alternative measurement, the BOD could be approximated by on-line UV-measurements. In this case, the OUR can be estimated as $K_1 BOD$. It should be carefully evaluated whether the investment needed to install such a type of controller is worth the improvements obtained, or whether the money could not be invested in a better way.

9.6 Conclusion

In this chapter, a controller for the minimum oxygen in the river was developed. For this, a prediction of the minimum oxygen concentration in the river is necessary. By using the Streeter-Phelps equations and using an on-line measurement of the OUR, the minimum oxygen concentration could be approximated reasonably well under critical conditions. With this type of predictions from the software sensor, it could be decided to overload the WWTP or not. While a small improvement in the oxygen concentration could be obtained, the ammonia concentration in the river was increased for a couple of days after the storm. This was due to the adverse effect of overloading the WWTP on its performance. Moreover, the oxygen predictor only takes the immediate oxygen depletion into account, neglecting the sediment oxygen demand downstream of the discharge point. This might lead to large errors when applied in practice. However, the concept of using software sensors to predict the effect processes with a time delay seems an interesting approach.

Chapter 10

General discussion and conclusions

In water quality managements, two main approaches to protect the quality of receiving waters can be followed (Tyson *et al.*, 1993): the approach following the Uniform Emission Standards (UES) or the approach following Environmental Quality Objective/Environmental Quality Standards (EQO/EQS). The Water Framework Directive, described in chapter 2, imposes new goals for all surface and groundwaters in the EU. A "good" water quality should be obtained by 2015. Both a "good" ecological status and a good chemical quality are required. This is a change in paradigm compared to the previous European Directives (like e.g. the Urban Wastewater Directive) that mainly focused on the emissions, rather than on the immissions.

The WFD explicitly mentions that ecological integrity is an important goal. This has important consequences for the current practices in the integrated urban water management. Traditional engineering solutions like minimising CSO volumes are no longer sufficient, since they do not guarantee that the good ecological status will be met. Therefore, new techniques and models will have to be applied in order to obtain a systems analysis which allows these advanced goals to be studied (like immission-based control, uncertainty analysis, ecological modelling). So far, most models have been dealing with the emissions from the sewer system and the treatment plant separately, while currently more research is being devoted to the resulting "immission concentrations". However, ecological modelling and predictions of ecosystems behaviour are still a problematic issue, although advances are being made (Goethals and De Pauw, 2001; Schleiter *et al.*, 1999).

As it is clear from the WFD that an integrated approach from an immission point of view is necessary to fulfil the requirements set in this Directive. In this work the possibilities and problems of immission based RTC in the Integrated Urban Wastewater Systems (IUWS) are investigated as a contribution to the tools useful in complying with the WFD. The IUWS is defined here as the combination of sewer system, treatment plant and receiving waters. Real-time control allows for the optimisation of existing infrastructure, without the need to extend the system. Real-time control of the subsystems, especially the sewer and the WWTP have proven to be able to reduce the amount of pollutants released to the receiving water. Also, the so-called integrated real-time control, in which interactions between the different subsystems are taken into account have been investigated and shown to perform better than the RTC of the subsystems (chapter 2).

10.1 Immission based real-time control

However, immission based real-time control, in which sensors in the river are used, have not been investigated so far. The possibilities of these type of control strategies were described in chapter 8. Two immission based control strategies were implemented and tested using a mathematical model that was based on the Tielt situation. In this simulation study, the objective was to keep the ammonia concentration in the river below a given threshold. This strategy takes into account the assimilation capacity of the river, which is not the case when applying emission based RTC strategies.

When the ammonia in the river was above the threshold concentration, the WWTP was hydraulically overloaded. The WWTP in Tielt is an extended aeration plant, and has sufficient aeration capacity to deal with the extra COD entering the plant. In addition the settler was not adversely affected by the increased hydraulic load. No other actions were taken at this stage, since the modelled effluent of the treatment plant was not adversely affected by this overloading.

The overloading of the WWTP was limited to the time interval during which the ammonia concentration was above the threshold. Once the ammonia was lower again, the overloading was stopped. This has as a main advantage that the WWTP is not overloaded during time periods in which the river was not in a critical situation. An emission based strategy could have overloaded the plant more than necessary for the river system.

It is clear that the control strategy applied in this integrated study is very simple and maybe even simplistic. Many other, more advanced control strategies to deal with storm water inflows to a WWTP like step feed control, aeration tank settling, etc. have been developed and may be integrated into an immission based control strategy. However, even with this simple strategy, the model showed improvements of the river water quality compared to the non-controlled case. The important point is that the sensor in the river indicates in which time periods this overloading is necessary. During these periods where the overloading is necessary, the advanced strategies should then deal with the extra flow directed towards the WWTP.

During the periods overloading is not necessary, i.e. when the assimilation capacity of the river is not exceeded, bypass of some diluted wastewater is allowed. This has several advantages, like a lower operational cost at the WWTP, less risk of sludge wash-out, less disturbance of the plant in case a second storm arrives, etc. The immission based control strategy provides the possibility for a balance between the protection of the environment and the costs for the protection of this environment. This is also a goal of the WFD: cost-effective measures to obtain the goals set.

As an alternative to the on-line ammonia measurement, a predictor for the minimum oxygen concentration in the river was developed and tested in chapter 9. The minimum oxygen could be predicted reasonably well under critical conditions. The control strategy based on this prediction could improve the oxygen concentration in the river only slightly. Moreover, problems with on-line measurements of the OUR need to be overcome before this can be implemented in practice.

Perspectives on immission based real-time control

In future research, the advanced control strategies that have been developed in the subsystems need to be integrated into an immission based strategy. In this way, an optimal combination of existing knowledge on RTC strategies and an integrated approach for the management of the IUWS can be achieved. A hierarchical control strategy that determines the setpoints and goals for the control systems in the subsystems is a possible solution. So far, these hierarchical control strategies have been constructed mainly by heuristic reasoning. It is the idea of the author that numerical techniques used in control theory could be extended or adapted for use within an integrated approach. The example of model based predictive control described by Rauch and Harremoës (1999) gives an indication about the possibilities of these techniques within the integrated urban wastewater management. The uncertainty and inaccuracy of the models used in the controllers can be compensated by reliable on-line measurements.

In order to achieve an optimal transfer of knowledge, a multi-disciplinary team is necessary. It is felt that many research projects are unbalanced in a way that the authors tend to emphasise those aspects that they know best, while other parts or options are treated in a (too) simplistic way. Every research field related to the management of IUWSs advances very fast, so that in order to include new knowledge and techniques specialists from different fields should be consulted. The advantages of this interdisciplinary approach are shown by Rosen (2001) who applies techniques from chemical process industry to the monitoring and control of WWTPs.

Schütze *et al.* (2002b) state that 33% of semi-hypothetical catchments has potential for improvements of the water quality of the river by integrated RTC. This shows there is a large number of catchments for which integrated RTC might be a valuable option and should at least be taken into account when looking at different options for a given problem. Factors that hinder wider application of RTC so far are the greater complexity in operation, the increased risk of technical and software failures and conservatism (Harremoës, 2002). These factors indeed limit the practical use at the moment, but it is believed that they will (slowly) be overcome if more successful applications are implemented.

10.2 Integrated modelling: Problems and solutions

For the development of the immission based RTC strategies, mathematical models are a useful, if not necessary, tool. All the subsystems have been modelled separately in the past, in varying degrees of detail. These submodels have been used for understanding, planning, management, control and optimisation of the subsystems separately, in general with success for the goals set at the beginning of the studies.

Integrated modelling studies have put these, more or less, detailed models together. In this type of studies, the different submodels were used separately, and were connected by files. When using detailed hydraulic models for sewer or river modelling, long calculation times limit their practical use. Also, problems with the numerical stability of the models are

reported. This modelling approach is useful for applications in design of sewer systems or flood protection.

An integrated model for the design and tuning of immission based control strategies has some requirements that are not fulfilled by the above approach. Three main problems were encountered in this research:

- The calculation times are too long for use in optimisation studies which typically require a lot of simulations
- The two way interaction of the submodels is not possible, due to the sequential modelling of the IUWS
- The different submodels have different state variables due to their separate historical development, that cannot be linked easily to each other.

These three problems were handled in this thesis and the proposed solutions will be discussed in the following sections.

10.2.1 Short calculation times

As mentioned above, detailed mechanistic models need complex numerical algorithms to solve them, leading to long calculation times. Two techniques were proposed in this thesis to obtain shorter calculation times: model simplification and model reduction.

Model simplification

One of the clear examples of complex models within the IUWS are the “de Saint-Venant” equations. These partial differential equations can be used to describe the hydraulic behaviour of sewer systems and rivers in detail. However, the accuracy obtained with these equations is much higher than the accuracy obtained with the water quality models. Therefore, alternatives for the hydraulic models of these subsystems are proposed. The CSTR-in-series approach is used successfully in sewer systems (e.g. the Kosim models). Also in river water quality modelling the use of CSTRs-in-series is adopted. However, problems are encountered in modelling the difference in flow and wave velocity, while also backwater effects are considered problematic. Another disadvantage of these simplified models is that they require a lot of data to calibrate the parameters accurately.

The simplified models are called mechanistic surrogate models, as they form a “surrogate” for the real thing, i.e. the mechanistic model. In this work, a general procedure for the creation of mechanistic surrogate models is developed. The main idea of the procedure is that the collection of field data for the calibration of the surrogate model is too expensive or laborious. Therefore, first a complex mechanistic model is to be created with the data available or collected during measurement campaigns. With this mechanistic model, simulations are done during which data are collected. With these “virtual” data, the mechanistic surrogate model is calibrated which subsequently can be used in the integrated model for design and tuning of the immission based RTC strategy.

It is important to note that this technique can only be used for those models that are known to be reliable enough to generate virtual data, as is the case with the "de Saint-Venant" equations. For models that are more uncertain, a simplified model can be calibrated directly from the field data. For example, the existing water quality models for sewer and rivers are too uncertain to be used for the generation of virtual data (see e.g. Willems and Berlamont (2002)).

This technique of data generation with complex mechanistic data was used in the model simplification of the ASM2d model for the WWTP (chapter 5), and for the river hydraulics in the case study on the river Zwalm (chapter 6).

Artificial neural networks were used to describe the conversion terms in a grey box model of an activated sludge tank. Different training algorithms were used and for a simple conversion model successful one-step ahead prediction of the conversion rate could be obtained. However, due to the grey-box model structure, the small errors on the predicted conversion rate are accumulating in the predictions of the concentrations of the model variables on the next time step. This sequence led to an accumulation of errors, and a model that could not be used as a surrogate for the conversion model of an activated sludge tank. The use of different training algorithms might improve this situation, although neural networks perform better when correct inputs from measurements or mechanistic models are used (Lee *et al.*, 2002).

In a second case study, the flow and pollutant concentration in the river Zwalm were approximated by a tanks-in-series model. The data needed for calibration of this model were generated by a model of the same river, using the diffusive wave approximation of the "de Saint-Venant" equations. Two steps in the calibration of the CSTRs-in-series model were necessary. In a first step the geometry of the tanks had to be adapted from the classical, rectangular shape. A parabolic relationship between the cross-sectional area and the water depth was found to best fit the observed data. This type of relationship is useful when modelling small rivers or creeks, which are narrow near the bottom and become wider near the top of the profile.

In a second step, the hydraulic parameters of the model were fitted. Two approaches can be followed for this. First, a static Q-h relationship can be fitted to the data produced by the "de Saint-Venant" equations. Second, a parameter estimation using dynamic simulation can be used to optimise the parameters describing the Q-h relationship of the surrogate model. The parameters were optimised for every tank separately. In the validation phase, the different tanks were connected to each other to create the model of the complete river. The flood wave propagation through the river could be approximated very well by the CSTRs-in-series model. Also, the backwater effects present in the river could be predicted well. The prediction of the pollution wave, which proceeds at a slower velocity than the flood wave, was found to be less, but still sufficiently accurate. Moreover, the accuracy could be increased by increasing the number of tanks used. However, this again increases the calculation time. Hence, the final number of tanks used will be a compromise between accuracy of the model and the calculation time. However, it could be concluded that the CSTRs-in-series model can be used as a surrogate for the complex mechanistic model, both for the flood and pollution wave propagation. Comparing this work to the approach followed by Reda (1996), it can be concluded that in their work more field data could be used to calibrate the extra parameters of the model.

Model reduction

A second technique proposed in this work to decrease the calculation time is model reduction. In literature, model reduction often refers to the simplification of model equations, e.g. changing a two-step nitrification into a one-step nitrification model. Similar techniques were applied in this thesis for the ASM2d model. However, model reduction can also be seen as reducing the space and time boundaries used during the simulation.

In section 5.4, several ways to reduce the ASM2d model and the Takács settler model were examined. These range from simplifying the oxygen dynamics, to eliminating certain state variables and replacing the Takács model by a conceptual settler model. The simulation results of the different reduced models were compared to the results obtained by the simulations with the full model. It was concluded that it is difficult to decide whether a reduced model approximates the full model closely enough or not. Different measures of performance were checked: visual comparison of the time series, comparison of the average concentrations, standard deviations or extremes, comparison of the frequency distributions of different pollutants in the effluent. However, since the immission based RTC study in chapter 8 overloaded the WWTP during storm conditions, it was decided to use the complete model in the RTC study. In general, criteria for model selection and reduction need to be based on the goals of the study. As with any model, a balance should be found between the amount of data available, the model complexity and accuracy and calculation time. It is clear that a model for controller tuning does not need the same accuracy as a model used for calculation of immission concentrations of a specific chemical.

A second model reduction was applied on the integrated model of Tielt. Four types of possible model reductions were identified in chapter 4: relocation of upstream and downstream boundaries, reduction of the conversion model and reduction of the time boundaries. All these reductions are based on the fact that the controller under study, is only influenced by certain parts of the system and only influences part of the system, both in time and space. Only those parts need to be modelled when designing and tuning the control strategy. For example, the upstream parts of the sewer system and the river might not be influenced by the RTC strategy and can be left out. Similarly, the part of the river downstream of the last sensor, can be left out. This approach was applied in the development of the so-called “control model” in the Tielt case study. Both the sewer system and the river model could be reduced substantially without influencing the tuning of the control strategy.

Perspectives on reducing calculation times

This research was started 3 and a half years ago on a PC with a Pentium 100 MHz processor (using a Unix workstation for computations) and ended on a machine with a Pentium III 800 MHz. Still simulations are considered to be too slow. It may be concluded that the increase in computation power, is balanced by the increasing expectations of the modeller. Faster computers have become available, but modelling software and the models used still put the memory and processor to their limits, as could be noted from the number of nights

that these PCs have been calculating at a processor use of 100% and a completely filled physical and virtual memory.

These uses of simplified and reduced models hence may improve the development speed of new models and control strategies. The models applied in this study only describe a small part of the river basins that should be taken into account according to the WFD. In these cases, even more general models will have to be applied for the catchment to identify problematic substances or discharges. Then, the somewhat more detailed models can be used to study the identified problems. In this way, a hierarchical model structure can be constructed from river basin, to a single river, to a single sewer system, to a single detention tank. When used in RTC applications, the models high up in the hierarchy might be used in a supervisory management or control scheme by setting general performance levels for the subsystems. The subsystems then need to comply to these requirements in the best possible way. It is expected that this type of models will be used increasingly, when dealing with the WFD.

Another aspect strongly influencing the calculation time are the software implementations and numerical algorithms used for solving the model equations. It is clear that compiled code is superior to interpreted code (with respect to calculation time). Most integration and optimisation algorithms currently available in commercial software are rather old, and new techniques, like genetic algorithms, are only slowly being implemented. Also efficient stiff solvers are not implemented currently in WEST, which limits its performance for the integration of stiff model equations, which the biological models used often are. It should however be noted that Jeppsson (2002) found that for hybrid systems, stiff solvers may work slower than traditional integration algorithms. It is hoped that improved interaction between mathematicians, software engineers and modellers improves the algorithms used or implements the methods used in a computationally efficient way. A good example of the consequences of suboptimal implementation was given during the last week of this work, where the improvement of a function to read the input file, resulted in a decrease in simulation time with a factor 3-5, depending on the model. Also, the way the model equations are implemented has a large influence, and has to be a balance between readability of the code and its efficiency. An intermediate step with computer optimised code as implemented in WEST fulfils both requirements.

10.2.2 Simultaneous simulation of the IUWS system

The second problem encountered when creating the integrated model was the need for two way interaction between the different parts of the system. A sequential simulation prohibits these and, hence, a simultaneous simulation was used. To achieve this, all models had to be implemented into one software package, for which WEST was chosen. WEST was originally developed for the simulation of WWTPs, but in this study models of both the sewer system (based on the Kosim equations) and the river (based on the RWQM1 combined with CSTRs-in-series) were implemented. Due to the hierarchical model building environment of WEST, the creation of the integrated model from the individual models is relatively simple.

The structure of the model base present in WEST has been reorganised in order to allow for an efficient reuse of general model equations as mass balances for CSTRs. In this way, new biological conversion models (like submodels of the RWQM1) can easily be added. Also, the frequency of errors is reduced in this way. Moreover, the model base can easily be extended with other models. As a conclusion, the simultaneous simulation of the IUWS system is now possible, although simulation with the current implementation still requires, despite the use of simplified and reduced models, a long calculation time. The current software implementation does not allow the (Kosim) model to be simulated as fast as in the original implementation using convolution integrals. The creation of a simulator that can handle both continuous and discrete equations at the same time, might further reduce the calculation time and, hence, ease the design and tuning of immission based control strategies.

Perspectives on simultaneous simulation

Simultaneous simulations are necessary if two way interaction between the submodels is required. Two approaches are used: (1) write a coordinating software package that controls data transfer between models implemented in different packages. This approach is followed for example by Synopsis (Schütze, 1998) and the Integrated Catchment Simulator (Taylor *et al.*, 2000). The other approach is to implement all models in an open simulator like Matlab™ or WEST. Both approaches can be defended, but the coordinating program induces an overhead compared to the all-in-one packages. When aiming for integrated basin management, a good software package should have an extensive and open model base, a sound numerical basis, a user-friendly interface, proper documentation and routines for data handling. Especially this last property is important since a lot of time has to be spent now before the simulation outputs are transformed into a format that allows easy interpretation. Moreover, if management on a river basin scale needs to be implemented, a GIS interface is also necessary. It should be evaluated which of the existing implementations is better in a given situation. In this work, the very fast Kosim modelling approach was implemented into WEST in a much less efficient way, increasing the computation time to have the possibility of simultaneous simulations. Again, the best choice depends on the system under study and should be carefully looked at.

10.2.3 Connecting models with different state variables

The third and last problem encountered in this study, relates to the fact that the existing models of the subsystems use different state variables. This problem was handled by the construction of connectors that include a “logical transformation of the state variables” and have a closed mass and elemental balance. For every component in either subsystem, the elemental composition needs to be determined. The use of correction terms then allows to compensate for the difference in compositions in the different subsystems, while closing the elemental balances. The closed mass balance approach is an important principle, but is still a pragmatic approach, since it assumes constant compositions of a state variable during the complete simulation time. It is, however, known that the composition

of the particulate fraction in a sewer system changes during a storm, or differs between storms. Since no detailed knowledge or model is available for this, the above approach was used. However, it should be kept in mind that these changes do happen in reality and one should keep them in mind when judging the model results or uncertainties.

Perspectives on the connection of models

It is clear that the approach followed in this study does not include all variations that are observed in reality. When a more realistic description of the composition of state variables e.g. sewer sediments is needed, a stochastic approach may be chosen. In this approach, the relationship between for example COD and suspended solids is not fixed as in the approach used in this study, but described by a distribution function. In this way, the observed variation is taken into account. However, the worst case scenario, which can be obtained by a conservative choice of the deterministic parameters, is then not taken into account. The application of the model might in this case be decisive on the approach to be followed.

10.3 Final conclusions and perspectives

Mathematical models have since long been used in water quality management. In this work, these mathematical models have been used for the design and tuning of an immission based control strategy in the integrated urban wastewater management. A simultaneously simulating mathematical model using mechanistic surrogate models for the subsystems has been developed. However, a lot of work remains to be done in different fields.

The first field is the integration of knowledge between control engineering and integrated wastewater systems modelling. A combination of the possibilities in these two fields can increase the performance of the system. However, the control engineering field should focus on dealing better with non-linear systems in order to solve the problems in the IUWS.

The second field is the understanding of the processes in the subsystems. In this work, no attention has been paid to sediments or sedimentation and resuspension processes, even if they are important in most IUWS systems. The reason is that the predictive capabilities of the models are currently not sufficient to allow for a good simulation of the observed phenomena, even while using complex mechanistic models for the hydraulics of the sewer or river system.

Third, and related to the previous field, the identifiability and uncertainty analysis needs to be improved, both for the complex mechanistic and simplified models. Moreover, the uncertainty propagation from one submodel to another needs to be studied. A first step has already been made by Willems (2000). In addition, in many modelling studies the lack of sufficient water quality data is still problematic and data collection needs to be extended and/or coordinated better to reduce the uncertainty of the estimated parameters.

Fourth, the models currently used in the urban wastewater management are deterministic models. Stochastic models might be needed to better describe certain phenomena like sewer sediment behaviour. This needs to be included in the modelling approaches.

Fifth, in this work, the traditional water quality parameters have been focused upon. However, to achieve a "good" ecological and chemical status as stated by the WFD, also other parameters need to be improved. In Flanders, oxygen and ammonia problems are still very common and justify this approach. However, heavy metals, aromatic hydrocarbons, pesticides and other substances threaten the ecology in the receiving waters and should be dealt with properly in order to achieve a good status. It is believed that by implementing management practices to deal with these traditional parameters, also the amount of other dangerous substances that are spilled into the receiving water will be reduced. It should however be noted that Harremoës (2002) states that: "*Prediction of ecological effects of urban drainage is not possible by modelling, because of the lack of knowledge related to the cause-effect relationships. The policy has to be based on the empirical-iterative approach complemented by monitoring and analysis and calls for robust, flexible solutions adaptable to new insights and new paradigms*". It is believed that fundamental knowledge about aquatic ecology is not sufficient to be used in modelling today, and until this gap is filled, monitoring, rather than modelling, will provide feedback to the management of the IUWS.

Pesticides and nitrates have a different source (mainly agriculture) and need to be managed similarly to the other pollutants to obtain a good water quality using basin-wide tools like ESWAT (van Griensven and Bauwens, 2001). Also, the impact of the industry on the water quality needs to be looked upon and compared to the influence of municipal urban drainage (see e.g. Demuynck *et al.* (1997)).

Summarising, it can be stated that in order to improve the river water quality in our densely populated areas, an even wider integration is necessary. This not only includes models for sewer systems, WWTPs, rivers, agricultural runoff, industrial pollution, ground water flows and quality, drinking water production, but also, and maybe more important, socio-economic considerations and public participation and motivation. People need to be aware that there is more to water than the thirty cm between the tap and sink.

Water is scarce, and it is the hope of the author that this work may be a small contribution to the solution of a complex problem: the provision of clean (drinking) water to 6 billion people.

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Summary

In the literature review in chapter 2 of this thesis, it became clear that mathematical models are frequently applied to the individual parts of the integrated urban wastewater system (IUWS). Sewer systems, wastewater treatment plants and rivers have been modelled using both complex and simplified models. These models have been used successfully in the management of these subsystems. Different real-time control (RTC) strategies have been developed to deal with disturbances to the system (mostly stormwater in the sewer and treatment plants). In these control strategies, a typical goal is the minimisation of overflow volumes or pollution loads to the receiving water.

Lately, more attention is being paid to the joint consideration of the subsystems in order to be able to take the different interactions into account. This is also required by the Water Framework Directive (WFD) of the EU, which mainly focuses on the quality of the receiving water, which should be "good" both in terms of ecological status and chemical quality. In view of this legislation, management practices that take the immission concentration (i.e. the concentration in the river) into account are necessary in order to be able to comply with the requirements of the WFD.

Immission based RTC is one way of improving the performance of the IUWS, which allows to optimise the quality of the receiving water and uses the existing infrastructure in an optimal way. In order to design and tune such an immission based RTC strategy, a simultaneously simulating model is necessary. In this way, two way interaction between the different submodels is possible.

Three problems are encountered when developing an integrated model that is to be used for developing an integrated control strategy or for system optimisation. First, the state-of-the-art models are typically implemented in different software packages, making simultaneous simulations difficult to achieve, since communication typically requires file transfer from upstream to downstream. Moreover, the flow of information about the downstream state to the upstream models, which is necessary for an integrated control action is even more complicated or even impossible. Second, the state-of-the-art models use different variables to describe the aquatic system (e.g. BOD, COD, TOC, ... to describe organic pollution). Third, the hydraulic equations, which describe flow propagation in sewer pipes and rivers (the "de Saint-Venant" equations) are non-linear partial differential equations. These require complex numerical algorithms to solve, making the models slow and thus difficult to use for optimisation studies.

The first problem of the different software packages was solved by implementing all models in the WEST® simulation software. One of the key features of WEST is its possibility

to integrate multiple processes. To enable this coupling, a powerful model base structure was developed. This model base is aimed at maximal reuse of existing knowledge and is therefore structured hierarchically. The original model base for WWTPs was reorganised and extended to incorporate models of the sewer system and rivers. Moreover, a general concept to connect models with different state variables was developed. In these connectors logical transformations of state variables are incorporated, while also the mass and elemental balances are closed by using correction terms.

The calculation time of the integrated model is reduced by applying two concepts: model simplifications with mechanistic surrogate models and model reduction. Model simplification mainly focuses on replacing complex equations or concepts with more conceptual ones. The complex mechanistic models which are known to have a good predicting capability (if calibrated correctly) are used to generate data by virtual experiments transferring the knowledge compiled in their equations to the surrogate model. In this way, the mechanistic surrogate model can be calibrated on the basis of more data than could be collected by field measurements. This concept was applied to both the WWTP and the river system. Model reduction focuses on the elimination of parts of the model that are not influenced by the control strategy under study. In this way, upstream and downstream parts may be eliminated together with some conversion models. A last reduction focused on obtaining a shorter time period that had to be simulated for the optimisation of the control strategy.

In chapter 5, it was tried to replace the known ASM2d model (Henze *et al.*, 2000), by a grey box model. In this grey box, the mass balance was incorporated, while the conversion term was predicted by an artificial neural network (ANN). This concept was first tested on a simple conversion model with one type of substrate and one type of biomass converting this substrate. A neural network could be trained to reasonably predict the conversion rate one step ahead. However, due to the feedback of errors back into the model, long term predictions of the reactor could not be obtained. Therefore, an alternative approach to the reduction of the ASM2d and Takács settler model (Takács *et al.*, 1991) was followed. In this case, four different reductions were tested. The simulation results of the reduced models were compared to the complete model by looking at different properties of the effluent time series, such as average or maximum concentration, frequency distribution, plots, etc. It was concluded that it is not straightforward to decide whether two effluent series are sufficiently close to legitimate the use of the reduced model.

The equations within the modelling of the IUWS with a big impact on the calculation time are the “de Saint-Venant” equations. These equations were replaced by the concept of Continuously Stirred Tank Reactor (CSTRs)-in-series. The possibilities to calibrate such a CSTRs-in-series model to the data generated by a complex model were tested in chapter 6. An adapted geometry concept was necessary to obtain a reasonable description of the river geometry. With this concept, an equation with three hydraulic parameters could be calibrated to describe the flow-depth relationship for every river stretch. When connecting the different tanks, both the flood wave and pollution wave could be approximated sufficiently close to allow the use of this model within an IUWS model.

In a next part, a case study on the Lambro catchment (Italy) was used to test the capabilities of the integrated modelling approach chosen. The main goal of the study was to predict the immission concentration of LAS, a detergent with a good biodegradability. A

model of the WWTP and a model of the river were constructed separately using the data available. These data however, were not sufficient to allow for a detailed calibration of the system. However, for the WWTP a reasonable approximation of the observed behaviour could be obtained. The hydraulic properties of the river Lambro were approximated by using 47 tanks in series, using the measured boron concentrations as tracer data for the calibration. In a next step, the in-stream degradation constant was estimated. With this integrated model, the impact of a bypass and the effluent of the treatment plant on the immission concentrations of LAS were evaluated. In a last phase, the effect of an upgrade of the treatment plant on the LAS concentrations was evaluated.

In a last part of the thesis, an integrated model of the catchment of Tielt was constructed. With this model, an immission based control strategy was designed and optimised. This control strategy focused on minimising the maximum ammonia concentration in the river. For the sewer system, the Kosim model was used, which was calibrated on the basis of a complex model. This Kosim model could be reduced from 68 elements to 4 elements, since only the last four elements were important for the control strategy. For the river, no complex model was available and, therefore, a CSTRs-in-series model was constructed directly. For the tuning of the control strategy, no conversion model was used in the river. In a first strategy the WWTP was overloaded when the immission concentration of ammonia in the river reached a given threshold. In a second strategy, the first strategy was extended by the implementation of an extra pump in the sewer system. In this way, more water could be sent to the WWTP, with a reduction of the CSO volume as a consequence. Both strategies could reduce the ammonia concentration in the river in certain parts of the storms studied.

As a secondary objective for the control strategies the minimum oxygen concentrations in the river were checked. Only the river model was used, but a submodel of the RWQM1 model (Reichert *et al.*, 2001b) was used as a bioconversion model. It could be concluded that the control strategies did not have an inverse impact on the oxygen concentrations in the river. In a last phase, the robustness of the control strategies towards changes in the system properties was tested. Three properties were changed: the aeration capacity, the nitrification capacity and the nitrogen load. The control strategies had about the same robustness as the reference case for the maximum ammonia concentration. This means that the control strategy will, if implemented in practice, perform still reasonably well under different conditions.

In a last chapter, an predictor for the minimum oxygen concentration in the river was developed and used in a immission based control strategy. The effect on the oxygen concentration in the river was small. Moreover, the measurement problems of OUR in practice will decrease the performance of the controller. The concept of using software sensors in immission based control strategies was demonstrated to be an interesting approach.

Overall, in this thesis, a procedure to create an integrated simultaneously simulating model of the IUWS system has been outlined. This model can be used to design and tune immission based control strategies. These strategies are shown to be a valid option in urban wastewater management driven by receiving water objectives. However, some problems remain to be solved such a data collection for large basins, calculation times of basin-wide models, knowledge about the phenomena (e.g. ecology), conservatism of the management, etc.

Samenvatting

De literatuurstudie in hoofdstuk 2 maakt duidelijk dat wiskundige modellen veelvuldig worden toegepast voor het bestuderen van de afzonderlijke delen van het geïntegreerd stedelijk afvalwatersysteem. Zowel complexe als vereenvoudigde modellen worden gebruikt om rioleringssystemen, waterzuiveringsinstallaties en rivieren te beschrijven. Deze modellen werden reeds succesvol toegepast bij het beheer van de deelsystemen. Verschillende real-time controle (RTC) strategieën werden ontwikkeld om de verstoringen van het systeem (hoofdzakelijk regenwater in de rioleringen en de waterzuiveringsinstallatie) zo goed mogelijk te beheersen. Deze controlestrategieën hebben als doel de overstortvolumes of de hoeveelheid polluenten die in de ontvangende waterloop terechtkomt, te minimaliseren.

Pas sinds enkele jaren worden de verschillende deelsystemen meer als een geheel bekeken zodat de interacties in rekening kunnen worden gebracht. Dit wordt ook verwacht door de Kaderrichtlijn Water van de Europese Unie, die de nadruk legt op de kwaliteit van de ontvangende waters. Een goede kwaliteit wordt vooropgesteld zowel wat betreft de ecologie als wat betreft de chemische samenstelling. Door de Kaderrichtlijn Water wordt beheer vanuit een immissiestandpunt meer en meer een noodzakelijke voorwaarde om te kunnen voldoen aan de eisen opgelegd door deze richtlijn.

Immissiegebaseerde RTC is één van de manieren om het geïntegreerd stedelijk afvalwatersysteem beter te laten functioneren. Het is een manier om zowel de kwaliteit van de ontvangende waterloop als het gebruik van de bestaande infrastructuur te optimaliseren. Om een dergelijke controlestrategie te ontwerpen en af te stellen is een simultaan simulerend model nodig van het systeem. Enkel op deze manier kan de interactie in twee richtingen tussen de deelsystemen in rekening gebracht worden.

Drie problemen dienen opgelost te worden vooraleer een geïntegreerd model kan gebruikt worden voor het ontwerpen van een geïntegreerde controlestrategie. Het eerste probleem is dat de beschikbare state-of-the-art modellen geïmplementeerd zijn in verschillende softwarepaketten. Dit maakt simultane simulatie moeilijk omdat de communicatie tussen deze paketten verloopt via het bestanden die van stroomopwaarts naar stroomafwaarts doorgegeven worden. Daarenboven is het creëren van een informatiestroom van stroomafwaarts naar stroomopwaarts, die noodzakelijk is voor een geïntegreerde controlestrategie, nog moeilijker, zoniet onmogelijk. Een tweede probleem is dat de huidige state-of-the-art modellen van de deelsystemen typisch gebruik maken van verschillende toestandsvariabelen. Zo zijn er modellen die BOD, COD of TOC gebruiken voor het beschrijven van de hoeveelheid organische vervuiling in het water. Een derde en laatste probleem is dat de

"de Saint-Venant" vergelijkingen die de stroming in rioleringen en rivieren beschrijven niet-lineaire partiële differentiaalvergelijkingen zijn. De ingewikkelde numerieke algoritmes die nodig zijn om deze op te lossen, maken deze modellen traag en dus moeilijk te gebruiken voor optimalisaties.

Het eerste probleem van de verschillende softwarepaketten werd opgelost door alle modellen te implementeren in de WEST® simulatie software. Een van de belangrijke eigenschappen van WEST is de mogelijkheid om verschillende processen te integreren in een enkele simulatie. Om deze integratie mogelijk te maken, moest een goede structuur voor de modellenbank uitgewerkt worden. Deze modellenbank is verder specifiek gericht op een maximaal hergebruik van bestaande kennis en heeft daarom een hiërarchische structuur. De oorspronkelijke modellenbank die opgebouwd is voor waterzuiveringsinstallaties werd geherorganiseerd en uitgebreid met modellen van rioleringssystemen en rivieren. Daarenboven werd een algemeen concept ontwikkeld om modellen met verschillende toestandsvariabelen aan elkaar te koppelen. De logische omzetting van toestandsvariabelen is geïncorporeerd in deze connectormodellen, terwijl ook de massa- en elementenbalansen gesloten worden door het gebruik van correctietermen.

De rekentijd van het geïntegreerde model werd verkort door het toepassen van twee concepten: modelvereenvoudiging met mechanistische surrogaatmodellen en modelreductie. Modelvereenvoudiging heeft vooral tot doel om de ingewikkelde vergelijkingen of gedetailleerde modelconcepten te vervangen door meer conceptuele modellen. De complexe mechanistische modellen, die een goede voorspellingskracht hebben als ze correct gecalibreerd werden, worden gebruikt om gegevens te produceren via virtuele experimenten. Op deze manier wordt de kennis van het complex mechanistisch model overgedragen naar het surrogaatmodel. Het mechanistisch surrogaatmodel wordt vervolgens gecalibreerd op basis van meer gegevens dan er verzameld werden door veldmetingen. Dit concept werd toegepast op een model van de waterzuivering en op een riviermodel. Modelreductie is gebaseerd op het weglaten van die delen van het model die niet beïnvloed worden door de controlestrategie die getest wordt. Op deze mainer kunnen zowel stroomopwaarts als stroomafwaarts bepaalde delen van het model geëlimineerd worden, evenals sommige conversiemodellen. Een andere reductie kan doorgevoerd worden door een zorgvuldige selectie van de periode die gesimuleerd dient te worden voor de optimalisatie van de controlestrategie.

In hoofdstuk 5, werd er geprobeerd om het gekende ASM2d model (Henze *et al.*, 2000), te vervangen door een grey boxmodel. In dit grey boxmodel werd de massabalans behouden, terwijl de conversiesnelheden voorspeld werden door een artificieel neuraal netwerk. De methodologie werd eerst getest aan de hand van een eenvoudig bioconversiemodel waarbij slechts één soort biomassa en één soort substraat aanwezig was. Het neuraal netwerk werd getraind zodanig dat de conversiesnelheden op de volgende tijdstap met een behoorlijke nauwkeurigheid konden worden voorspeld. Bij gebruik van het grey boxmodel voor langetermijnvoorspellingen was het model niet in staat om het originele model voldoende nauwkeurig te benaderen, hoofdzakelijk doordat de kleine fouten terug werden ingevoerd in het neuraal netwerk en accumuleerden. Daarom werd een modelreductie van het ASM2d model en het model voor een nabezinker van Takács (Takács *et al.*, 1991) voorgesteld. Hierbij werden vier verschillende modelreducties uitgetest. De resultaten van de verschillende modelreducties werden beoordeeld door de vergelijking van de

effluent-tijdreeks van de gereduceerde modellen met de tijdreeks van het volledige model. Verschillende criteria werden gehanteerd bij deze vergelijking zoals de gemiddelde waarde, de maximum concentratie, de frequentiedistributie, enz. Het was echter niet eenduidig vast te stellen op welke manier kon beslist worden of de twee effluent-tijdreeksen voldoende dicht bij elkaar lagen om het gebruik van het gereduceerd model te verantwoorden.

De vergelijkingen die bij de modellering van het geïntegreerd stedelijk afvalwatersysteem een grote invloed hebben op de rekentijd zijn de zogenaamde "de Saint-Venant" vergelijkingen. Deze vergelijkingen werden vervangen door het CSTR (*continuously stirred tank reactor*)-in-serie concept. De mogelijkheden en limitaties van een dergelijk model om na calibratie aan de hand van data gegenereerd met een complex model, de rivier hydraulica te benaderen, werden onderzocht in hoofdstuk 6. De beschrijving van de geometrie van een tank diende aangepast te worden vooraleer een degelijke beschrijving van de geometrie van de rivier kon worden bekomen. Nadien werden de drie parameters van een niet-lineair verband tussen de waterhoogte en het uitgaande debiet gecalibreerd voor iedere tank afzonderlijk. Als validatie werden de verschillende tanks aan elkaar gekoppeld en het gedrag van het gehele systeem werd nagegaan. Zowel de water- als de vervuilingsgolf konden voldoende dicht worden benaderd zodat dit model bruikbaar is binnen een model van het geïntegreerd stedelijk afvalwater systeem.

In een volgend deel van de thesis, werd de gevalstudie van het bekken van de Lambro (Italië) gebruikt om de mogelijkheden van het geïntegreerd model na te gaan. De hoofddoelstelling van deze studie was het voorspellen van de immissieconcentratie van LAS, een biodegradeerbare detergent. Eerst werd een apart model van de waterzuivering en de rivier opgesteld op basis van de beschikbare data. Deze gegevens waren niet voldoende om een gedetailleerde calibratie van deze modellen toe te laten. Niettemin werd een redelijke benadering van het waargenomen gedrag van de waterzuiveringsinstallatie bekomen. Het hydraulische gedrag van de rivier werd benaderd door 47 gemengde tanks in serie. Hiervoor werd gebruik gemaakt van meetgegevens van boor dat dienst deed als inerte tracer. In een volgende stap werd de eerste orde degradatieconstante in de rivier geschat. In een laatste fase werden de twee modellen aan elkaar gekoppeld zodat de impact van het effluent en de bypass van de waterzuivering op de immissieconcentratie van LAS konden worden nagegaan.

In het laatste deel van de thesis werd een geïntegreerd model van het stedelijk afvalwatersysteem in Tielt opgebouwd. Met behulp van dit model, werd een immissiegebaseerde controlestrategie ontwikkeld en afgesteld. De gebruikte controlestrategie heeft tot doel de maximum ammoniumconcentratie in de rivier te verminderen. Het rioleringssysteem werd beschreven met een Kosim model dat gecalibreerd was met behulp van een complex model. Het volledige Kosim model kon gereduceerd worden van 68 tot 4 elementen omdat de controlestrategie enkel deze laatste 4 elementen beïnvloedde. Voor de rivier was er geen complex model beschikbaar, waardoor een CSTR model gebruikt werd dat niet kon gecalibreerd worden. Tijdens het afstellen van de controlestrategie werden geen conversies in de rivier in rekening gebracht. Twee controlestrategieën werden uitgetest. Bij de eerste strategie werd de waterzuivering overbelast in het geval de ammoniumconcentratie in de rivier hoger was dan een vooraf bepaalde grens. In de tweede strategie werd de eerste strategie uitgebreid met een extra pomp in het rioleringsstelsel. Op deze manier kon meer

water naar de waterzuivering gestuurd worden, met een reductie van het overstortvolume als gevolg. Beide strategieën waren in staat om de maximum ammoniumconcentratie in de rivier te verlagen tijdens bepaalde delen van de storm.

Een secundair objectief voor de controlestrategieën betrof de minimum zuurstofconcentratie in de rivier. Hiervoor werd enkel het riviermodel gebruikt, maar nu werd een submodel van het RWQM1 model (Reichert *et al.*, 2001b) gebruikt voor het doorrekenen van de conversies in de rivier. Hieruit bleek dat de gebruikte controlestrategieën geen negatieve invloed hadden op de concentraties aan opgeloste zuurstof in de rivier. Tenslotte werd de robuustheid van de controlestrategieën t.o.v. veranderingen in de systeemeigenschappen getest. Drie eigenschappen werden aangepast: de aeratiecapaciteit, de nitrificatie capaciteit en de stikstofbelasting. Hieruit bleek dat de controlestrategieën ongeveer dezelfde robuustheid hadden als het referentiescenario. Dit betekent dat het kan verwacht worden dat deze controlestrategieën ook een positief effect zullen hebben in praktijk, waar andere omstandigheden gelden dan tijdens het afstellen ervan.

Als alternatief voor de meting van ammonium, werden in hoofdstuk 9, een voorspeller voor de minimum zuurstofconcentratie in de rivier ontwikkeld en gebruikt in een analoge immissiegebaseerde controlstrategie. Het effect van deze strategie op de zuurstofconcentratie in de rivier was eerder klein. Bovendien zijn er in praktijk problemen te verwachten met het meten van de zuurstofopnamesnelheid. Het principe van het gebruik van een software sensor in immissiegebaseerde controlestrategieën is echter een interessante optie.

In deze thesis werd een procedure ontwikkeld die gebruikt kan worden voor de opbouw van een simultaan simulerend geïntegreerd model van het stedelijk afvalwatersysteem. Dit model kan vervolgens gebruikt worden voor het ontwerp en de afstelling van een immissiegebaseerde controlestrategie. Deze strategieën zijn een volwaardig alternatief om de waterkwaliteitsobjectieven van de ontvangende waterloop te bereiken.

Curriculum Vitae

Personalia

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Opleiding

1987-1993 Secundair onderwijs, Latijn-Wiskunde, St.- Franciscuscollege, Wetteren

1993-1998 Bio-ingenieur in de milieutechnologie, Universiteit Gent
Scriptie: Nitriet in actief slib: belang en opvolging met een nieuwe on-line sensor; Promotor: Prof. W. Verstraete

Bijkomende opleidingen

In het kader van mijn doctoraatsopleiding volgde ik volgende vakken

1999 Hydraulica van de de waterlopen: Prof. F. De Troch

2000 Programmeren II: Prof. H. Tromp

2000-2002 Academische initiële lerarenopleiding, zal beëindigd worden in juli 2002.

Werkervaring

1998-2002 Aspirant van het Fonds voor Wetenschappelijk Onderzoek - Vlaanderen. Het onderzoek ter voorbereiding van het doctoraat werd uitgevoerd aan de vakgroep Toegepaste Wiskunde, Biometrie en Procesregeling (BIOMATH) van de Universiteit Gent.

Conferenties

Congressen en symposia

21-23 apr 1997	International symposium on environmental biotechnology, Oostende (B)
24-25 sep 1998	Aquatech, Amsterdam (NL)
21-23 okt 1998	Integrated Modelling Users Group Conference: IMUG 98, Brussel (B)
22-23 sep 1999	13th Forum for Applied Biotechnology, Gent (B)
12-14 apr 2000	Integrated Modelling Users Group Conference: IMUG 2000, Praag (Cz)
9 mei 2000	Wastewater planners user group, Birmingham, Groot-Brittanië
3-7 jul 2000	1st World Water Congress of the International Water Association: Paris 2000, Parijs (F)
14-16 sep 2000	Conference on Monitoring and Modelling Catchment Water Quantity and Quality (8th General Assembly of the European Network of Experimental and Representative Basins), ERB2000, Gent (B)
18-20 sep 2000	5th International Symposium on Systems Analysis and Computing in Water Quality Management: WATERMATEX, Gent, (B)
19-22 feb 2001	2nd International Conference on Interactions between sewers, treatment plants and receiving waters in urban areas: Interurba II, Lissabon (P)
3-7 jun 2001	1st IWA (International Water Association) Conference on Instrumentation, Control and Automation: ICA 2001, Malmö (S)
24-25 sep 2001	15th Forum for Applied Biotechnology, Gent (B), Gent (B), secretary of the conference

COST working group meetings

9-11 apr 2000	"IUWS course", Praag(Cz)
23-24 feb 2001	COST 624 "Optimal management of wastewater systems" Working Group No. 2 "Integrated system", Lisbon (Pt)

Publicaties

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